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Numerical simulation of a droplet icing on a cold surface

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Simulazione numerica del congelamento di una goccia su una superficie fredda

Sommario

L'obbiettivo del presente lavoro di tesi consiste nel simulare numericamente il fenomeno del congelamento di una goccia d'acqua posta a contatto con una superficie fredda. In particolare, uno degli scopi è simulare e determinare la causa o le cause che portano alla formazione della caratteristica punta che può essere osservata in cima alla goccia stessa una volta che essa si è congelata. A tale scopo, è stato utilizzato il codice JA-DIM sviluppato all' *Institut de Mécaniques des Fluides de Toulouse*. Con l'obbiettivo di simulare l'espansione dell'acqua nel corso del passaggio dal suo stato liquido a quello solido, nel codice in oggetto è stata implementata una formulazione originale che accoppia il calcolo termodinamico, il metodo Immersed Boundary e la formulazione detta Volume of Fluid (VoF). Infine, è stata svolta un'analisi sui parametri che maggiormente influenzano la velocità di congelamento, al fine di determinare soluzioni tecniche che possano permettere di ritardare la formazione di ghiaccio su una superficie.

Numerical simulation of a droplet icing on a cold surface

Abstract

The objective of the present work is to numerically simulate the icing phenomenon of a water droplet when deposed on a cold surface. In particular, one of the objective is to simulate and determine the cause(s) for the characteristic pointy tip that appears on the top of the frozen drop once the solidification has completed. In order to accomplish this task the research code JADIM developped at the *Institut de Mécaniques des Fluides de Toulouse* has been used. With the aim to simulate the expansion experienced by the water during the transition from its liquid to its solid state in the code an original formulation has been implemented in which the thermal computation, the Immersed Boundary Method (IBM) and the Volume of Fluid (VoF) approach have been coupled. Furthermore, an analysis on the main parameters which affect the icing velocity has been performed in order to determine possible technological solutions to delay the accretion of ice on the surfaces.

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List of Symbols

A	area	m^2
c_p	specific heat capacity	$J/(kg \cdot K)$
\dot{h}	specific enthalpy	J/kg
Η	total entalpy	J/kg
J	mass flux	$kg/(m^2 \cdot s)$
k	thermal conductivity	$W/(kg \cdot K)$
L	latent heat	J/kg
p	pressure	Pa
q	heat flux	W/m^2
r	radius	$m^{'}$
s	position of the interface	m
S_i	balance equations' source terms	
T	temperature	K
${oldsymbol U}$	vector of absolute velocity	m/s
v	specific volume	m^3/kg
α	thermal diffusivity	m^2/s
λ	thermal conductivity	W(mK)
μ	dinamic viscosity	$Pa \cdot s$
ρ	density	kg/m^3
σ	Stefan-Bolzamann constant	W/m^2K^4
au	volume fraction	_

Sub- and Superscripts

value referred to air
apparent
average value
final value assumed by the variable
value referred to liquid water
value referred to initial condition
value referred to ice
value referred to interface
value referred to liquid
value referred to melting, solidifying, phase-change
maximum value
value referred to solid
value referred to temperature
value referred to velocity
value referred to solid boundary

Acronyms

- ADFs Aircraft De-icing Fluids
- *CFD* Computational Fluid Dynamics
- FVM Finite Volume Method
- *IBM* Immersed Boundary Method
- PCM Phase Change Material
- PDE Partial Differential Equation
- *VoF* Volume of Fluid

1. Introduction

1.1. Ice accretion on airplanes

The formation and accretion of ice on airplane's surfaces are open issues which have to be studied and understood since aircraft accidents continue to occur due to these problems and, even if catastrophic events do not occur, the aerodynamic efficiency and the manoeuvrability of the aircraft are influenced, causing changes in both the overall drag and lift forces applied to the aircraft. Icing accidents can be prevented in two different ways: icing conditions can be avoided, or the aircraft system can be designed and operated in an ice tolerant manner. In any case, for all aircrafts, ice avoidance is a desirable goal for increased safety [1].

Ice builds up on aircraft in two ways: in flight or on the ground. On the ground, precipitation falls onto the airplane and, if there are the right conditions of temperature, freezes on upper surfaces much like what happens if one leaves his car out overnight. So, ground icing mainly forms on the upper surfaces of the wings and tail. That type of ice is managed by de-icing the plane with a fluid (typically propylene glycol) at the airport, operation that requires significant amounts of both money and time, as well as specific areas and tools.

Flight icing occurs when the airplane is flying through clouds made up of small liquid water droplets. These liquid water droplets can be sustained as liquid also below the freezing point. In fact, it turns out that if the water is very pure, so if it is condensed out of the atmosphere, and there is nothing for that water to freeze on, it can be sustained below the normal freezing point. Given that, when the airplane is flying through the cloud, the water droplets impact the aircraft and then freeze because now they have a surface to freeze on [2]. In this second case, ice builds up on the frontal surfaces: leading edge of the wings, the nose and the tail surfaces.

In order to avoid ice accretion there are two possible solutions: system capable of preventing ice or removing ice. The de-icing system works on the basis of allowing ice to form before being broken off, using pneumatic boots that inflate to crack the ice. The anti-icing system prevents ice from forming by blowing hot air from within the compressor of the engine or by heating the surfaces with electrical resistances.

1.1.1. Anti-icing methods, environmental aspects

As the amount of air travel has increased, the volume of de-icing chemicals used and discharged into the environment has also increased, with the resulting attention by regulators on the potential negative environmental impacts of de-icing chemicals. Deicing and anti-icing of aircraft are operations made in order to remove and to inhibit for a period of time the formation of ice on wings, fuselages, and other parts of the airplane that provide lift during takeoff. Common practice is to de-ice (remove accumulation) then anti-ice (protect from further accumulation) aircraft before takeoff, because takeoff is the most delicate phase and anti-icing techniques have a determined duration in time, especially in case of severe atmospheric conditions.

De-icing fluids are usually applied to the aircraft as a hot mixture (water and propylene glycol) under pressure using tank trucks that have spray nozzles on extendible arms in order to reach all necessary sensitive surfaces of the aircraft (cf. Figure 1.1). The pressure of the liquid hitting the surface of the aircraft mechanically removes ice, which is also melted by the solution. Between 20% to 50% of the de-icer that is applied to the aircraft is estimated to remain, meaning that as much as 80% of the fluid can end up on the airport's runoff. The high costs in time and money and environmental effects are not negligible.



Figure 1.1: Ground de-icing operation

Typically for aircrafts, glycol de-icers are manufactured as a mixture of propylene glycol, water, and other additives such as corrosion inhibitors, surfactants and wetting agents. The toxicity exhibited by the aircraft de-icing fluids (ADFs) is in part due to the presence of the glycols (which typically make up 45% to 65% of the total fluid by weight), but is also due to the additives contained in the fluids. Although additives comprise a small percentage of ADFs, they may be responsible for a disproportionate share of the toxicity of the ADFs. Several toxicity tests have been performed using pure ethylene and propylene glycol but a few studies have been performed using formulated ADFs [3].

The general environmental impacts due to the presence of ADFs in the airport's stormwater runoff are: aquatic life effects such as fish kills, growth of biological slimes, elimination of aquatic life, effects on wildlife, birds and cattle, human health problems (worker and human exposure - headaches and nausea), effects on groundwater, water supplies and soils. Thus airport runoff that usually contains significant amounts of de-icing material cannot be normally discharged directly into the environment but must instead be contained and treated to reduce the pollutants before release into the environment, which contribues to increase costs for the entire de-icing operation [3].

1.2. Ice effect on aircraft flight dynamics

The presence of ice formations alters airflow over the wing and tail since it reshapes the surface of these lift-producing parts, and potentially can cause aerodynamic stall, a condition that can lead to a temporary loss of control. The roughness is enough to change the aerodynamics of the wing such that there is more drag and less lift. The amount of lift a wing creates depends on the relative angle between the airstream and the airfoil. As the angle of attack is increased, more lift is generated, but at some point air cannot correctly flow over the upper surface, and aerodynamic stall can occur.

The point at which aerodynamic stall takes place depends on the contour of the airfoil. If the surface is contaminated with slight roughness (ice effect), it will reduce the lift and change the point at which stall takes place. For scheduled air carriers, including commercial passenger airlines, icing has been a contributing factor in 9.5 % of fatal air carrier accidents [2].

Moreover, the ice's accretion on both the lift-producing parts and the fuselage has negative influence on the fuel consumption, reducing flight efficiency. In fact, the presence of frozen water increases the total weight of the plane which causes a direct impact on the engine's power needed to move the plane. Another negative effect of this phenomenon is that ice has an irregular shape which causes all the surfaces to be not as smooth as designed, which has a direct impact on the drag forces acting over the aircraft, which again requires more thrust and an anomalous fuel consumption.

1.3. Case study

Given all the problems written above, this work is meant to study numerically the mechanism of solidification of a droplet on a cold plate, trying to investigate and understand the dynamics of this process, referring also to the experimental results.

By studying this simplified problem, the tools required for more complex problems will be developed in order to comprehend the build up of ice on aircraft's surfaces and fight against it with effective solutions. While a number of theoretical and numerical studies have been conducted in recent years to develop ice prediction tools for improved ice protection system designs, many details of important microphysical processes that are responsible for the ice formation and accretion on frozen cold surfaces are still unclear [4].

The most important parameters which can influence the numerical simulations are the initial shape of the droplet, depending on its volume, contact angles and on the action of both gravity and surface tension, and of course all the boundary conditions of the case study. The main characteristics of the process which need to be taken into account are the change in density and other physical properties such as the thermal conductivity between liquid to solid state of water, which is controlled by the evolution of the icing front, and the solidification time. In the following chapters some considerations and simplifications done in order to analyse the problem and to set up the simulations are presented, as well as some information about the code used and all the results achieved.

2. Physical phenomenon and governing equations

As the objective of this work is to investigate the phenomenon of a water droplet becoming ice once deposed on a cold surface, the first analysis which needs to be done regards the solidification of a phase changing material (PCM), in particular water, but most of the following considerations are valid for any PCM. The two main issues that will be studied are linked to the heat exchange, because the most frequent way to guarantee the solidification is by cooling a liquid beneath a certain temperature, with the consequent dilatation or size reduction subsequent a phase change.

The solidification of a liquid is a phenomenon driven by several different contributions: the most important ones are obviously linked to thermal fluxes as heat transfer and latent heat release but also changes in thermophysical properties, mass transfer and surface effects should not be neglected. The typical condition of a solidifying liquid , which is interesting to study, is the one where the considered liquid is initially at a temperature higher than its transition one (also called phase change, solidifying/melting or freezing temperature) in an environment (all of it or just a part) at a lower temperature. As a consequence of the difference in temperature between different parts of the domain, there will be heat fluxes and, more specifically, the phase change material will be cooled and a certain portion of it will reach a temperature lower to the phase change one. Depending on the nature of the studied material, the phase change temperature could be a range of temperatures, typical of alloys, meaning that the solidifying process starts at a certain temperature and it develops to the ending one, or a single one, classical behaviour of pure substances, also called isothermal phase change.

Another condition often occurring in flight condition is due to the so-called *super-cooled water droplets*. In this second condition the liquid is already at a temperature below its freezing point, in a metastable state, and it lacks a nucleation point for instantly becoming solid (the entire droplet or just a portion of it, depending on the size): this phenomenon is responsible of the so called *clear/rime ice* which cause, for example, particular structures on the leading edge of airplane wings like those displayed in Figure 2.1: the localisation is due to the fact that the nucleation point is the impact point on the wings. However because of the complexity and the peculiarity of the state in which it occurs, this problem will not be studied in this work despite its importance in real flight conditions.

The region in which the phase change occurs, called freezing front in case of liquid to



Figure 2.1: Example of clear ice

solid transition, can present very different structures depending on several factors but for most pure material in ordinary conditions it appears locally planar and of negligible thickness, while in alloys it is characterized by a dendritic structure; consequently the final crystal lattice strongly depends on the characteristics of the solidifying process [5].

Another peculiarity of the phase change problems is the change of thermophysical properties of the solidifying substance, which means that the same material has different characteristic in its solid or liquid state. For example, thermal conductivity in both ice and water changes little with temperature compared to the difference between them. Moreover, water is one of the few substance which increases its volume in the freezing process instead of having a greater density in the solid state (other example are antimony and bismuth).

The icing of a water droplet on a cold plate, which is the objective of this work, is influenced by many different contributions like the initial shape of the droplet, its temperature and the presence and the eventual motion of the surrounding air.

For these reasons it is convenient to consider first a certain number of assumptions and also a simplified problem, the so-called Stefan's problem, which has an analytical solution and can be used to validate numerical simulations regarding more general and complex geometries and conditions.

2.1. Droplet phase change

The objective of this work is the study of a droplet freezing on a cold plate, in order to obtain a better understanding of the parameters influencing the process. So one of the first tasks required is to identify the phenomena with the biggest influence on the problem to be included in the numerical simulations.

The main field of interest is the thermal one, given that this is a phase change problem, but the initial configuration has to be determined as well, depending on various parameters which could have a large influence.

2.1.1. Density

Density, in general, is a function of pressure and temperature: while the first will be constant due to the absence of particular processes which could change it (also the vertical pressure variation is negligible as a result of the small domain of interest), the second will change as main driver of the present simulations. Thus, the behaviour of the density of the involved substances has to be studied in order to be able to predict its influence. For this reason, in Figure 2.2 and 2.3 the values of the density of air and water are shown, as a function of temperature at a constant pressure equal to 1 atm [6].



Figure 2.2: Density of air vs T



Figure 2.3: Density of water vs T

While both quantities vary with temperature it is clear that the variation of real interest is the one between liquid water and ice more than the small changes in density of the three substances themselves. In fact, considering the range of temperatures shown, a variation from $-15^{\circ}C$ to $25^{\circ}C$ causes density of air to change of about 10% if compared to its initial value, but this change is only 0.1% if the denominator is the initial density of water.

For this reason densities of liquid water, ice and air will be considered as constants through all the simulation, which means that all the three phases will be considered as incompressible while the phase change will be a compressible process in order to try to simulate and comprehend the influence of the difference in density between the solid and liquid phase of water.

2.1.2. Heat transfer

The heat transfer mechanisms are, as well known, conduction, convection and thermal radiation. The main difference between the three of them is the requirement for each type of transfer, meaning that conduction needs a medium as well as convection, where in the latter case the medium is in motion (in fact the word convection can be seen as the sum of conduction and advection), while thermal radiation only requires a temperature difference between two bodies. Thus, depending on the temperature field (environment and boundary conditions) and the materials involved, each one of these mechanisms can have a great importance in the problem or be negligible.

2.1.2.1 Conduction

Conduction is the transfer of heat from one part of a body at a higher temperature to another part or another body (in physical contact) at a lower temperature, due to the transfer of energy at a molecular level. While in solids conduction is due to the combination of vibration of the molecules arranged in a lattice and to the motion of free electrons, in gases and liquids the molecules are in constant motion and the ones at a higher temperature periodically collide with the molecules of a lower energy level and exchange energy and momentum, causing as a macroscopic effect the heat flux[7].

The heat flux for each direction can be expressed in terms of the *Fourier's law* (2.1), as a function of the temperature gradient, the area perpendicular to the direction of transfer A and the thermal conductivity λ , which is a thermophysical property of the material through which the transfer happens:

$$q_x = -\lambda A \frac{dT}{dx} \quad [W] \tag{2.1}$$

Usually, the thermal conductivity λ is a function of temperature and eventually other parameters (such as pressure in gases): for this reason, given the nature of the problem (both thermal and time-varying), it is useful to observe the behaviour of this property for the substances involved with temperature changes.

The thermal conductivity of air can be calculated with the formula (2.2), using coefficients resumed in Table 2.1 and temperatures expressed in kelvin: [7]

$$\lambda_{air}(T) = \sum_{n=0}^{5} \left(C(n)T^{n} \right)$$
(2.2)

Given a range of temperatures (i.e. $T \in (-20, 50)^{\circ}C$), Figure 2.4 can be obtained by simple computation, which shows a quasi-linear behaviour of λ (which could be also deduced by simply looking at the power of the coefficients in Table 2.1). Since in the

C(0)	C(1)	C(2)	C(3)	C(4)	C(5)
-2.276510^{-3}	1.259810^{-4}	-1.481510^{-7}	1.735510^{-10}	-1.066710^{-13}	2.476610^{-17}

Table 2.1: Coefficient for equation (2.2)

simulations the temperature variation will be narrower than that shown in Figure 2.4, it is an acceptable assumption to consider the thermal conductivity of air as a constant.



Figure 2.4: λ_{air} vs T

The same consideration can be made for the thermal conductivity of water, given its moderate change in the temperature range of interest, as shown in Figure 2.5.

The third substance involved in the thermal exchanges in the considered system is water in its solid form: ice. Its thermal conductivity can be expressed as well as a function of temperature as in (2.3), where temperature is expressed in Celsius [8], which can be plotted showing in Figure 2.6 a stronger variation than the previous substances. Nonetheless, at least in a first instance, it will be considered constant in order to obtain a simpler modelling because both the range of temperature is not so significant but mostly because the effect of its change should be negligible if compared with the differences between the thermal conductivities of the other materials involved. In fact, the same reasoning done for the densities could be made: the difference between the conductivities of the three substances is much larger than the variations of each one of them with temperature:

$$\lambda_{ice}(T) = 1.16 \cdot \left(1.91 - 8.6610^{-3} \cdot T + 2.9710^{-5} \cdot T^2\right) \quad \left[\frac{W}{mK}\right]$$
(2.3)

Thus, from a thermal point of view, the considered system will be constituted of three different regions each one characterized by a different but constant thermal conductivity. As a result, the temperature field's derivative is expected to show dis-



Figure 2.5: λ_{H_2O} vs T

continuities along these interfaces, where the thermal conductivity itself presents a discontinuity.

Moreover, even the densities (and the same considerations can be made for the specific heat capacity c_p) have been previously set as constants through the three different substances so it can be stated that the thermal diffusivity α is a constant property for air, water and ice:

$$\alpha_i = \frac{\lambda_i}{\rho_i c_{p,i}} \quad \left[\frac{m^2}{s}\right] \tag{2.4}$$

This parameter acquires its importance from the heat equation: if only conduction is considered the energy equation can be written as:

$$\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (\lambda \nabla T) = \dot{q} \tag{2.5}$$

Due to the fact that in each phase the thermal conductivity is constant and there is no internal generation (\dot{q} is located only in the interface), Eq. (2.5) can be written as the well known Laplace equation (2.6), where the thermal diffusivity α has been isolated. These equation is true in each phase, being α_i the corresponding thermal diffusivity:

$$\frac{\partial T}{\partial t} = \alpha_i \nabla^2 T \tag{2.6}$$



Figure 2.6: λ_{ice} vs T

2.1.2.2 Convection

The convection heat transfer mode is the combination of two mechanism: energy is transferred due to random molecular motion (diffusion), but also by the macroscopic motion of a fluid. If a temperature gradient is applied, the movement of the fluid enhances the heat exchange.

A distinction can be made, based on the nature of the flow: *forced convection* is the heat transfer in presence of a flow imposed by external means (as a fan or a pump), while *free (natural) convection* happens when the temperature gradient causes a gradient of density and consequently a flow induced by buoyancy forces.

Regardless of the nature of convection, the appropriate heat flux from a boundary surface exposed to a fluid stream could be expressed as in (2.7), known as *Newton's law* [9]:

$$q = hA(T_w - T_{fluid}) \quad [W] \tag{2.7}$$

The heat transfer coefficient h defined in (2.7) is sensitive to multiple parameters, as the geometry, the physical properties of the fluid and, sometimes, even the temperature difference $\Delta T = T_w - T_{fluid}$ between the wall and the fluid.

In case of forced convection the momentum equations are not coupled with the thermal ones, so momentum could be solved first and the energy equation after, given the velocity field.

On the contrary, natural convection can only appear if:

- fluid has a temperature-dependent density
- there is a body force field (usually gravitational field)
- temperature gradient has not the same direction of the the gravity vector

If even one of these conditions is not satisfied natural convection cannot activate.

In the case of study the temperature gradient is expected to be mostly aligned with the gravity vector, in fact it would be exactly in the same direction in the absence of the droplet. This would happen because the cold plate is on the bottom of the domain of calculation while initially the surrounding air is hotter: because of conduction, the air will become colder from the bottom to the top. Consequently, being cold air denser than the hot one, a stable stratification is expected without natural convection.

However, the different conductivity of water will distort the thermal field in some way but given the dimension of the droplet, this distortion is expected to be negligible, at least initially.

Assuming the values typical of the problem resumed in Table 2.2, the order of magnitude of the heat flux due to both conductive and convective mechanisms is shown respectively in (2.8) and in (2.9), where the notation with two superscripts indicate the flux for unity of area. In order to have the two fluxes of the same order of magnitude, a value of the convective factor h of about 260 for natural convection would be necessary, larger than the values quoted in the literature [7].

$$q_{cond}^{"} = -\lambda_a i r \frac{dT}{dx} \sim -\lambda_{air} \frac{\Delta T}{\Delta x} \sim 6500 \quad \left[W/m^2\right]$$
(2.8)

$$q_{conv}^{"} = h_{conv} \left(T_w - T_\infty \right) \sim h_{conv} \cdot 25 \quad \left[W/m^2 \right]$$
(2.9)

$\lambda_{air} [W/mK]$	$T_{max} \ [^{\circ}C]$	$T_{max} [^{\circ}C]$	$\Delta x \ [m]$
0.026	18	-7	10^{-4}

Table 2.2: Typical values of a freezing droplet problem

2.1.2.3 Thermal radiation

The last cited mechanism, thermal radiation, is an electromagnetic radiation emitted by every body by virtue of its temperature. While the other mechanisms require the presence of a medium, radiation can only be hindered by it, since there are materials transparent to radiation while others are not.

Given the Stefan-Boltzmann law, which relates the energy flux emitted by a *black body*, meaning an ideal body which absorbs/irradiates all electromagnetic radiation, to its temperature, a formulation for the heat exchange between two black bodies can be written as (2.10) [7]:

$$q = \sigma A_1 F_{1-2} (T_1^4 - T_2^4) \quad [W]$$
(2.10)

where

$$\begin{cases} \sigma = 5.669 \cdot 10^{-8} \quad \left[\frac{W}{m^2 K^4}\right] & \text{Stefan-Boltmann constant} \\ T \quad [K] & \text{Absolute temperature} \\ F_{1-2} \quad [-] & \text{View factor, between 0 and 1; it represents the fraction} \\ & \text{of energy leaving body 1 intercepted by body 2} \\ A_1 \left[m^2\right] & \text{Radiating surface of body 1} \end{cases}$$

In the case of non-ideal bodies, from a thermal radiation point of view called *grey bodies*, the heat flux has a similar expression except for a coefficient which decreases the magnitude of radiation compared with the one typical of a black body. While in other contexts this heat flux could be quite important, especially when high temperatures are involved (difference between the forth power of absolute temperature can become large), such as in combustion, but given the typical temperature in freezing processes for water, it is almost always negligible.

As done for natural convection, also for thermal radiation the order of magnitude of the specific heat flux can be estimated: even overestimating it by considering both the cold plate and the air as black bodies and the view factor equal to one, the heat flux linked to this mechanism is just a small percentage of that due to conduction. In fact, using the same values of Table 2.2 the ratio between radiation and conduction appears to be less than 2% (2.11):

$$q_{rad}^{"} \sim \sigma (T_{max}^4 - T_{min}^4) \sim 120 \quad [W/m^2]$$
 (2.11)

In conclusion, this heat exchange mechanism will be considered as negligible and so it will not be considered in the simulations.

2.1.3. Droplet shape

The second step in order to study the solidification of a water droplet on a cold plate is to determine the initial shape assumed by the droplet deposed on the surface. Its configuration is due to the sum of the forces acting both on the surface and on the volume: the surface tension, the shear stress, buoyancy, electromagnetic forces etc.

A reasonable assumption to be made is that in determining the shape of the droplet the main effects to be taken into account are the surface tension and the gravity/buoyancy forces. Given that the shear stress has no great importance, as well as electromagnetic forces, this implies the absence of significant electromagnetic field or flow around the droplet. While the first assumption is not too constraining, the second implies that, at least initially, everything is static with no flow interacting with the water on the plate.

Given these assumptions and the geometry of the problem, where gravity is perpendicular to the surface where the water is deposed, the result is an axisymmetric droplet in static equilibrium.

As previously said, the two forces influencing the droplet shape are surface tension and gravity which have contrasting effects: while gravity seeks to flatten the drop as a consequence of the bigger density of water in comparison to the surrounding air, surface tension, in order to minimize the surface area compared to the volume, would give the droplet a spherical shape.

In order to quantify the influence of these two effects the adimensional parameter known as *Bond number* or *Eötvös number* can be used; it is a measure of the importance of the liquid drop's weight (gravity) with respect to the surface tension force [10]. A small value of this number indicates that drop's weight has a small influence in the determination of the shape of the droplet which can consequently be assimilated to a sphere or a spherical cap, according to the characteristic contact angle on the surface. On the other hand, a large value for Bo, implies a great influence of gravitational force

and consequently a flattened drop. Causes of a small *Bond number* can be low gravity environment, low difference between the density of the droplet and the surrounding fluid (meaning that buoyancy force equalize the weight), high value of the surface tension and/or small dimension of the drop itself. *Bo* is defined as:

$$Bo = \frac{g \cdot \Delta \rho \cdot d^2}{\gamma} \tag{2.12}$$

Given a water droplet in standard gravitational conditions surrounded by air the typical values are:

$$\begin{cases} g = 9.81 \quad \left[\frac{m}{s^2}\right] & \text{Gravitational acceleration} \\ \Delta \rho \sim 1000 \quad \left[\frac{kg}{m^3}\right] & \text{Difference between densities of the droplet and air} \\ d \quad [m] & \text{Characteristic length} \\ \gamma = 0.073 \quad \left[\frac{N}{m}\right] & \text{Surface tension} \end{cases}$$

thus *Bo* is a function of the characteristic length of the droplet. If the volume of water is small enough, the droplet's shape is well approximated by a spherical cap, otherwise it is flattened by the effect of gravitational force.

Despite the great importance of this parameter, it is not the only one involved: the second fundamental aspect to look at in order to determine the shape of the water droplet is the coupling of the water with the substrate of the cooled plate. This means that the same volume of water can assume different configurations as function of the material/treatment of the surface below, due to different contact angles. Moreover different configurations cause variation in the characteristic length used to calculate the *Bond number*, even if usually not large enough to strongly vary *Bo* to the point of changing from a gravity influenced condition to the opposite one.

As firstly described by Thomas Young in 1805, the contact angle, θ_C in Figure 2.7, of a liquid drop on an ideal solid surface is defined by the mechanical equilibrium of the drop under the action of three interfacial tensions.



Figure 2.7: Definition of contact angle θ_C

It can be evaluated from the so-called Young's equation (2.13), where γ_{l-g} , γ_{s-l} and γ_{s-g} are liquid-gas, solid-liquid and solid-gas interfacial tensions respectively:

$$\gamma_{l-g} \cdot \cos\left(\theta_C\right) = \gamma_{s-g} - \gamma_{s-l} \tag{2.13}$$

Conventionally if the contact angle for a specific substrate is grater than 90° the surface is called hydrophobic while if it is smaller, hydrophilic. Wetting is a phenomenon resulting from coupling a fluid and a solid, which is strongly influenced by the surface's treatment of the substrate as well as dirt and so on; because of this, it is a characteristic that could change in time, as a function of the environment.

Consequently, if the volume of water is small enough to verify the condition $Bo \ll 1$, knowing the characteristic contact angle for the substrate under consideration, the droplet shape can be deduced simply by equating the fixed volume to the volume of a spherical cap having the desired contact angle.

Considering that a spherical cap has two degrees of freedom, it is possible to write down some relations between its typical parameters, in order to use the most convenient ones in the different cases.



Figure 2.8: Spherical cap and its parameters

Naming R the radius, H the height, θ_c the contact angle, a the wetted radius and V the volume, as shown in Figure 2.8, the following relations are derived using basic trigonometry:

$$\begin{cases}
H = (1 - \cos \theta_c) \cdot R \\
a = R \cdot \sin \theta_c \\
R = \frac{H^2 + a^2}{2H} \\
V = \pi H^2 \cdot \left(R - \frac{H}{3}\right)
\end{cases}$$
(2.14)

Usually, the known parameters are the volume of water, deposed on the plate using a graduated syringe, and the contact angle which is typical of the solid-liquid coupling; given the relations in (2.14), the other variables can be obtained easily in order to successively insert the required ones in the code.

2.2. The Stefan's problem

The Stefan's problem is name after Jožef Stefan, the Slovene physicist who studied this subject at the end of the XIX century, better known for his studies on radiation which led to the formulation of the Stefan-Boltzmann law.

The term "Stefan problem" is generally used for heat transfer problems with phasechanges such as from the liquid to the solid. In the hyperbolic Stefan problems, the characteristic features of Stefan problems are present but unlike the classical ones, discontinuous solutions are allowed because of the hyperbolic nature of the heat equation.

The problem is a boundary value problem for a partial differential equation (PDE), characterized by two regions, one for each of the two phases, in which the solutions of the underlying PDE are continuous and differentiable. But there is also an interface region, characterized by a discontinuity, where another condition (Stefan's condition) is applied in order to obtain closure. Peculiarity of the problem is the fact that the position of the interface evolving in time is a variable itself, so the boundary conditions are applied with respect to a time dependent position, unknown a priori.

2.2.1. Assumptions

In order to obtain an analytical solution some simplifications are to be made, which are reasonable for pure materials and in case of moderate thermal gradients and temperatures, suitable in this case which involves water as already seen in the previous section:

- The heat transfer is driven by the sole conduction, assuming negligible both convective and radiative transfer
- Sharp and locally plane interface
- Thermophysical properties constant with temperature in each phase, while different between the two phases
- Phase change temperature fixed and known

2.2.2. Statement of the problem

Considering a mono-dimensional and semi-infinite domain filled with phase-change material in the positive x-axis direction, at an initial temperature greater than the melting one $(T_i > T_m)$, which means it is all liquid at t = 0. Calling s(t) the position of the interface between the two phases, the equations for this problem are:

• solid phase: $0 \le x < s(t)$

$$\frac{\partial T_s}{\partial t} = \alpha_s \frac{\partial^2 T_s}{\partial x_s^2} \tag{2.15}$$

• liquid phase: $s(t) < x < \infty$

$$\frac{\partial T_l}{\partial t} = \alpha_l \frac{\partial^2 T_l}{\partial x_l^2} \tag{2.16}$$

On the other side, in order have a solution for a set of differential equations, also boundary conditions are needed: • Dirichlet's condition to the fixed boundaries: imposed temperature at the wall and asymptotic imposed temperature at infinity

$$T(x=0) = T_{wall} \tag{2.17}$$

$$T(x \to \infty) = T_i \tag{2.18}$$

• Stefan's condition at the interface (x = s(t)), which is constituted by the continuity of the temperature field and the heat transfer balance, considering the two fluxes and the latent heat

$$-\lambda_l \frac{\partial T_l}{\partial x}\Big|_{s^+} + \lambda_s \frac{\partial T_s}{\partial x}\Big|_{s^-} = \rho_s L \frac{ds}{dt}$$
(2.19)

$$T_s|_{s^-} = T_l|_{s^+} = T_m \tag{2.20}$$



Figure 2.9: 1D Stefan problem

2.2.3. Solution

Given these conditions the problem can be solved, finding the position of the freezing front and the temperature fields in both solid and liquid: the results are successively presented [11].

The temperature profiles, as well as the interface position, are a function of three dimensionless parameters: *Stefan number* (2.21), the ratio between the sensible heat in the liquid phase and the sensible heat in the solid phase ϕ (2.22) and the square root of the ratio of the thermal diffusivities α (2.23)

$$Ste = \frac{\rho_s c_{p,s} \left(T_m - T_{wall} \right)}{\rho_s L} \tag{2.21}$$

$$\phi = \frac{\rho_l c_{p,l} \left(T_i - T_m \right)}{\rho_s c_{p,s} \left(T_m - T_{wall} \right)}$$
(2.22)

$$\alpha = \sqrt{\frac{\alpha_s}{\alpha_l}} \tag{2.23}$$

Given these adimensional quantities, the following transcendent equation has to be solved for K_N :

$$\frac{e^{K_N^2}}{erf(K_N)} - \frac{e^{-K_N^2\alpha^2}}{erfc(K_N\alpha)}\frac{\phi}{\alpha} = \frac{K_N\sqrt{\pi}}{Ste}$$
(2.24)

and then the desired quantities are a function of the parameter K_N , the physical properties and the initial and boundary conditions:

• position of the interface

$$s = 2K_N \sqrt{\alpha_s t} \tag{2.25}$$

• temperature profile in the solid phase

$$T_s(x,t) = T_{wall} + \frac{(T_m - T_{wall})}{erf(K_N)} erf\left(\frac{x}{2\sqrt{\alpha_s t}}\right)$$
(2.26)

• temperature profile in the liquid phase

$$T_l(x,t) = T_i - \frac{(T_i - T_m)}{erfc(K_N\alpha)} erfc\left(\frac{x}{2\sqrt{\alpha_l t}}\right)$$
(2.27)

Using the physical properties, resumed in Table 2.3, and the initial and boundary condition in Table 2.4 temperature profiles, as the one presented in Figure 2.10, can be obtained and will be used in chapter 5 in order to validate the model and the code developed.

	$\lambda \ [W/mK]$	$ ho \ [kg/m^3]$	$c_p \left[J/(kgK) \right]$	$\alpha \ [m^2/s]$
Water	0.6	1000	4186	1.410^{-7}
Ice	2.2	917	2040	1.210^{-6}

Table 2.3: Physical properties of water and ice

$T_i [^{\circ}C]$	$T_{wall} \ [^{\circ}C]$	$T_m [^{\circ}C]$
20	-7	0

Table 2.4: Boundary and initial conditions for Stefan problem



Figure 2.10: Temperature profile at a fixed time result of the Stefan problem

Results as the one in Figure 2.10 have been obtained with a MATLAB script which solve the transcendental equation (2.24) and give as outputs a matrix where temperature is function of time and space.

As expected, we can observe that temperature asymptotically tends to the initial temperature (set in this case at $T_i = 20^{\circ}C$) but, more important, it can be seen a change in the temperature profile derivative at the interface water-ice, as a result of the change in the thermal conductivity between the two different substances. In fact, if there is no internal heat generation, the flux is conserved and the balance can be written in the form below:

$$q = \lambda_{ice} \frac{\partial T}{\partial x} \Big|_{s^{-}} = \lambda_{water} \frac{dT}{dx} \Big|_{s^{+}}$$
(2.28)

Consequently, due to the fact that $\lambda_{ice} \neq \lambda_{water}$, also the derivative of temperature has to have a discontinuity in correspondence of the solid-liquid interface. In particular the thermal conductivity of ice is bigger than water's one so the slope of temperature in the water is steeper than in the ice, as can be seen in Figure 2.10. However, the latent heat from the phase-change has an influence on this process and (2.28) it's not correct, while the exact condition is given by (2.19) and the internal generation contribue to mitigate the discontinuity but it hasn't the precise value necessary to eliminate it.

Moreover, this consideration can be extended to the other interfaces involved in the original problem of the droplet, especially the ones involving air due to the significant difference of thermal conductivity ($\lambda_{air} \sim 0.023 \ W/mK$) and the fact that, along that interface, there is no phase change involving any kind of latent heat.

Useful characteristic of this problem is the dependence of the temperature field on the error function (2.29); this function tends to 1 quite rapidly, in particular erf(3) >0.9999 so in the future simulations it will not be necessary a calculation domain too big in order to simulate the asymptotic boundary condition (temperature being constant at infinity as stated in (2.18).

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$$
 (2.29)

Knowing the position of the solid-liquid interface from (2.25), the velocity of the interface itself can be deducted by simple derivation:

$$v_{interf}(x) = K_N \sqrt{\frac{\alpha_s}{t}}$$
(2.30)

It can be observed that the velocity is inversely proportional to the square root of time, which means that the displacement of the icing front will be way faster at the initial stages of the process than during the final phases. Moreover, velocity is not defined for t = 0 and $\lim_{t\to 0} v_{interf}(x) = \infty$. The cause is to be sought between the hypotheses of Stefan's problem: the wall is supposed to be at constant and imposed temperature equal to T_{wall} through the entire process, while the initial condition on the fluid is a constant temperature imposed in the entire domain. The consequence is that at the initial time $t = 0^+$ there is a finite temperature difference in no spacial step which in agreement with (2.1) cause an infinite thermal flux. As a by-product, a sudden temperature change and a consequent infinite velocity of the interface are found, because the latter is by assumption positioned where temperature is equal to T_m , the phase change temperature, so if temperature instantly change from the initial one to the wall temperature the interface moves at infinite velocity.

In reality, the initial phase of the freezing process of some liquid in contact with a wall at a temperature below its melting temperature is strongly influenced by impurities and the microscopical shape of the solid which lead to one or several nucleation points. Starting from these *nuclei* the liquid freezes and a lack of it is the cause of the supercooled water droplets already mentioned. For these reasons even if all the other hypotheses of the Stefan's problem are satisfied, the very initial phase of the icing process is not exactly described by its solution.

2.2.4. Fluid displacement generated by density variation

As well known, the density of the solid and liquid phases can be different and this phenomenon causes a movement (i.e. a bottle full of water cracks if the water is cooled and becomes ice). The governing equation of this phenomenon is the continuity, and under the hypothesis that initially there is only liquid it can be written as follows, with the subscript θ meaning *initial*:

$$\rho_{liq}V_{liq} + \rho_{sol}V_{sol} = const = \rho_{liq}V_{liq,0} \tag{2.31}$$

Under the mono-dimensional assumption it can be simplified being the volume the product of a constant area and an height. As in Figure 2.9 the height of the solid phase has already been identified as the interface s(t) while the total height of the two phases will be generically expressed as H:

$$\rho_{liq} \cdot (H - s(t)) + \rho_{sol} \cdot s(t) = const = \rho_{liq} H_{liq,0}$$

$$(2.32)$$

Then the expression can be derived with respect to time:

$$\frac{dH}{dt} = \frac{ds}{dt} \cdot \left(1 - \frac{\rho_{sol}}{\rho_{liq}}\right) \tag{2.33}$$

Given that the liquid is incompressible, the velocity of the superior border $\frac{dH}{dt}$ is also the velocity in each point of the fluid, which for this reason will be identified as $v_{liq}(t)$. From continuity expressed as (2.33), it can be seen that it is just a function of the velocity of the freezing interface and the density ratio between solid and liquid. In particular if there is no difference in densities, there is no movement and the governing equations are the (2.15) (2.16).

Otherwise, if the velocity of the fluid is not negligible (the solid phase is, by assumption, unmoving) the equation (2.16) has to be modified as follows:

$$\frac{\partial T_l}{\partial t} + v_{liq} \frac{\partial T_l}{\partial y} = \alpha_l \frac{\partial^2 T_l}{\partial x_l^2} \tag{2.34}$$

The (2.34) can be solved coupled with (2.15) and boundary conditions alike those of the classical Stefan problem. The procedure used to obtain the solution is shown in Appendix A and gives the following results for the temperature field in the liquid and the transcendent equation:

$$T_{l} = T_{0} + (T_{m} - T_{0}) \frac{erfc\left[\alpha\delta\left(\frac{x}{2\delta\sqrt{\alpha_{s}t}} - r\right)\right]}{erfc\left[\alpha\delta\left(1 - r\right)\right]}$$
(2.35)

$$\frac{e^{-\delta^2}}{erf(\delta)} - \frac{\phi}{\alpha} \frac{e^{-(\alpha\delta)^2}}{erfc[\alpha\delta(1-r)]} \frac{e^{2r(\alpha\delta)^2}}{e^{(r\alpha\delta)^2}} = \frac{\delta\sqrt{\pi}}{Ste}$$
(2.36)

being the parameter r an indicator of the expansion experienced by the fluid while changing from its liquid to its solid state:

$$r = 1 - \frac{\rho_s}{\rho_l} \tag{2.37}$$

It is important to verify that if there is no change in density between the solid and the liquid phases of PCMs, and consequently the parameters r is equal to 0, it imply a zero velocity as stated by (A.3) and the transcendental equation (2.36) corresponds to Eq. (2.24), the one already presented.

2.3. Experimental results

In this section will be summarily presented the experimental results obtained by Emeryk Ablonet [12] which are the basis for the following simulations. The experimental setup consisted in an aluminium plate cooled by a cryostat, covered with a thin layer of Teflon in order to depose the droplet: being the atmosphere not controlled, humidity has the tendency to form a substrate of ice, which is removed by changing the Teflon layer. So, the two different parameters which were changed during the experiment were the temperature of the cold plate by acting on the cryostat and the volume of water deposed. The first one of the two variables mentioned is the temperature boundary condition of the simulations, named as T_w . Instead, the second parameter determines the initial configuration of the droplet, according to the considerations on the *Bond number* described in the previous sections; the other peculiarity of the initial shape of the drop is the contact angle, which is determined by the Teflon layer but considering that it is positioned there to avoid an operative problem, it is not necessarily a constant in every simulation and it could be an interesting parameter to study. The images obtained using an high-speed camera were processed and at the end the result are images as those in Figure 2.11 and Figure 2.12.





Figure 2.11: Droplet's volume $20\mu L$

Figure 2.12: Droplet's volume $65\mu L$

The parameter changing between the two images is the volume of water deposed on the plate: the left one as a volume of $20\mu L$ which, considering a spherical cap with a contact angle $\theta_{water-Teflon} \simeq 130^{\circ}$ and using the 2.14, gives a radius $R = 1.73 \cdot 10^{-3}$. Injecting this radius as characteristic length in the Bond number 2.12, it is obtained a value of Bo = 0.4. The same procedure can be made for a bigger volume as the one in Figure 2.12, leading to Bo = 0.9. In agreement with the theory, the smaller droplet closely resemble a spherical cap while the bigger one is flattended by the action of the gravity force, so it has an elliptic shape with the y-axis (the gravity direction) shorter than the x-axis. In Figure 2.13 it can be seen an intermediate phase of the freezing process with the position of the solid-liquid interface highlighted in red: a peculiarity is the concave shape of the front.

While along the axis of the droplet the freezing front is quite planar for symmetry reasons, at the triple line interface (ice, water and air) its shape constantly changes with time depending on the evolution of the icing process. Moreover, it has reported difficult to have an accurate measure of this point due to the refraction caused by the curvature of the drop-air interface in the direction perpendicular to the plane showed in these figures.

So, at least alongside the symmetry axis the idea is that the phenomenon could be compared with the exact solution of Stefan's problem considering that its assumptions should be respected and the multidimensional phenomena shouldn't have a significant effect. Consequently, according to the equation which provides the position of the interface in relation with time (2.25), a square root tendency is expected. However the results of the experience weren't so clear and has yet to be determined if the hypothesis made are verified. In fact observing Figure 2.14 definitive conclusions can't be drawn: a linear and a square root tendency are traced (respectively dashed and



Figure 2.13: Intermediate phase of freezing process

dotted) and the red triangles represent the inferior part of the freezing interface while the blue triangles the superior one. As already stated, the superior part, corresponding with the triple interface, is affected by both a bigger error while determining it and a significant influence of boundary effects. Differently the red points represent the front in correspondence with the axis of the droplet and here a closer conformity with the Stefan's solution was expected, while the tendency looks maybe more linear than square root.



Figure 2.14: Evolution of icing front vs time

At last, in Figure 2.16 can be observed the pointy tip which is characteristic of every droplet which changes its phase: interesting fact is that this protrusion appears only in the final stage of the freezing process as can be deduced by comparing the latter image and Figure 2.15. Even if the droplet has almost completely become ice (the volume of liquid water above the red line is small in comparison with the initial volume of liquid), it is this small fraction remaining that will generate the characteristic tip. It has been verified that this phenomenon has no particular relation with the contact angle, meaning that the protusion appears both in case of sphare shaped drop (case that occurs with great value of the contact angle θ_c , on hydrophobic surfaces) and when the water spreads on the underlying plate (hydrophilic surfaces, with contact angles inferior to 90°). [13]

Probable causes of this particular structure on the iced droplet could be the *Marangoni* effect or the density variation.

The Marangoni effect can be sintetically described as the phenomenon which leads a fluid with a high surface tension to pull more strongly on the surrounding fluid than one with a low surface tension: the presence of a gradient in surface tension will naturally cause the liquid to flow away from regions of lower surface tension. The surface tension gradient can be caused by concentration gradient or, as in this case, by a temperature gradient (surface tension is a function of temperature).

However some experiences suggest that the difference in density is the main (maybe unique) driver for the protusion to develop: in fact the the same procedure was repeated for peanut oil droplets, instead of water droplets, reporting that no protusion formed. [14]



Figure 2.15: Last phase of icing process



Figure 2.16: Characteristic point of an iced droplet

3. Numerical code

3.1. Finite volume method

Physic problems which involves fluid's fluxes, mass and heat transfers, are ruled respectively by the principles of conservation of mass, momentum, energy and chemical species, and these principles are written by mean of partial differential equations. Being the PDE difficult to solve directly, The Finite Volume Method is a numerical technique that turns the PDEs representing the conservation laws over very small volumes into discrete algebraic equations over finite volumes (elements or cells).

As for other numerical techniques as finite difference or finite element method, the first step in the solution process consists in the discretization of the geometric domain, which in the FVM is discretized into finite volumes. The PDEs are then transformed into algebraic equations by integrating them over each discrete element. The system of these new algebraic equations has to be solved to compute the values of the variables for each element. In this method, some of the terms in the conservation equation are turned into face fluxes and evaluated at the finite volume faces. Because the flux entering a volume is identical to that leaving the adjacent volume, the FVM is conservative. This conservation property of the method is the main advantage that makes it the preferred method in CFD. Another important attribute of the FVM is that it can be formulated in the physical space on unstructured polygonal meshes. Finally in the FVM is quite easy to implement the boundary conditions, since the unknown variables are evaluated at the centroids of the volume elements, not at their boundary faces. These characteristics have made the FVM quite suitable for the numerical simulations of a variety of applications involving fluid flow and heat and mass transfer.

3.1.1. The discretization process

The numerical solution of a PDE consists in finding the values of the generic dependent variable ϕ at specified points from which its distribution over the domain of interest can be constructed. These points are the grid elements (or grid nodes) and result from the discretization of the original geometry into a set of non overlapping discrete elements, a process known as *meshing* [15]. Then the resulting variables are generally positioned at cell centroids or at vertices depending on the adopted discretization procedure. Whatever method has been chosen the focus is always on replacing the continuous exact solution of the PDE with discrete values. The distribution of the variable ϕ is hence discretized, and it is usual to refer to this process of converting the
governing equations into a set of algebraic equations for the discrete values of ϕ as the *discretization process* and the chosen method employed to do this conversion as the discretization methods.

The geometric discretization of the physical domain results in a mesh on which the conservation equations are solved. This requires the subdivision of the domain into discrete cells or elements that completely fill the computational domain to generate a mesh system. This is accomplished by a variety of techniques resulting in a wide range of mesh types. These meshes are classified according to several characteristics: structure, cell shape, variable arrangement,orthogonality, etc. In all cases the mesh is composed of discrete elements defined by a set of vertices and bounded by faces. Of course, information related to the topology of the mesh elements, in addition to some derived geometric information, are needed. These include element to element relations, face to elements relations, geometric information of the surfaces, element centroid and volume, face centroid, area and normal direction (the direction of the normal to a boundary face always points outward of the domain). For certain mesh topologies, details about the mesh can be easily deduced from the element indices as in structured grids, while for others it has to be constructed and stored in lists, as in the case of unstructured grids.

3.1.2. The semi-discretized equation

The first step of the finite volume discretization process consists in integrating the equations over the elements into which the domain has been subdivided, then the Gauss theorem is applied in order to transform the volume integrals of the convection and diffusion terms into surface integrals. Then the surface and volume integrals are transformed into discrete ones and integrated numerically through the use of *integration points*. To explain this, we can use an example for a two-dimensional transport problem. The conservation equation for a general scalar variable ϕ can be expressed as:

$$\underbrace{\frac{\partial (\rho\phi)}{\partial t}}_{ransient \ term} + \underbrace{\nabla \cdot (\rho \boldsymbol{v}\phi)}_{convective \ term} = \underbrace{\nabla \cdot (\Gamma^{\phi} \nabla \phi)}_{diffusion \ term} + \underbrace{Q^{\phi}}_{source \ term}$$
(3.1)

being ρ the density, **v** the velocity vector in each point and Γ^{ϕ} the diffusivity, depending on the generic variable being transported ϕ . The steady-state form of the above equation is obtained by dropping the transient term and is given by

$$\nabla \cdot (\rho \mathbf{v}\phi) = \nabla \cdot \left(\Gamma^{\phi} \nabla \phi\right) + Q^{\phi} \tag{3.2}$$

By integrating the above equation over the element C shown in Figure 3.1, equation (3.2) is transformed to

$$\int_{Vc} \nabla \cdot (\rho \mathbf{v}\phi) \, dV = \int_{Vc} \nabla \cdot \left(\Gamma^{\phi} \nabla \phi\right) \, dV + \int_{Vc} Q^{\phi} dV \tag{3.3}$$

Replacing the volume integrals of the convection and diffusion terms by surface integrals through the use of the divergence theorem, the above equation becomes



Figure 3.1: Conservation in a discrete element

$$\oint_{\partial V_c} (\rho \mathbf{v}\phi) \cdot d\mathbf{S} = \oint_{\partial V_c} \left(\Gamma^{\phi} \nabla \phi \right) \cdot d\mathbf{S} + \int_{V_c} Q^{\phi} dV$$
(3.4)

where **S** represents the surface vector, **v** the velocity vector and ϕ the conserved quantity.

3.1.2.1 Flux Integration

Denoting the convection and diffusion flux terms by $\mathbf{J}^{\phi,C}$ and $\mathbf{J}^{\phi,D}$, their expressions are given by

$$\mathbf{J}^{\phi,C} = \rho \mathbf{v}\phi \tag{3.5}$$

$$\mathbf{J}^{\phi,D} = -\Gamma^{\phi} \nabla \phi \tag{3.6}$$

Moreover, defining the total flux \mathbf{J}^{ϕ} as the sum of the convection and diffusion fluxes, the following relation can be written as:

$$\mathbf{J}^{\phi} = \mathbf{J}^{\phi,C} + \mathbf{J}^{\phi,D} \tag{3.7}$$

Replacing the surface integral over the generic cell C by a summation of the flux terms over the faces of element C, the surface integrals of the convection, diffusion, and total fluxes become:

$$\oint_{\partial V_c} \mathbf{J}^{\phi,C} \cdot d\mathbf{S} = \sum_{f \sim faces(Vc)} \left(\int_f (\rho \mathbf{v}\phi) \cdot d\mathbf{S} \right)$$
(3.8)

$$\oint_{\partial V_c} \mathbf{J}^{\phi,D} \cdot d\mathbf{S} = \sum_{f \sim faces(Vc)} \left(\int_f \left(\Gamma^{\phi} \nabla \phi \right) \cdot d\mathbf{S} \right)$$
(3.9)

$$\oint_{\partial V_c} \mathbf{J}^{\phi} \cdot d\mathbf{S} = \sum_{f \sim faces(Vc)} \left(\int_f \mathbf{J}_f^{\phi} \cdot d\mathbf{S} \right)$$
(3.10)

In these equations the surface fluxes are evaluated at the faces of the element rather than integrated in it. This transformation has important consequences on the properties of the FVM, the most important one is that this method is conservative. In order to proceed with the discretization, the surface integral at each face of the element in addition to the volume integral of the source term have to be evaluated. Using a Gaussian quadrature the integral at the face f of the element becomes

$$\int_{f} \mathbf{J}^{\phi} \cdot d\mathbf{S} = \int_{f} \left(\mathbf{J}^{\phi} \cdot \mathbf{n} \right) dS = \sum_{ip \sim ip(f)} \left(\mathbf{J}^{\phi} \cdot \mathbf{n} \right)_{ip} \omega_{ip} S_{f}$$
(3.11)

where ip refers to an integration point and ip(f) is the number of integration points along the surface f. There are many options available with their accuracy depending on the number of integration points used and the weighing function ω_{ip} . For a simple mean value integration, also known as the trapezoidal rule, only one integration point located at the centroid of the face is used with a weighing function of value equal to 1 $(ip=\omega_{ip}=1)$. This approximation is second order accurate and is applicable in two and three dimensions. Another option in two dimensions, which is third order accurate, involves two integration points (ip = 2) with weights $\omega_1=\omega_2=1/2$. We can use also three integration points; it is clear that the computational cost rises with the number of integration points used in the approximation[15]. With ip(f) denoting the number of integration points along face f, the general discretized relations for convection and diffusion terms become

$$\oint_{\partial V_c} (\rho \mathbf{v} \phi) \cdot d\mathbf{S} = \sum_{f \sim faces(Vc)} \sum_{ip \sim ip(f)} \left(\omega_{ip} \left(\rho \mathbf{v} \phi \right)_{ip} \cdot \mathbf{S}_f \right)$$
(3.12)

$$\oint_{\partial V_c} \left(-\Gamma^{\phi} \nabla \phi \right) \cdot d\mathbf{S} = \sum_{f \sim faces(Vc)} \sum_{ip \sim ip(f)} \left(\omega_{ip} \left(-\Gamma^{\phi} \nabla \phi \right)_{ip} \cdot \mathbf{S}_f \right)$$
(3.13)

3.1.2.2 Source term integration

With the aim of calculating the source term is used a volume integration. Adopting again a Gaussian quadrature integration, the volume integral of the source term is computed as:

$$\int_{V} Q^{\phi} dV = \sum_{ip \sim ip(V)} \left(Q^{\phi}_{ip} \omega_{ip} V \right)$$
(3.14)

As already done for the surface flux integration, there are different options for volume integration with their accuracy depending on the number of integration points used (ip) and the weighing function ω_{ip} . For one point Gauss integration $ip = \omega_{ip} = 1$ with the integration point located at the centroid of the element. This approximation is very common and is second order accurate and is applicable in two and three dimensions. As

for the flux integration, the accuracy increases with the number of integration points but so does also the computational cost.

3.1.3. The discrete equation using one integration point

While the above terms can be discretized with any specified number of integration points, it is common for the FVM to use one integration point, giving a second order accuracy. This way in fact is a good compromise between accuracy and flexibility while keeping the method simple and relatively of low computational cost. Following the mid-point integration approximation, the semi-discrete steady state finite volume equation for the element C can be simplified to

$$\sum_{f \sim nb(C)} \left(\rho \mathbf{v} \phi - \Gamma^{\phi} \nabla \phi \right)_f \cdot \mathbf{S}_f = Q_C^{\phi} V_C \tag{3.15}$$

The purpose of the second stage of the discretization process is to transform equation (3.15) into an algebraic equation by expressing the face and volume fluxes in terms of the values of the variable at the neighbouring cell centers. The second discretization step so is based on the *linearization of the fluxes*.

3.1.3.1 Flux linearization

The face flux can be split into a linear part which is a function of the ϕ values at the nodes on the two sides of the face (in this case ϕ_C and ϕ_F), and a non-linear part, which includes the portion that cannot be expressed in terms of ϕ_C and ϕ_F where the subscripts C and F stand for *center of the element* and a generic point *outside the element* respectively, divided by the considered face. The resulting equation can be written as follows:

$$\mathbf{J}_{f}^{\phi} \cdot \mathbf{S}_{f} = \underbrace{FluxT_{f}}_{totalflux} = \underbrace{FluxC_{f}}_{flux\ linearization} \phi_{C} + \underbrace{FluxF_{f}}_{flux\ linearization} \phi_{F} + \underbrace{FluxV_{f}}_{non-linearized\ part} (3.16)$$

where $FluxT_f$ represents the total flux through face f, and is decomposed into three terms. The first two terms represent the contributions of the two elements sharing the face and are written with the linearization coefficients $FluxC_f$ and $FluxF_f$. The third term describes the nonlinear contribution that cannot be expressed as a function of ϕ_C and ϕ_F and is given by the non-linear term $FluxV_f$. All the values of $FluxC_f$, $FluxF_f$ and $FluxV_f$ obviously depend on the discretized term and the scheme used for its discretization. The flux linearization is obtained by substituting eq(3.16) into the left hand side of eq(3.15). Repeating for all cell faces we have

$$\sum_{f \sim nb(C)} \left(\mathbf{J}_{f}^{\phi} \cdot \mathbf{S}_{f} \right) = \sum_{f \sim nb(C)} \left(FluxT_{f} \right) = \sum_{f \sim nb(C)} \left(FluxC_{f}\phi_{C} + FluxF_{f}\phi_{F} + FluxV_{f} \right)$$
(3.17)

The linearization of the volume flux is performed by expressing it as a linear function of the element node value ϕ_C and is given by

$$Q_C^{\phi}V_C = FluxT = FluxC\phi_C + FluxV \tag{3.18}$$

Substitution of Eqs.(3.17) and (3.18) in Eq.(3.15) gives the algebraic relation

$$a_C\phi_C + \sum_{f \sim nb(C)} \left(a_F\phi_F\right) = b_C \tag{3.19}$$

where the relations between equation coefficients and flux coefficients are expressed by

$$a_{C} = \sum FluxC_{f} - FluxC$$

$$a_{F} = FluxF_{f}$$

$$b_{C} = -\sum_{f \sim nb(C)} FluxV_{f} + FluxV$$
(3.20)

3.1.4. Transient Semi-Discretized Equation

For unsteady problems the temporal term in Eq.(3.1) is retained, consequently it is not sufficient the integration over the volume but in order to take account of the time evolution, an integration over time is also needed. In this case the integrated equation becomes:

$$\int_{t}^{t+\Delta t} \int_{V_{c}} \frac{\partial \left(\rho\phi\right)}{\partial t} dV dt + \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} \left(\rho \mathbf{v}\phi\right)_{f} \cdot d\mathbf{S} \right) \right] dt - \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} \left(\Gamma \nabla\phi\right)_{f} \cdot d\mathbf{S} \right) \right] dt = \int_{t}^{t+\Delta t} \left[\int_{V_{c}} Q^{\phi} dV \right] dt \quad (3.21)$$

Further simplification of this equation requires a choice based on the time integration accuracy required. For fixed grids, where the volume and the surface of each element are constant in time, the first term can be integrated as:

$$\int_{t}^{t+\Delta t} \int_{Vc} \frac{\partial \left(\rho\phi\right)}{\partial t} dV dt = \int_{t}^{t+\Delta t} \frac{\partial}{\partial t} \left(\int_{Vc} \rho\phi dV\right) dt = \int_{t}^{t+\Delta t} \frac{\partial \left(\overline{\rho\phi}\right)}{\partial t} V_{c} dt \qquad (3.22)$$

where

$$\overline{\rho\phi}_C = \frac{1}{V_C} \int_{V_C} \rho\phi dV = (\rho\phi)_C + O\left(\Delta^2\right)$$
(3.23)

Substituting, Eq.(3.21) reduces to

$$\int_{t}^{t+\Delta t} \frac{\partial \left(\rho\phi\right)}{\partial t} V_{c} dt + \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} \left(\rho \mathbf{v}\phi\right)_{f} \cdot d\mathbf{S} \right) \right] dt - \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} \left(\Gamma \nabla\phi\right)_{f} \cdot d\mathbf{S} \right) \right] dt = \int_{t}^{t+\Delta t} \left[\int_{Vc} Q^{\phi} dV \right] dt \quad (3.24)$$

and using the midpoint rule (explained previously), (3.24) becomes:

$$\int_{t}^{t+\Delta t} \frac{\partial (\rho\phi)}{\partial t} V_{c} dt + \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} (\rho \mathbf{v}\phi)_{f} \cdot d\mathbf{S} \right) \right] dt - \int_{t}^{t+\Delta t} \left[\sum_{f\sim nb(C)} \left(\int_{f} (\Gamma \nabla \phi)_{f} \cdot d\mathbf{S} \right) \right] dt = \int_{t}^{t+\Delta t} Q_{C}^{\phi} V_{C} dt \quad (3.25)$$

Going forward beyond this point requires assumptions as regard as the variable is changing in time.

3.2. JADIM research code

Jadim is a research code developed by Jacques Magnaudet and Dominique Legendre's team in the Interface group at *Institut de Mécaniques des Fluides de Toulouse*. The code permits to describe in an accurate way such physical mechanisms present in multiphasic flows. Jadim is a numerical tool which resolves Navier-Stokes equation in 3D for incompressible fluids and instationnarities.

A second order space and time finite volume method with a structured mesh is used (third order Runge-Kutta scheme for non-linear term resolution coupled with a Crank-Nicholson scheme for the semi-implicit part).

The pressure is computed from a projection method, the Poisson's equation is solved using a Fourier solver for monophasic case and an iterative sparse solver for two fluid model. The large eddy simulation (LES) of turbulent flow uses a dynamic mixed subgrid-scale model [16].

There are also implemented:

• heat transfer computation

- Volume of fluid (VOF)
- Immersed Boundary Method (IBM)

3.2.1. One fluid formulation

The multiphase flow is modellized using the so called one fluid formulation, as to say that under the assumptions of:

- the fluids are Newtionian and incompressibles
- there is no mass transfer at the interface
- the surface tension is constant

the fluid flow can be described by the classical one fluid formulation of the Navier-Stokes equations:

$$\begin{cases} \frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \boldsymbol{\Sigma} + \mathbf{g} + \mathbf{F}_{\sigma,s} \\ \nabla \cdot \mathbf{U} = 0 \end{cases}$$
(3.26)

where Σ is the viscous stress tensor, **g** is the acceleration due to gravity, and ρ and μ are the local density and dynamic viscosity, respectively and $F_{\sigma,s}$ is the capillarity contribution.

In order to solve problems with more than one fluid, it is necessary to introduce the volume fraction defined as $\tau = \frac{V_1}{V_{tot}}$; once this parameter is computed (or imposed) in the domain, local density and local dynamic viscosity can be deduced from τ by a linear interpolation as follow:

$$\rho = \tau \rho_1 + (1 - \tau) \rho_2 \tag{3.27}$$

$$\mu = \tau \mu_1 + (1 - \tau) \,\mu_2 \tag{3.28}$$

where ρ_1 and μ_1 are the physical properties of the first fluid and the volume fraction has an integer value in cells completely filled with fluid one or two, and it has an intermediate value if the interface cuts the considered cell, that is to say it vary continuously through 0 and 1: $\tau \in [0, 1]$. [17]

With this previous formulation, a new variable has been introduced in the system, so it is necessary to add another equation in order to close the problem, which is the transport equation for the volume fraction, that has to be solved to locate the interface between the two phases:

$$\frac{\partial \tau}{\partial t} + \boldsymbol{U} \cdot \nabla \tau = 0 \tag{3.29}$$

3.2.2. Spatial discretization

The previous equations (3.26) and (3.29) are discretized by means of a staggered grid using a finite volume method, where the spatial derivatives are approximated using second-order centered schemes. This means that each variable has its own control volume of integration. An example for the positions and the control volume is represented, for a two-dimensional case, in 3.2. The extension to the generic three-dimensional problem is obvious.



Figure 3.2: Control volumes and variables

As said, in the above figure a 2D's staggered grid is illustrated with the positions where the different variables are calculated and the control volumes in which they have to be integrated. The variables in this case are the pressure P, the volume fraction τ , and the velocities U and V for the x and y direction respectively; the corresponding staggered control volumes are denoted with CVP, CVU and CVV.

3.2.3. Temporal discretization

The time scheme used in the Jadim code to compute the advective terms in the Navier-Stokes equations is a third-order Runge-Kutta type scheme, while the viscous stresses in the same equations are solved using a semi-implicit Crank-Nicolson method.

The incompressibility is ensured by using a projection method, which consists in splitting the velocity field into two contributions: the first is the rotational one, which gives a predicted velocity field calculated semi-implicitly, while the second is the potential one, obtained from a pressure correction solution of a pseudo-Poisson equation, whose divergence is zero. Since the viscosity contribution is calculated implicitly, the constraining criterium on the time step linked to viscosity is avoided. The capillary force, if present (this is not the case), introduces an additional time step constraint that is based on an advective time step where the velocity would be the maximum velocity of a capillary wave. The different time step criteria are summarized in the following Table 3.1

Summarizing, the main steps to follow in the time advancement in order to calculate the velocity and pressure fields are:

• update of the volume fraction τ : calculation of ρ^{n+1} and μ^{n+1} solving the equation (3.29)

gravitational effects	$\Delta t < \sqrt{rac{\Delta x}{g}} ightarrow + \infty$
advection	$\Delta t < \sqrt{3} rac{\Delta x}{U}$
viscosity	$\Delta t < rac{\Delta x^2}{ u} ightarrow + \infty$ $(implicit)$

Table 3.1: Time step constraints

- momentum semi-implicit resolution: a third order Runge-Kutta type scheme is used for the advancement through time. The advective and body terms are calculated explicitly, while viscous terms, as previously said, are calculated using a semi-implicit Crank-Nicolson algorithm. This results lead to the calculation of the predicted velocity field U^* comprising the vorticity of U^{n+1}
- capillary contribution: a second predicted velocity field U^{**} is computed from U^* and $F_{\sigma,v}$
- projection step: pressure field P^{n+1} is found solving a pseudo-Poisson equation from U^{**} and U^{n+1} is calculated with a projection method

3.3. The Immersed Boundary Method

As stated in the previous chapter, the aim of this work is to simulate the solidification of a droplet placed on a cold plate and the main challenge is to make a good representation of the solid-fluid interaction. This kind of interactions are encountered in a large number of industrial and natural applications, including chemical processes, aeronautics, transportations, biomecanics, geophysics, oceanography and many others. Modeling solid-fluid interaction is often difficult because of the complexity of the solid shape and the motion in the fluid flow. Reproducing the dynamics of multiple interacting objects of arbitrary geometry with possible deformations is even more challenging if the flow is non-uniform in his composition, density or temperature [18].

The methods used for modeling solid-fluid interactions may be divided into two main groups, depending on the way the interfaces between the solid and the fluid are described. The first group, usually named as *body-fitted grid methods*, makes use of a structured curvilinear or unstructured grid to conform the mesh to the boundary of the fluid domain. The problem can be encountered in situations involving complex moving boundaries, is that one needs to establish a new body-conformal grid at each time-step which leads to an excessive computational cost and a subsequent slowdown of the numerical procedure. In addition, one can have issues associated with regridding such as grid-quality and grid-interpolation errors. The second group of methods is referred to as *fixed-grid methods*. These techniques make use of a fixed grid, which eliminates the need of regridding, and the presence of the solid object is taken into account using source terms added to fluid flow equations. Fixed-grid methods have been mainly developed in recent years, such as distributed Lagrange multiplier based methods, immersed boundary methods (used in this work), lattice Boltzmann methods, penalty methods and ghost-fluid methods. All these numerical methods have been developed and shown to be effective in computing fluid-particle systems and fluidstructure interactions; the focus here will be on the Immersed Boundary Method (IBM). The term *immersed boundary method* was first used in reference to a method developed by Peskin (1972) to simulate the cardiac mechanism with the associated blood flow. The particular feature of this method was that it was based on a cartesian grid, which did not conform to the geometry of the heart. Since this new procedure was introduced, numerous modifications have been made and a great number of variants of this approach now exist. If a cartesian grid is used, which is generated with no regard to the solid object's shape, so the solid boundary would cut through this cartesian mesh. Because the grid does not conform to the solid boundary, incorporating the boundary conditions would require some modifications in the equations in the vicinity of the boundary, which is the key factor in developing an IB algorithm and which distinguishes one IBM from another (see methods in [19]). In particular, there will be a force added to the right-hand side of momentum equations to mimic the boundary condition:

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{U} \cdot \nabla) \mathbf{U} = -\frac{1}{\rho} \nabla P + \frac{1}{\rho} \nabla \cdot \boldsymbol{\Sigma} + \mathbf{g} + \boldsymbol{F}_{\sigma,s} + \boldsymbol{f}$$
(3.30)

where the terms are the same of Eq. (3.26) with the addition of IB force **f**. Among the different IBMs developed one can distinguish between the so-called *continuous forcing methods* and the *discrete forcing methods*. In the first class of procedures the force is added to momentum equation before the discretization, as done by Peskin in simulating the blood flow associated with a beating heart, where the IB was represented by a set of elastic fibers and the fiber stress was transmitted from IB to the grid by means of a regularized Dirac function. In these kind of methods the force formulation does not depend on the used numerical scheme and they are very effective in problems involving elastic boundaries.

Differently, in the second group of methods, the force is added to the momentum equations after the discretization and its formulation depends on the used numerical scheme. These are more effective if rigid boundaries are involved, even if there can be implications for numerical accuracy as well as stability. Moreover, they can be categorized into those methods that are formulated so as to impose the boundary condition on the immersed boundary through indirect means, and those that directly impose the boundary condition on the IB [19]. In any case, the smoothing of the forcing function inherent in these approaches can lead to an inability to provide a sharp representation of the IB and this can be especially undesirable for high Reynolds number flows.

4. Implementation in JADIM

The core idea of this project of thesis is to replicate the behaviour of a droplet of water freezing on a cold plate by using the immersed boundary method (IBM) to simulate the accretion of ice and its outcomes on the surrounding fluids. As already seen in Chapter 2, a peculiarity of this process is the final shape assumed by the solidified droplet due to the change of density during the phase change from liquid water to its solid state.

There are two substantial differences between the approach of IBM in this work and the classical immersed boundary formulation: its purpose and its definition. Firstly, here the IBM is not used in its common sense because its function is not limited to simulate a moving boundary but it also take account of what happens at its interior. Secondly, the objective is to couple the immersed boundary method not only with the volume of fluid method but also with the temperature field in the domain, that is to say that the presence and the movement of the object simulated using this technique is strictly linked with the temperature more than with a law imposed by force's field.

In classical examples of IBM application are Peskin's study of the heart or generic situation involving complex moving boundaries as object falling in a flow under the influence of the flow itself and gravity, the temperature is not considered and the studied phenomena are linked to the interaction of the solid boundary with the environment (the surrounding fluid motion). Otherwise, the problem developed in this work is centred on heat transfer and the thermal field plays a crucial role and the immersed boundary has to influence and be influenced by it.

In fact the core idea is to simulate the ice has a fluid which can not be moved and has different thermophysical properties, the first way to obtain this result is the *rheological method* which consists in defining an artificial higher viscosity to characterize the water below phase change temperature [20], while the second one is based on using an IBM layer in order to obtain a similar result.

The choice of this second option as developed in this work is linked to the aim of taking account of both the temperature field (heat fluxes and temperature diffusion) and the force field (expansion due to the density variation) associated with the phase change of water. It is obvious that:

- the IBM layer develops through the process
- its existence is due to temperature field
- once created it influences the heat transfer

In the standard approach the IBM already exists at the starting time and its position is imposed a priori or it depends by a steady shape of the object moving in the domain following certain laws depending on many different parameters. Differently, the model developed has an IBM object which depends on the temperature, with temperature function of time, so it is time-temperature dependent. In particular the ice (simulated with the IBM layer) could not be present at the initial time and, surely, its volume changes with time: it increases if a cooling problem is studied.

At a fixed time step, if it is assumed that there is both ice and water (an intermediate time when the solidification process is already started but has not finished yet) the force/velocity field can be divided into two parts. The first one is where there is ice, here velocity is imposed equal to zero by having the IBM layer; the second, where there is the other fluid, has an imposed velocity due to evolution of the IBM frontier. Through time, the IBM object increases its volume and its frontier moves forward following the temperature field but, differently from the classical formulation, the velocity imposed on the surrounding fluid by this advancement it is not equal to the velocity of the frontier itself (for an incompressible flow) but a different one determined by the ratio between the two densities of ice and water. In fact, the water becomes ice and it is *absorbed* by the IBM and the velocity on the exterior is due to the conservation of mass, as shown in (2.31)-(2.33). In a certain way, it can be said that the IBM object incorporates a portion of water while advancing, and the remaining part of liquid is pushed upwards (in the direction perpendicular to the ice front) by expansion.

The other main effect of the phase change is the variation of thermophysical properties, in particular the thermal diffusivity named α , consequently the basic idea developed is to use the IBM sub-layer as a switch to modify this property. As already said, this layer of IBM will be created as a function of temperature, as a consequence its dynamics is linked to the thermal fluxes, which are, in turn, led by the thermal diffusivity of the different phases of water.

4.1. Definition of the IBM function

As stated, the objective is to define a parameter which has the purpose to indicate the presence of ice in each cell of the domain. This parameter obviously has to be function of temperature, in particular function of the phase change temperature and it will be used to compute every physical property in the domain. This new variable, in analogy to the volume fraction τ , should show the volume fraction of ice; so it will assume the value of 1 in the ice and 0 in the liquid water. As known, the phase of water is a function of temperature, and being a pure substance the phase change happens at a fixed temperature and this would means a discontinuity in the new variable:

$$\begin{cases} if \quad T > T_m \Rightarrow water \Rightarrow \alpha_{ibm} = 0\\ if \quad T < T_m \Rightarrow ice \Rightarrow \alpha_{ibm} = 1 \end{cases}$$
(4.1)

where α_{ibm} represents the parameter discussed and $T_m = 0^{\circ}C$ is the phase change temperature.

At this point, the formulation for the volume fraction of ice as just defined is characterized by discontinuity with a step distribution which it is not suitable for a numeric simulation for stability reasons so a smoother formulation is required.

Obviously, the first step in order to smooth α_{ibm} is to move from the real isothermal phase change to a range of solidification temperatures; the more this range is wide the more the variable is simple to be computed but it also moves away from the real solidification/melting process. Once the range of solidification has been chosen it is necessary to define a law of variation through which it is possible to link the two ends of the function. There are a great number of possible mathematical function which can achieve this purpose as linear, sine/cosine, different powers, hyperbolic tangent, etc. The last two have been discarded for different reasons: the hyperbolic tangent has the flaw of rapidly grow until its upper limit but it takes too long to assume its final value at the extremities (0 and 1), while the power solution has been tested in a previous work at IMFT [20] and has been proven to be unsatisfactory.

Firstly the range of temperature has to be chosen fixing the values of both the temperature at its extremities, named minimum and maximum temperatures T_{min} and T_{max} . Then the required characteristics of the function defining α_{ibm} are to assume the value of 0 and 1 respectively at the minimum and maximum temperatures and to have an intermediate value between them. Given this requirements the possible formulations with linear and cosine options are:

$$\alpha_{ibm} = \frac{T_{max} - T}{T_{max} - T_{min}} \tag{4.2}$$

$$\alpha_{ibm} = 0.5 \cdot \left[\cos \frac{\pi \cdot (T - T_{min})}{T_{max} - T_{min}} + 1 \right]$$
(4.3)



Figure 4.1: Example of the different formulation for the function α_{ibm}

The most natural choice as a range of temperature between which the phase change is hypothesized to happen would be symmetrical in respect of the solidification temperature, but another smart assumption would be to have it shifted towards the liquid phase, assuming the phase change temperature as inferior border. This second choice as the meaning of assuming that the solidification can only take place in the liquid, while if the temperature is below the phase change temperature, the fluid is certainly in its solid state.

In any case, the choice of the width of the range of temperature assumed, as well as its positioning, requires some tests in order to identify the best compromise, or it can be influenced by the study of a certain parameter of the problem or another.

Given the previous functions, they would fit in a case like the *Stefan problem* where only water is present, however in a more general case where another fluid, like air, is considered, a slight modification is required for the purpose of preventing the cooled air to be taken account as ice. Remembering that a volume fraction τ has already been implemented in the code in order to discriminate two different fluid, is sufficient to multiply the (4.2) and (4.3) for this volume fraction:

$$\alpha_{ibm,lin} = \tau \cdot \frac{T_{max} - T}{T_{max} - T_{min}} \tag{4.4}$$

$$\alpha_{ibm,cos} = 0.5 \cdot \tau \cdot \left[\cos \frac{\pi \cdot (T - T_{min})}{T_{max} - T_{min}} + 1 \right]$$

$$(4.5)$$

paying attention to have the volume fraction set the right way, as to say its value must be equal to 1 for the PCM's phase and 0 for the other (air).

4.2. The IBM function as a switch for thermophysical properties

Once the α_{ibm} function has been defined, the portion of the domain where water should be solid is identified but nothing more has been done yet. The successive step consists in changing the properties of the liquid which have an interest in the simulations.

While the mean to take account for the increased opposition the ice has towards the motion is directly implemented in the equation by the immersed boundary method and will be addressed in the next paragraph, the thermophysical properties as the thermal diffusivity and the density has to be changed as well.

In order to obtain a coherent result, the set of equation used for the one fluid formulation needs to be modified. As for two fluid it was necessary to introduce the volume fraction τ , in the case where another substance is introduce it is necessary to have another parameter which has the same meaning. This parameter has already been built and it is α_{ibm} which represents the volume fraction of ice as regards the water. Consequently expression as (3.27) and (3.28) have to be modified as follows, being ϕ a generic intensive property:

$$\phi = (1 - \tau) \phi_1 + \tau \left[(1 - \alpha_{ibm}) \phi_2 + \alpha_{ibm} \phi_3 \right]$$
(4.6)

where the subscripts from 1 to 3 refer respectively to the surrounding fluid, the liquid phase of PCM (water) and its solid phase.

4.3. The immersed boundary method and the momentum equation

Newton's laws are relations between motion of bodies and the forces acting on them, in particular Newton's second law states that the acceleration of a body is proportional to the net force acting on it and is inversely proportional to its mass. In a more general form it can be written as:

$$\boldsymbol{F} = \frac{dm\boldsymbol{U}}{dt} \tag{4.7}$$

which corresponds to the physical principle that force is equal to the variation of momentum with time.

Considering a control volume and all possible forces acting on it (body, surface...) the final momentum equation formulation obtained is [21]

$$\frac{\partial \boldsymbol{U}}{\partial t} + (\boldsymbol{U} \cdot \nabla) \, \boldsymbol{U} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \boldsymbol{U} + \boldsymbol{F}$$
(4.8)

It is clear from the above equation (4.8) that forces and velocities are strictly linked and the firsts can be a consequence of the latter or vice versa, being mutually dependent variables. In the considered problem forces are unknowns while the velocities have known formulation, so, by the mean of immersed boundary, velocity will be imposed and the consequent forces computed.

4.3.1. Velocities calculation

As previously stated, velocities are a given input of the problem, because in the ice layer, by assumption, there is no motion while the surrounding fluid is pushed by the expansion due to the phase change and continuity equation as shown by (2.33):

$$\boldsymbol{v_{liq}} = \left(1 - \frac{\rho_{ice}}{\rho_{water}}\right) \boldsymbol{V_{front}}$$
(2.33')

This equation represents the evolution of the icing front as it absorbs a portion of water but, at the same time, the density ratio causes an augmentation of volume and consequently the motion. However, the velocity to be imposed by the immersed boundary, at this point is still unknown because it depends on the solidification interface advancement which has to be calculated starting from the other variables of the problem. Once this variable is found, the consequent velocity above can be computed and directly imposed to the fluid, because the density ratio is given as an input constant.

4.3.1.1 Scalar transport equation

In order to obtain the solidification front velocity a new equation is needed, the so called *scalar transport equation*; it represents the transport of a scalar quantity operated by a velocity. In the considered case, the scalar being transported is the parameter α_{ibm} and the velocity which acts the transport is the unknown that has to be found.

$$\frac{\partial \alpha_{ibm}}{\partial t} + \boldsymbol{V_{front}} \cdot \nabla \alpha_{ibm} = 0 \tag{4.9}$$

given the definition of normal vector of a scalar field

$$\boldsymbol{n} = \frac{\nabla \alpha_{ibm}}{||\nabla \alpha_{ibm}||} \tag{4.10}$$

introducing (4.10) in (4.9) the second one can be manipulated as follow:

$$\frac{\partial \alpha_{ibm}}{\partial t} + \boldsymbol{V_{front}} \cdot \boldsymbol{n} ||\nabla \alpha_{ibm}|| = 0$$
(4.11)

Equation (4.11) can be inverted in order to find the searched velocity of the solidification front V_{front} :

$$\boldsymbol{V_{front}} \cdot \boldsymbol{n} = \frac{-\frac{\partial \alpha_{ibm}}{\partial t}}{||\nabla \alpha_{ibm}||} \tag{4.12}$$

Last step, in order to simplify the computation of this term, being α_{ibm} a function of phase and temperature (4.4) (4.5), and being temperature a function of time in turn, the *chain rule* can be used to obtain the following formulation:

$$\boldsymbol{V_{front}} \cdot \boldsymbol{n} = \frac{-\frac{\partial \alpha_{ibm}}{\partial T} \frac{\partial T}{\partial t}}{||\nabla \alpha_{ibm}||}$$
(4.13)

At this point, all the right hand side of (4.13) can be calculated by knowing the temperature field and temperature evolution in time, giving as result the product between the velocity of the front and its normal, which means the absolute value of velocity following the normal direction. Momentum equation consists in three scalar equation for each cartesian direction, consequently the known velocity that has to be introduced in these equations has to be decomposed in its scalar components. This operation can be done by simply multiplying the found absolute value by the three components of the normal vector (4.10):

$$n_i = \frac{\frac{\partial \alpha_{ibm}}{\partial x_i}}{||\nabla \alpha_{ibm}||} \tag{4.14}$$

being i the generic direction of the cartesian reference system.

4.3.2. Momentum computation

The forcing term \mathbf{f} has to be evaluated, starting from the knowledge of the velocity, and different approaches have been developed in the last years, in particular the already cited direct and indirect forcing methods.

In general, the shape of the solid object is complex and the location of the boundary condition for the velocity is unlikely to coincide with the grid nodes, so that interpolation techniques are usually employed to enforce the boundary condition by imposing constraints on the neighboring grid nodes. Another strategy has been developed [18] which consists in using the *solid volume fraction* α_{ibm} in the transition region between the solid and the fluid instead of a classical interpolation. The expression of the forcing term become:

$$\boldsymbol{f} = \alpha_{ibm} \frac{\boldsymbol{U} - \boldsymbol{U}^*}{\Delta t} \tag{4.15}$$

where Δt is the time step used for the time-advancement, **U** the local velocity imposed to the immersed solid object and U^* is a predictor velocity without considering the immersed object.

Using the solid volume fraction, which may be viewed as a smoothing of the immersed boundary, is an alternative way to using a regularizing function in conjunction with a Lagrangian marking of the boundary. The latter technique is largely used in immersed-boundary methods in order to allow for a smooth transfer of momentum from the boundary to the fluid. The advantage of the present choice is that (i) it is simple to implement, (ii) no interpolation is needed between the Eulerian grid and possible Lagrangian markers, since no marker are used here, so that the computational cost is reduced when multiple objects are simulated, and (iii) the results appears to be in good agreement with respect to other available higher-order immersed-boundary or boundary-fitted approaches.

In the particular case studied, the velocity \mathbf{U} imposed to the object is divided in two different parts, function of the value assumed by the solid fraction:

$$\begin{cases} U = 0 & \alpha_{ibm} \ge 0.95 \\ U = v_{liq} & 0 < \alpha_{ibm} < 0.95 \end{cases}$$
(4.16)

This separation has been done in order to obtain the double purpose of both force a zero velocity to the solid phase and a non-zero velocity to the fluid, where the latter is imposed by the interface. In fact, with this formulation is the solidification zone which push the liquid in accord to Eq. (4.13). The upper limit of the phase change region has been fixed equal to 0.95 in order to guarantee real zero velocity in the solid, that is to say where α_{ibm} has the precise value of 1.

The velocity U^* is computed every Runge-Kutta cycle by using the classical Navier-Stokes equation without the immersed boundary forcing term (3.26). The successive steps consists in calculating the forcing term f^k , where k is the index for the Runge-Kutta loop. Then using Eq. (3.30), which takes account of the presence of the immersed boundary, a new velocity \tilde{U}^{k+1} is calculated but it is not divergence free. So a Poisson pseudo-equation is solved to get the potential auxiliary function Φ^{n+1} , being n the current time step.

4.4. Pressure correction

The Poisson pseudo-equation is written in the following form:

$$\frac{\boldsymbol{U}^{n+1} - \tilde{\boldsymbol{U}}^{n+1}}{\Delta t} = -\frac{1}{\rho} \nabla \Phi^{n+1} \tag{4.17}$$

being the Φ the potential auxiliary function defined as:

$$P^{n+1} = P^n + \Phi^{n+1} \tag{4.18}$$

The successive step consists in applying the divergence operator to Eq. (4.17), where, by assumption the divergence of the corrected velocity U^{n+1} is equal to zero. This operation implicates the Poisson pseudo-equation to become:

$$div\left(\tilde{\boldsymbol{U}}^{n+1}\right) = div\left(\frac{\Delta t}{\rho}\nabla\Phi^{n+1}\right) \tag{4.19}$$

which has to be integrated on the cell volume according to the volume of fluid method.

$$\int_{V} div \left(\frac{1}{\rho} \nabla \Phi^{n+1}\right) dV = \int_{V} \frac{1}{\Delta t} div \left(\tilde{\boldsymbol{U}}^{n+1}\right) dV \tag{4.20}$$

which applying the Gauss-Green theorem gives:

$$\int_{S} \frac{1}{\rho} \nabla \Phi^{n+1} \cdot \boldsymbol{n} dS = \frac{1}{\Delta t} \int_{S} \tilde{\boldsymbol{U}}^{n+1} \cdot \boldsymbol{n} dS$$
(4.21)



Figure 4.2: Exemplification of Φ

Using the conventions shown in Figure 4.2, the left hand term of Eq. (4.21) can be written in the following way:

$$\int_{S} \frac{1}{\rho} \nabla \Phi^{n+1} \cdot \boldsymbol{n} dS = \left(\Phi_{i,j+1} - \Phi_{i,j} \right) \frac{A_N}{\rho_N \Delta y_N} + \left(\Phi_{i+1,j} - \Phi_{i,j} \right) \frac{A_E}{\rho_E \Delta x_E} + \left(\Phi_{i,j} - \Phi_{i,j-1} \right) \frac{A_S}{\rho_S \Delta y_S} + \left(\Phi_{i,j} - \Phi_{i-1,j} \right) \frac{A_W}{\rho_W \Delta x_W} \quad (4.22)$$

where the letters N, S, E, W indicate the cardinal directions.

The previous equation can also be written in a more compact structure by assuming:

$$a_i = \frac{A_i}{\rho_i \Delta x_i, y_i} \tag{4.23}$$

being once again i the index for the different cardinal direction. Which gives the final equation as:

$$\int_{S} \frac{1}{\rho} \nabla \Phi^{n+1} \cdot \mathbf{n} dS = a_N \Phi_{i,j+1} + a_E \Phi_{i+1,j} + a_S \Phi_{i,j-1} + a_W \Phi_{i-1,j} + (a_N + a_E + a_S + a_W) \Phi_{i,j} \quad (4.24)$$

Starting from the simple example represented in Figure 4.3, some considerations regarding the case study and the pressure correction method can be made.



Figure 4.3: Imposition of a velocity

If the objective is to impose a fixed velocity value starting from the wall through the above fluid domain, this can be easily done by acting on the coefficients of the previous Eq.(4.24). In particular, considering this example, the chosen velocity V_P must be preserved in the flow so it has not to be corrected doing the steps written above. This means that the corrected velocity U^{n+1} and the predicted velocity \tilde{U}^{n+1} must correspond, with the last of them equal to the velocity to be preserved. In order to grant this equality, referring to Eq.(4.17), it can be seen that the gradient of the auxiliary potential Φ has to be zero. That is to say that the wall-normal derivative of Φ must be 0; in other words, called $\Phi_{i,j}$ the potential in the first cell over the wall, the potential in the i, j - 1 position has to be neglected. The easiest way to do that is by eliminating the contribution of $\Phi_{i,j-1}$ from Eq.(4.24) imposing the coefficient a_S to be 0. In a more general way, considering a one dimensional solidification problem where the ice advance starting from a south wall towards the north direction, an icing front velocity can be calculated as in Eq.(4.13) and must be preserved in order to push the fluid above the ice-water interface. The way to accomplish that is by imposing $a_S = 0$ in the fluid domain in order to preserve the front velocity, same way as done for the wall example illustrated before. Resuming, the coefficients' modifications required in order to have a fluid motion due to the expansion during the phase change and a fixed solid region are, for the simple 1D case:

$$\begin{cases} a_N = 0 & if \quad \alpha_{ibm} > 0.5 \\ a_S = 0 & if \quad \alpha_{ibm} < 0.5 \end{cases}$$

$$(4.25)$$

where 0,5 is an indicating value for the interface between the two phases.

4.5. Solidification latent heat

When the solidification process occurs to liquid water, not only the thermophysical properties change but the so-called *latent heat* has to be taken in account. Latent

heat expresses the amount of energy in the form of heat required to completely effect a phase change of a substance and it is an intensive property; in particular this energy is absorbed or released during a constant temperature phase change process by the thermodynamic system.

The numerical treatment of this phenomenon has been studied by many authors and a variety of possible solution has been proposed: in the field of fixed-grid methods, the usual technique exploits the enthalpy formulation for the energy equation. Enthalpy is a measurement of energy in a thermodynamic system and in a simplified case, it takes account for two different contributions, the first one directly linked to the temperature field and the second one to the phase change effect, that is to say the latent heat. With enthalpy can also be measured a lot of different phenomena as combustion or other chemical reactions but in the considered form it can be expressed as follows:

$$\begin{cases} H = c_{p,l}T & \text{in the liquid domain} \\ H = c_{p,s}T + L & \text{in the solid domain} \end{cases}$$
(4.26)

being L the latent heat, which for the considered case of water at sea level pressure has the value of $334000 \frac{J}{kg}$. The previous equation 4.26 can be profitably written in general formulation, true in all the domain, exploiting the already defined solid fraction α_{IBM} :

$$H = \left[\alpha_{IBM}c_{p,s} + \left(1 - \alpha_{IBM}\right)c_{p,l}\right]T + \alpha_{IBM}L \tag{4.27}$$

The advantage of this formulation is that it can be easily introduced in the heat equation and solved for temperature using a fixed grid method. Two different methods are described by Voller et al. [22]:

- The latent heat source term
- The apparent heat capacity

The starting point is always the heat equation in the classical form of enthalpy, which for the simple case of conduction can be expressed as 4.28. The first of the two method mentioned, it changes the equation by adding a source term S, while the second one maintain the same form for the equation but it propose a different formulation for the heat capacity c_p .

$$\frac{\partial \rho H}{\partial t} = \nabla \cdot (k \nabla T) \tag{4.28}$$

4.5.1. The latent heat source term

The development of this method consists in modifying the governing energy equation 4.28 with a non-linear source term, which can be obtained by introducing the enthalpy formulation 4.27 in it. The product rule for the derivatives allows to expand the left hand side of the equation:

$$\frac{\partial \rho H}{\partial t} = H \frac{\partial \rho}{\partial t} + \rho \left(\frac{\partial c_p T}{\partial t} + \frac{\partial \alpha_{IBM} L}{\partial t} \right)$$
(4.29)

being also the thermophysical properties ρ_{c_p} and k function of the solid fraction α_{IBM} , they can be written in the usual form:

$$\begin{cases}
\rho = \rho_s \alpha_{IBM} + (1 - \alpha_{IBM}) \rho_l \\
c_p = c_{p,s} \alpha_{IBM} + (1 - \alpha_{IBM}) c_{p,l} \\
k = k_s \alpha_{IBM} + (1 - \alpha_{IBM}) k_l
\end{cases}$$
(4.30)

Further manipulations lead to the searched formulation for the heat equation and its source term:

$$\begin{cases} \frac{\partial T}{\partial t} \cdot \left[\rho_l c_{p,l} + \alpha_{IBM} \cdot \left(\rho_s c_{p,l} + \rho_l c_{p,s} - 2\rho_l c_{p,l}\right) + \alpha_{IBM}^2 \cdot \left(\rho_l c_{p,l} - \rho_l c_{p,s} - \rho_s c_{p,l} + \rho_s c_{p,s}\right)\right] = \\ = \frac{\partial}{\partial x_i} \left(k \cdot \frac{\partial T}{\partial x_i}\right) - S \\ S = \frac{\partial \alpha_{IBM}}{\partial t} \cdot \left\{\rho_l L + T \cdot \left(\rho_l c_{p,s} + \rho_s c_{p,l} - 2\rho_l c_{p,l}\right) + \\ + \alpha_{IBM} \left[2\rho_s L - 2\rho_l L + 2T \cdot \left(\rho_l c_{p,l} + \rho_s c_{p,s} - \rho_l c_{p,s} - \rho_s c_{p,l}\right)\right] \right\} \end{cases}$$
(4.31)

In the simple case in which the temporal changes in the liquid density are neglected, that is to say considering ρ_l equal to ρ_s , the previous equation assumes the short form shown also in [22]:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) - S \tag{4.32}$$

where ρ is a constant and both c_p and k have to be written in function of the parameter α_{IBM} as shown in Eq.(4.30). While the heat source term reduces to the following formulation:

$$S = \rho \frac{\partial \alpha_{IBM}}{\partial t} \left[L + T \left(c_{p,s} - c_{p,l} \right) \right]$$
(4.33)

in which the second term is considerably smaller than the first one given the small temperature values involved in a water's solidification problem, and then in first approximation it can be neglected.

The energy equation was already implemented and solved in the code JADIM by using the following formulation:

$$T^{n+1} = T^n + dt * (Adv + Cond + ...)$$
(4.34)

Knowing the temperature at the current time step T^n , the different thermal fluxes are computed (for example the conductive and advective contributions, but also other special cases) and then the temperature at the subsequent time step T^{n+1} can be found by multiplying these terms for the chosen time step.

It is between these thermal contributions that the latent heat source term has to be added. In order to be coherent with the existing formulation, the source term in Eq.(4.32) has to be divided by the product ρc_p . The resulting formulation for the temperature equation including the new source term is:

$$T^{n+1} = T^n + dt * (Adv + Cond + ... + \frac{S}{\rho c_p})$$
(4.35)

where S is computed using the same approach presented in the calculation of the velocity imposed by the phase change expansion, that is to say by exploiting the chain rule in order to split the time derivative of α_{IBM} in two simpler derivative contributions.

In conclusion, starting from the simplified equation which does not take account of the density temporal changes (4.33), the source term in the temperature equation has been expressed in the form:

$$S = \frac{\partial \alpha_{IBM}}{\partial T} \frac{\partial T}{\partial t} \frac{[L + T \left(c_{p,s} - c_{p,l} \right)]}{c_p}$$
(4.36)

Physically speaking, during a phase change (solidification process) a portion of the heat flux is not transferred through the material but it is employed by the substance to change its state from liquid to solid, absorbing it. This method consists in numerically simulating this physical phenomenon by injecting heat in the phase change interface through the source term. This source term *warms* locally the substance, simulating the lessening of the heat transfer process due to the phase transition.

4.5.2. The apparent heat capacity

This method is based on the idea of reformulating the governing equation in terms of a single unknown variable, with the non-linear latent heat effects isolated in a coefficient called *apparent heat capacity*. This property can be properly defined as the derivative of H with respect to temperature T, so:

$$c_{app} = \frac{dH}{dT} \tag{4.37}$$

This means, using the definition of H, that it can be written:

$$c_{app} = c_p + L \frac{d\alpha_{IBM}}{dT} \tag{4.38}$$

with

$$c_p = c_{p,s}\alpha_{IBM} + c_{p,l}\left(1 - \alpha_{IBM}\right) \tag{4.39}$$

Using the chain rule it can be stated that

$$\frac{\partial H}{\partial t} = \frac{dH}{dT} \frac{\partial T}{\partial t} \tag{4.40}$$

and by substituting into Eq.(4.28) the governing equation becomes

$$\rho c_{app} \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) \tag{4.41}$$

This last equation is often called the apparent heat capacity equation and it is identical in form to the basic Fourier heat conduction equation. As result, this formulation can be easily implemented into existing codes, by changing the usual *specific heat* with the *apparent heat capacity*, which contains both actual properties of the examined fluid $(c_{p,l} \text{ and } c_{p,s})$ and an added term incorporating the latent heat. The second part has the purpose to create a virtual heat capacity in the interface region between the solid and the fluid; this can be easily seen by moving the product ρc_{app} to the right hand side of Eq.(4.41). As result we obtain a thermal diffusivity which corresponds to those of ice in the solid region and of water in the liquid one, but it is artificially decreased (even of two orders of magnitude) in the interface zone, because of the higher specific heat computed in this part of the domain. The aim of this is to hinder the heat transfer from the liquid towards the solid, in order to approximate the influence of the latent heat on the solidification process.

5. Simulations

The objective of this section consists in performing a set of simulations by using the developed version of JADIM, mainly with two aims: firstly to validate the work done and secondly to calibrate the different parameters at our disposal in order to best fit the analytical solutions. In order to achieve this result, the different analytical solutions found in Chapter 2 for the Stefan problem will be compared with some one-dimensional tests performed with JADIM, trying to find the best function between those presented, then to analyse the effects of the other tools which have been implemented in the original code. Once these tests will be done, the second step consists in verifying the convergence to the analytical result by refining the used grid. The third step, instead, has the aim to extend the simulation from a simple 1D domain to the actual drop of water lying on a cold plate. In order to achieve this result the third phase (air) has to be introduced as well as another spatial dimension.

5.1. 1D simulations

One-dimensional simulations will be performed first, in order to validate and calibrate the code and, for this purpose, the Stefan problem will be used as criterion for comparison. The Stefan problem is characterised by the solution of a partial differential equation in just one dimension, and it has been solved by imposing isothermal condition of temperature at the wall and to infinity. It is clear that while the first condition can be easily implemented in the numerical simulations as a boundary condition, the second one presents some difficulties. In order to have a valiant set of results it is necessary to have a domain long enough for the temperature to be constant at great distance from the isothermal wall, so not influenced by the conditions on the studied part of the domain. Fortunately, the solution for the profile temperature involves the error function, which is characterized by a rapid convergence to its final value as shown in Figure 5.1; in particular, for a value of its argument equal to 2.5, the approximation erf(x) = 1 gives an error inferior to $1\%_0$. For this reason it is sufficient to verify a posteriori, once the simulation is completed, that the temperature profile is unchanged in a sufficient number of cells towards the end of the domain, remaining equal to the initial temperature value. In order to perform the one-dimensional simulations, on the other two walls of a rectangular domain (the ones just necessary to have an enclosed space) will be applied a symmetrical condition, with no heat or mass fluxes passing through them, which has the target to successfully represent a single dimension domain.



Figure 5.1: Error function

5.1.1. Choice of the IBM function

The first parameter analysed is the α_{IBM} function: it defines the transition zone, where the fluid has intermediate thermo-physical characteristics between those of the ice and those of the water.

It is important to highlight that every function is an approximation due to the fact that the real phase change for a pure substance is isothermal, consequently the modelling of the phase change by using a range of temperature causes the introduction of an error in comparison to the analytical solution. In fact, while in the Stefan problem a solidification temperature is defined, which divides the solid from the liquid phase, in the following simulations this temperature could be the middle of the *solidification* range of temperature or one of its extremities. The first choice seems to be more adherent to reality, meaning that, since an approximation is necessary, both the solid and the liquid phase are symmetrically charged with the consequent error and the phase change temperature corresponds to the average value of those affect by the transition. On the other hand, an asymmetrical choice is oriented towards a better modelling of the solid phase: being the transition simulated only in the liquid part of the domain, it is expected to individuate the solid-liquid interface in a more precise way, because in this case the freezing front is pinpointed by the temperature corresponding to the actual phase change temperature. Otherwise, the average do not correspond to the real solidification temperature, which could cause an inaccurate behaviour of the liquid part.

For the above mentioned reasons, the different formulation of α_{IBM} (4.4) and (4.5) will be tested with various values of the extremity range temperatures T_{max} and T_{min} , in order to understand both the influence of the choice between the two different transition functions and of the width of the phase change zone.

$$\alpha_{ibm,lin} = \tau \cdot \frac{T_{max} - T}{T_{max} - T_{min}} \tag{4.4}$$

$$\alpha_{ibm,cos} = 0.5 \cdot \tau \cdot \left[\cos \frac{\pi \cdot (T - T_{min})}{T_{max} - T_{min}} + 1 \right]$$
(4.5)

Consequently the simulation resumed in Table 5.1 are performed and compared to the exact solution. These simulation have all the same dimension of the grid and the same time spacing, in order to make them comparable between themselves.

	Temperature range				
Linear	[-2,2]	[-1,1]	[0, 1]	[0, 0.1]	
Cosine	-	[-1,1]	[0, 1]	-	

Table 5.1: Summary of the simulation performed

The observed results are some temperature profiles at different time steps, with the respective maximum and mean error as well as the position of the interface, pinpointed by the unitary value of the function defining the IBM fraction.

For the sake of brevity, the results will be resumed in some short paragraphs and a comparison between them done afterwards, showing some of the best/worst graphs. A presentation of these charts for each case would result redundant, being them similar to each other, for this reason a comparison would be more effective, highlighting the differences more than the similarities.

With this purpose, some summarising tables will be presented, showing:

- the maximum error regarding temperature, that is to say the maximum difference between the numerical and the analytical solution, named $err_{T,max}$
- an average error, which is calculated by operating the average through different time steps of the previous maximum error. The average is not computed on the space domain because it would be easy to manipulate by adding point at the hotter extremity which, by assumption, remain at a constant temperature. This error will be marked as $err_{T,avg}$
- the maximum error in the positioning of the freezing front $err_{int,max}$
- the average error in the positioning of the freezing front $err_{int,avg}$

5.1.1.1 Linear function, $4^{\circ}C$ width of the temperature range, centred

er	$r_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
6	3.1%	5.7%	27%	17%

Table 5.2:	Errors	for	linear	function,	range	[-2, 2]
				/		. / .

While the error done on the temperature is not too high, the error regarding the position of the freezing front in quite big, the explanation is to be found in the fact that the value of $\alpha_{IBM} = 1$ corresponds to the temperature of $-2^{\circ}C$; instead, in the analytical solution, it is just one point corresponding to the transition temperature.

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
4.3%	4.1%	14.2%	9.2%

Table 5.3: Errors for linear function, range [-1, 1]

5.1.1.2 Linear function, $2^{\circ}C$ width of the temperature range, centred

The results presented in Table 5.3 concerning the simulation using a narrower range of temperature shows a better adherence to the exact solution in each of the analysed parameters as expected, because of the better approximation to a isothermal phase change.

5.1.1.3 Cosine function, $2^{\circ}C$ width of the temperature range, centred

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
5.2%	4.3%	12.2%	7.6%

Table 5.4: Errors for cosine function, range [-1, 1]

The case here in Table 5.4 shows similar errors on temperature, even if slightly higher but a better positioning of the freezing front, probably due to the fact that as was presented in Figure 4.1, the cosine function is steeper near the extremities of the temperature range, causing the highest value of α_{IBM} to be closer to zero.

5.1.1.4 Linear function, $1^{\circ}C$ width of the temperature range, asymmetrical

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
5.2%	4.2%	4.7%	2.2%

Table 5.5: Errors for linear function, range [0, 1]

As shown in Table 5.5 adopting an asymmetrical solidification zone, the temperature profile is worse than the centred case even if the width has been diminished. On the other hand, the error on the position of the freezing front has been drastically reduced, because in this case the analytical solidification temperature is pinpointed.

5.1.1.5 Cosine function, $1^{\circ}C$ width of the temperature range, asymmetrical

The errors for the cosine function in the range of temperatures indicated in Table 5.6 are almost identical to those of the linear function already presented.

5.1.1.6 Linear function, $0.1^{\circ}C$ width of the temperature range, asymmetrical

This simulation is performed with the narrowest range of temperatures and it has the aim to show how, having a quasi-isothermal phase change condition, the results are the closest to the analytical solution. However the disadvantage is that when the latent

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
5.3%	4.1%	4.8%	2.3%

Table 5.6: Errors for cosine function, range [0, 1]

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$
2.8%	2%	3.5%	1%

Table 5.7: Errors for linear function, range [0, 0.1]

heat is taken in account or the density change, it becomes instable or skip one or both these two major issues. The cause is to be found in the fact that with the two extremities of the phase change zone so close one to each other is more than likely that the α_{IBM} function never takes the intermediate values between 0 and 1.

5.1.2. Comparison and graphs

It is clear from the simulations performed that in these simple cases done in order to test the different solid fraction function α_{IBM} , the errors increase in correspondence to a wider temperature range chosen in order to simulate the phase change zone. This has shown to be a general statement, valid both in the case of a centred interval and an asymmetrical one.

However this second choice influence the solution as regards a more precise result on the temperature profile or the position of the freezing front. As already mentioned and clearly understandable from the comparison between Figure 5.2 and Figure 5.3, in the first case it is not the $0^{\circ}C$ which corresponds to the lower extremity of the range of variation of the function α_{IBM} . In fact, in addition to the numerical points being misplaced, the distance from the analytical curve it increases through time due to the diffusion of temperature: initially, the temperature profile is steeper which cause the error to be smaller.

The temperature profile is shown in Figure 5.4 and the main features to be highlighted are first of all a good adherence between the numerical and the analytical solutions, secondly it can be seen that the main discrepancy is some cells before the phase change temperature. The cause is to be found in the fact that in numerical solution the variation of the slope between ice and water (characterized by different thermal diffusivities) changes is more gradual way, and in particular the temperature profile shown refers to a phase change zone beginning at $-1^{\circ}C$. In fact, the two curves are again really close one to each other once the phase change temperature of the exact solution is surpassed.

5.1.3. Effects of the volume expansion

In this paragraph will be investigated the behaviour of the main feature developed in the present work: the velocity induced in the liquid domain by the volume expansion due to the density change between the solid and the liquid phase of the water.

The velocity in the fluid not only has to be computed in the right way, but it also has to assume the right value with respect to the temperature field which is influenced



Figure 5.2: Position of the freezing front, cosine function [-1, 1]



Figure 5.3: Position of the freezing front, linear function [0, 0.1]



Figure 5.4: Temperature profile, cosine function [-1, 1]

by this motion and it also influence it. For the present reason a particular attention will be paid to this parameter, in the attempt to have a suitable approximation of the analytical result. As for the precedent paragraph, the effects of the different solid fraction functions will be studied, with a particular attention to their influence on the computation of the velocity.

However, the velocity induced in the upper fluid is a fraction of the velocity of the freezing front: its trend is shown in Figure 5.5. The condition given to solve the Stefan problem are:

- Initial condition constant through the entire domain
- Wall temperature constant and sub-solidification

The consequence is that the calculated velocity has the following expression, deduced in Appendix A:

$$V_{fluid} \propto \sqrt{\frac{1}{t}}$$
 (5.1)

which for t = 0 it has a singularity point and $\lim_{t\to 0^+} V_{fluid} = \infty$. This condition will be unlikely simulated with particular precision due to the finite factors in the numerical computation. For this reason, the first values of velocity will be without doubt the more subject to errors and difficult to be computed to ensure numerical stability. In fact, in the formulation already presented (4.13), the partial derivative of the solid fraction with respect to temperature has a finite value (constant if the chosen function is linear) depending on the amplitude of the temperature range for the phase change to occur, consequently it is the second factor which has to raise to a larger value. It is clear that its value depends on the time spacing considered, the smaller the greater it becomes.

$$\boldsymbol{V_{front}} \cdot \boldsymbol{n} = \frac{-\frac{\partial \alpha_{ibm}}{\partial T} \frac{\partial T}{\partial t}}{||\nabla \alpha_{ibm}||}$$
(4.13)

However, the first factor can't be too high because it is necessary to have a certain number of cells inside the intermediate values of the α_{IBM} function in order to compute the velocity, otherwise there will be no velocity at all due to the lack of the interval in which it is calculated. For the present reason, the choice of the amplitude of the temperature range for the solid fraction function will be a trade-off between the precision in the computation of the temperature profile and a correct calculation of the velocity, because as for the temperature it has been shown previously that the more the isothermal phase change it is approximated the more the error decreases.



Figure 5.5: Velocity induced in the fluid by expansion

5.1.3.1 Linear function, $2^{\circ}C$ width of the temperature range, centred

The results of this simulation presented in Table 5.8 show how the error concerning the temperature field is increased by adding the velocity computation with respect to the case without any expansion. The reason is to be searched in the link between temperature and velocity, the introduction of the second one corresponds to the introduction of an approximation in its calculation which leads to an additional error as regard as the temperature diffusion. On the other hand, a growth of the error in the interface position can be attributed to the fact that a stronger diffusion of temperature causes smoother temperature gradients which causes a bigger gap between the cell with the temperature value of $-1^{\circ}C$ and the analytical point of phase change at 0 Celsius degrees (for each time step).

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$	$err_{vel,max}$	$err_{vel,avg}$
6.4%	5.4%	15.1%	9.5%	16.5%	8.1%

Table 5.8: Errors for linear function, range [-1, 1]

5.1.3.2 Cosine function, $2^{\circ}C$ width of the temperature range, centred

The same considerations done for the previous case are still true for the present simulation, Table 5.9 when in comparison with the non-expansion problem. The differences between the cosine and the linear function are not so significant and the main improvement with this choice is related to the position of the interface once again because the steeper cosine function tends to move the freezing front position closer to the actual value.

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$	$err_{vel,max}$	$err_{vel,avg}$
6.1%	4.6%	12.2%	7.8%	13.7%	7%

Table 5.9: Errors for cosine function, range [-1, 1]

5.1.3.3 Linear function, $1^{\circ}C$ width of the temperature range, asymmetrical

The following step performed consisted in studying a narrower range of temperature, together with the asymmetrical choice of the solidification range in order to have a correspondence between the unitary value of the solid fraction function and the actual phase change position. this fact is confirmed by the results shown in Table 5.10, where a reduction of the errors concerning the interface positioning can be noticed. However, this result is worse than the case without velocity due to the already mentioned introduction of a further error in the temperature calculation.

err	T,max	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$	$err_{vel,max}$	$err_{vel,avg}$
6.	.2%	5%	8.3%	4.3%	23.6%	8.7%

Table 5.10: Errors for linear function, range [0, 1]

5.1.3.4 Cosine function, $1^{\circ}C$ width of the temperature range, asymmetrical

The results presented in Table 5.11 are similar to the previous ones and the same kind of considerations can be done. As can be observed in this case the errors are slightly increased with respect to the linear function choice because in a narrower range of solidification, the steeper trend of the cosine function is a disadvantage.

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$	$err_{vel,max}$	$err_{vel,avg}$
6.5%	5.2%	8.3%	4.4%	23.6%	8.9%

Table 5.11: Errors for cosine function, range [0, 1]

5.1.3.5 Linear function, $0.1^{\circ}C$ width of the temperature range, asymmetrical

The last simulation consists in testing the behaviour of the linear function in the range which proved to be the best in the one dimensional simulation without the expansion induced velocity. The first consideration can be done by observing the temperature field errors: while without expansion the errors when moving from a larger temperature range to this one were more or less halved, in this case this improvement does not happen. The reason is to be found in the velocity error: the maximum error is 100% because the velocity is not calculated at all. Also the mean value of the error is very high which means that the time steps when velocity is not computed are a significant percentage of the total. It can be stated that such solidification range is too tiny for the present purpose because it happens too frequently that there is no range of solidification but the solid fraction function presents a stepped trend and, as already explained, it is inside the freezing interface that velocity is calculated and imposed.

$err_{T,max}$	$err_{T,avg}$	$err_{int,max}$	$err_{int,avg}$	$err_{vel,max}$	$err_{vel,avg}$
6%	5.5%	-	-	100%	53.8%

Table 5.12: Errors for linear function, range [0, 0.1]

5.1.3.6 Comparison and graphs

The first consideration is about the choice of the α_{IBM} function in relation to the temperature range of solidification: from the above results it can be affirmed that a behaviour more adherent to the analytical result is obtained when using the cosine function with a reasonable large phase change width. The reason is linked to the fact that the cosine function is quite steep for its intermediate value. However, if the range is narrower the odds of calculating the desired parameters in this region are smaller, this can explain why when considering the [0, 1] range, the linear function returns better results.

As for the non expansion case, the position of the interface is always better found when choosing an asymmetrical range with its minimum temperature corresponding to zero degrees.

In conclusion, an interesting consideration can be done regarding the choice of the solidification range: in fact, while for the no-velocity case a narrower width of phase change gives better results both for temperature and interface position, this link does not subsist when expansion is taken into account by computing the velocity. This is due to the mutual influence between temperature field and fluid displacement caused by expansion: if velocity isn't calculated well, also thermal diffusion is affected. For this reason a trade-off choice has to be made, between a large solidification range which allows an optimal velocity evaluation but a misrepresented phase change region and a narrower one with a better freezing front individuation.

In Figure 5.6 is presented an example of a satisfying result for the velocity computation through time for the mono-dimensional case. It is clear how the tendency is well approximated, while as expected the values are underestimated for the above mentioned reasons. In any case, due to the inverse proportionality to the square root of time the biggest errors are located in correspondence of the first time steps while with the time proceeding the numerical points tends to get closer to the analytical curve.



Figure 5.6: Velocity induced in the fluid by expansion and numerical points

5.1.3.7 Grid convergence

A parameter which needs to be studied is the influence of the grid dimension, the distance between two neighbouring nodes in the space where equation are solved. For this reason, simulations with the same boundary condition have been performed on a domain of the same size but with a different number of cell inside it. For the sake of brevity, this simulation have been done considering just the cosine function, with a phase change range of [-1, 1], because it looked like as the most promising between the possible choices analysed concerning the velocity computation and a good compromise for the other studied parameters. In Figure 5.7, Figure 5.8 and Figure 5.8 are shown the results of the maximum and time averaged errors for the temperature field, the velocity induced in the fluid and the freezing front position respectively. The node spacings presented here assume the value of $2 \cdot 10^{-6}$, 10^{-6} , $5 \cdot 10^{-7}$ and 10^{-7} while the time step is constant and equal to 10^{-7} .

It is possible to notice how with a smaller distance between the nodes, using a finer mesh, the errors concerning temperature and velocity decrease both in their maximum and in their averaged values. This phenomena is due to a better solution of the equation in the domain, and in the case of velocity, also to the fact that it decreases the possibility of having no points in which the velocity is computed. This second statement is supported mostly by the sudden increase of the maximum error with the widest mesh, which is an indicator of at least one time where velocity is not calculated.

On the other hand, in Figure 5.9 no improvement can be observed by refining the mesh, in particular in the average value for the position of the freezing front. The reason is to be found in the fact that, as already said, the interface pinpointed with these limits of temperature does not correspond to the one of the analytical solution and, as a consequence, it is useless to increase the number of points in the domain if the objective is to obtain a better approximation. For this reason in Figure 5.10 is shown the same analysis considering the linear function with solidification range between [0, 1] which is the one which guarantees the best result for this parameter. Indeed, considering this function, the errors for the solid-liquid zone tend to decrease when increasing the number of cells, as expected.



Figure 5.7: Grid convergence for temperature, cosine function [-1, 1]

Figure 5.8: Grid convergence for velocity, cosine function [-1, 1]



Figure 5.9: Grid convergence for interface position, cosine function [-1, 1]



Figure 5.10: Grid convergence for interface position, linear function [0, 1]

In this section has been shown how refining the mesh is possible to decrease the errors regarding most of the parameters of interest. However the more the number of cells is high, the more the computation time is long. The computation time is the length of time required to perform a computational process and, maintained constant a series of other parameters, it is directly linked to the number of points in the domain. For this reason, ideally with an infinitesimal distance between points, the error should tends to zero but in the normal application a trade-off solution is necessary. In particular from the simulations performed it can be affirmed that the $2 \cdot 10^{-6}$ mesh returns results not satisfying while the other meshes gives better results. The mesh with the smallest spacing guarantees no sufficient advantages with respect to the other two to be selected, so the choice will be between the two with $\Delta x = 10^{-6}$ or $5 \cdot 10^{-7}$.

5.1.4. Simulation of the latent heat

In this section the two methods presented for taking in account for the latent heat of solidification will be tested in order to decide which one is convenient to employ in the further simulation of the actual water droplet. The choice is between the introduction of a source term in the temperature equation which directly heat the phase change region and the modification of the specific heat capacity in order to obstruct the heat transfer and obtain a similar outcome.

5.1.4.1 Latent heat source term

The results originated by the procedure explained in the previous chapter is here tested, using as basis for comparison the Stefan problem as for the other cases.

The first test was performed using the cosine function and imposing the already test [0, 1] as range of phase change: however the simulation diverged. The latent heat source was too intense and temperature in the freezing region rose to values exceeding even the initial temperature of the water, causing the solid fraction to disappear. Consequently in the successive simulation the transition zone has been widened, considering the [-1, 1] range of temperature. The results were more satisfying and are presented in Figure 5.11 and 5.12 and Table 5.13: in particular the figures presented refers to the different time steps and it is clear how the source term gives worse result for the first instants, when the involved gradients are high, while with time proceeding it improves.

$err_{T,max}$	$err_{T,avg}$
35%	18%

Table 5.13: Errors for cosine function latent heat source, range [-1, 1]

In any case, as stated by Voller and Swaminathan [23] the method is not particularly stable and would require iterative loops in order to guarantee convergence. In the case without expansion some results have been obtained even if the stability is influenced by the width of the phase change range and the total difference of temperature in the domain but the link have not been found, not allowing to have a valid formulation. On the other hand, when in the transition zone is also added the velocity imposition due to the density variation a stable case without iteration has not been found. Given


Figure 5.11: Temperature profile with latent heat source term $t = 2 \cdot 10^{-4} s$

the fact that iteration would have to be implemented in each loop of the calculation of each time step causing the computation time to substantially grow, this method even have been discarded for the final simulations.

5.1.4.2 Apparent heat capacity

The formulation described in the previous chapter 4.38, allows to calculate the apparent heat capacity in the entire domain and gives as a result the physical heat capacity in the liquid water and in the ice where the derivative with respect to the temperature of the solid fraction is zero, instead in the phase change region the heat capacity is incremented. The result is a method to compute the thermal diffusivity α which is sensitive to the solidification process: considering the middle value of the transition zone, according to the volume fraction formulation, thermal conductivity and density are the exact mean value between those of the solid and the liquid water, independently of the width of the considered range. On the other hand, the apparent heat capacity c_{app} is directly linked to the chosen range, because of the temperature derivative of the solid fraction in its formulation: the more the range is narrow, the more this derivative's value is high and consequently an higher c_{app} is calculated. These three parameters are employed to calculate the thermal diffusivities, whose values are shown in Table 5.14

A low value for c_{app} , considering the pure conduction equation, means that it is necessary a strong variation of temperature with respect to space in order to observe a much smaller variation of temperature with respect to time. This, as anticipated and physically correct has the consequence that in the zone where the phase change happens the heat is obstructed and thermal diffusion hindered, acting as an insulating. However it is possible to notice from Table 5.14 how thermal diffusivity drops in correspondence of the transition zone, this causes temperature to grow in a sudden way in



Figure 5.12: Temperature profile with latent heat source term $t = 5 \cdot 10^{-4} s$

α_{ice}	$1.2 \cdot 10^{-6} \frac{m^2}{s}$
α_{water}	$1.4 \cdot 10^{-7} \frac{m^2}{s}$
$\alpha_{app} \ [0,1]$	$4.3 \cdot 10^{-9} \frac{m^2}{s}$
α_{app} $[-1,1]$	$8.6 \cdot 10^{-9} \frac{m^2}{s}$
$\alpha_{app} \ [-2,2]$	$1.7 \cdot 10^{-8} \frac{m^2}{s}$

Table 5.14: Different values of thermal diffusivity

this range. The direct consequence of this tendency is that the difference of temperature experienced between two neighbouring cells is important and it could cause a lack of cells involved in phase change. In fact this technique has been developed to deal with solidification/fusion of metals: firstly for this class of material the solidification range is not an approximation but it is strictly physical with the three phases divided by the so-called *solidus liquidus* lines, but the other characteristic is that a latent heat of solidification similar to water's is experienced in phase change region of about 100 degrees, causing the apparent heat capacity to be less steep.

A trade-off condition will likely to be searched between having a smoother function for the thermal diffusivity and not to diverge strongly from the original problem. Another possible disadvantage of this technique is that the freezing front has not to advance no more than one cell per time step, otherwise the latent heat related to the missing cell would be lost.

The simulations performed have shown that this method tends to underestimate the latent heat due to the phase transition as a consequence of the above reason, a steep profile of temperature which cause a little number of cells to assume the low values for thermal diffusivity.

In particular, the cell(s) with low thermal diffusion, simulating the phase change

$err_{T,max}$	$err_{T,avg}$
23%	18.4%

Table 5.15: Errors for apparent heat capacity method, range [-1, 1] employing linear function

region, appears to be located between the two chosen limits of temperature, shifted towards the inferior boundary. The temperature ranges tested are those already presented in the table that is to say 4,2 and 1 degrees of width.

The first analysed has been the one with the narrowest gap between the two limits, which have been positioned in $[0, 1]^{\circ}C$; the results haven't been particularly satisfactory for the following reasons:

- the high value of the derivative of the solid fraction function with respect to temperature causes the lowest value of thermal diffusivity which, as a consequence, leads to never more that one cell for each time step where the phase change occurs
- the phase change heat, consequently, is underestimated
- the solidification temperature is located at more than the physical transition temperature

these three effects do not compensate each other and, together, have the consequence of a phase change region which moves faster than expected and located at a higher temperature value.

Then the widest range has been tested, with the choice of 4 degrees Celsius of width and a centred range. The aim of this choice was to analyse the effect of an increased value of the thermal diffusivity in the phase change region in order to avoid the loss of latent heat of solidification. However, even if the growth of latent heat have been partially obtained, it was not sufficient to compensate the choice of a non-physical transition temperature. In fact, also in this case the cells with low thermal diffusion are located closer to the inferior limit of temperature and the resulting thermal diffusivity is always two degrees of magnitude smaller than the ice's one, resulting in a steep variation in the temperature gradient. Concluding, the phase change region appears to be too close to the lower limit of the selected range, leading to a non physical transition region with no satisfying countermeasure on the latent heat hand, given by the higher values of the thermal diffusivity calculated.

Consequently, the trade-off choice is a 2 degrees width range with [-1, 1] as minimum and maximum temperature, with a temperature profile shown in Figure 5.13. The consequences are:

- the transition temperature is located between -1 and 0, with a fair correspondence with the physical problem
- the latent heat of solidification is always underestimated
- the errors are mainly located in the ice region

The first two points, in this case, tend to compensate each other as regard as the spatial location of the phase change region. This effect is due to the fact that, given the underestimation of the latent heat, the numerical transition region moves faster than the analytical one, however it is shifted closer to the lower temperature, resulting in a the fair correspondence mentioned above. The last point is a direct consequence of the smaller amount of heat due to the phase change, so this reduced heat transfer through the ice leads to smoother temperature gradients in the solid region. Geometrically it can be seen as a smaller gap in the temperature experienced by the ice (ΔT) caused by the excessive value of c_{app} , in correspondence of the same spacial location of the interface (Δx), resulting in a lower slope of temperature behaviour, given the quasilinear ice conduction. Globally, the errors, shown in Table 5.15, are lower than the previous two cases even if still not enough satisfactory.



Figure 5.13: Temperature profile, apparent heat capacity method

Concluding, a comparison between the two ways of simulating the phase change latent heat can be made; while in the considered range of time the two methods give similar results, the main difference occurs for higher simulation times. The latent heat source term presents the higher errors in first phases of the simulation, when temperature time gradients are important while tends to improve its behaviour with the simulation going forward. Differently, the latent heat capacity method, due to its underestimation of the solidification effects, has a worsening behaviour for long simulation times. However, this second method has proved to be stable with different temperature conditions in the domain (wall and initial) as for various solidification range choices as regard as both width and function, without the necessity of additional convergence loops.

5.2. Droplet simulation

The successive step has been the simulation of an actual droplet of water on a cooled surface. Differently from the one dimensional case, here not just two phases has been considered but a third one has been introduced considering the entire domain, the considered phases are:

- Air: in the domain surrounding the droplet
- Water: the initial droplet
- Ice: the result of the solidification process

while the characteristics of air are constant (density, thermal diffusivity and viscosity) as well the amount in the space, the characteristics of water become those of the ice in the way described in the precedent chapters and its volume decreases as the solidification process goes forward.

The one dimensional case had the aim to understand the behaviour of the research code and the modification introduced, while the three phase problem has no analytical solution to be compared to but some experimental results and other numerical works can be used as guidelines and benchmarks for the present work [12] [24].

Given the nature of the problem, the thermal properties are predominant that is to say the thermal conductivity, the heat capacity and the density: the three of them are proficiently united in the already mentioned thermal diffusivity. As anticipated, those characteristics can be assumed as constants in the three different phases due to the limited temperature variations involved, in particular because the differences between them are much higher than the respective variations with temperature. The values adopted in the following simulation are resumed in Table 5.16.

	$\alpha \left[\frac{m^2}{s} \right]$	$\rho\left[\frac{kg}{m^3}\right]$
Air	$2.166 \cdot 10^{-5}$	1.2
Water	$1.433 \cdot 10^{-7}$	1000
Ice	$1.176 \cdot 10^{-6}$	917

Table 5.16: Physical characteristics of the substances involved in the simulations

Given the shape of the droplet, the problem is treated using an axi-symmetrical domain, filled with a regular Cartesian mesh. The analysis performed before suggests to chose a grid dimension of at least 10^{-6} m, which is a decent compromise between accuracy and numerical computation time. However, this small spacial dimension is an obstacle when trying to simulate actual droplet volumes as those studied in Ablonet's work [12] which involves volumes of water deposed on the cooled plate between 10 and 70 μL : this kind of volumes would require something like 140 million of cells. The direct consequence is that the volume of water will be reduced in order to reduce the computational cost, in fact JADIM is a research code which is not optimized as regard as calculation velocity and parallel computation.

When small volumes of water are considered, as stated in Chapter 2, the shape of the droplet is driven by the surface tension while gravitational effect is negligible. The result is a droplet with a spherical cap structure, in accordance with very low values of the adimensional Bond number $(Bo \ll 1)$.

The simulation are performed in a 2D box, where on the x-axis is imposed the axi-symmetrical condition. An example of a generic starting condition is shown in Figure 5.14 where the south wall is the axis of symmetry. The cooled wall is the west one, where a constant temperature below the solidification point is imposed as well as zero velocity. The thermal condition imposed on the other two walls is the a zero heat flux which means that the boundaries of the domain are adiabatic. As regard as the temperature values, the entire system is considered initially at the room temperature of $18^{\circ}C$ and the cooling surface is assumed to have the constant value of $-5^{\circ}C$. This second hypothesis is not a totally physical one, because in laboratory experiences the possibilities are the following two:

- the cooling plate is initially switched off and a thermal transition time occurs
- the cooling plate has already reached the assumed temperature

in the first case the assumption of this work's simulations corresponds to a zero thermal inertia of the plate, while in the second one would cause a stratified air domain which would be altered with the deposition of the droplet.



Figure 5.14: Initial droplet shape

One of the main differences moving from a mono-dimensional domain to an axisymmetric one consists in the computation of the velocity imposed by the density variation due to the phase change: the freezing front is not just a straight line parallel to the cooled wall but assumes more complicated shapes, always perpendicular to the solidification direction in each point. The implication of this is that the freezing front is not directly link to the position of the cooled boundary but has to be found according to the thermodynamics of the problem. In particular, the solidified region can be easily detected thanks to the solid fraction function previously mentioned and a function calculating its gradient for each point has been employed in order to determine the searched freezing direction. This routine gives as result the gradient of the function α_{IBM} , which is proficiently used to calculate its norm which appears both in the freezing front velocity's absolute value formulation (4.13) and in its unit vectors (4.14).

At this point, obtained the absolute value of the solidification front velocity and its unit vectors, knowing the density ratio between solid and liquid phase, the velocity due to the expansion can be calculated, projected along the two axis and properly applied on the liquid phase to cause its motion.

As result of the previous analysis, the solid fraction function chosen for the following simulations is the linear one, with a solidification range between -1 and 1 Celsius degrees. This choice has been made in order to properly simulate the motion of the liquid phase which is the more innovative achievement presented in this work and gives decent results as regard as the thermal behaviour.

The simulations performed have mainly the aim to reproduce the solidification process and its effect on the final droplet's shape. The two leading drivers for the tip which can be observed on a solidified droplet of water have supposed to be the so-called Marangoni effect and the solidification's expansion; given that in the present work the Marangoni effect is not taken in account (the code doesn't support its computation), the aim is to verify the hypothesis that the second one has the biggest influence or, at least, is sufficient to cause the protrusion's formation at the top of the droplet [14]. However, every day experience teaches that not in every condition water's freezing leads to pointy formations, in particular initial water's flat shapes do not tend to cause this particular behaviour. Consequently, the same amount of water can present different shapes as a result of the solidification's process, according to the initial shape which is determined by the cold plate surface's material and the consequent contact angle.

5.2.1. The solidification process

In the present section the results of the solidification process will be shown in the form of a series of figures representing the evolution of the solid fraction function (ice) in the domain and final shape assumed by the droplet as the freezing process is completed. In order to facilitate the comprehension and increase the spontaneity for the readers, the following figures are rotated by 90° counterclockwise: in that way the cooled plate is positioned on the bottom and freezing proceeds in the y direction. Moreover, a part of the air domain has been cut out of the figures with the aim to focus the attention on the droplet, this part of air is however necessary because, without it, the thermal inertia of the environment becomes negligible with respect to that of the water, which causes temperature to fall down too quickly, altering the entire process.

The first instants of the solidification process, shown in Figure 5.15, allow to ap-



Figure 5.15: Beginning of the solidification process, solid fraction



Figure 5.16: A different position of the freezing point, solid fraction



Figure 5.17: The freezing front affecting the entire surface of the drop, solid fraction



Figure 5.18: The final shape of the droplet, solid fraction

preciate how the freezing front is higher in correspondence of the liquid-air interface. This phenomenon is due to the higher thermal diffusivity of the air, which cools more rapidly than the liquid and it cools the droplet itself from the outside.

Once a solid layer is formed, also the conduction in the solid becomes more effective and the temperature in the part of the droplet closer to the axis decreases quite uniformly as can be seen in Figure 5.16, where the effect of the outside air is less prominent. As a confirmation of these facts, the effects of the different values of the thermal diffusivities can be appreciated in Figure 5.19 where it is clear how the lower value for this parameter of the water hinder the thermal diffusion, being the liquid fraction remarkably warmer than the rest of the domain.



Figure 5.19: Temperature field in correspondence of an intermediate solidification step

In Figure 5.17 it can be seen how the previously described effect of the air cooling faster leads the temperature on the surface of the droplet to decrease in value and the solidification process on this region to start from the outer layer even if the water below is still outside the phase change range of temperature. This phenomenon predicted in the present simulation can be also seen in the laboratory experiences as shown in Figure 2.13, where a thin layer of ice can be noticed on the top of the droplet.

In the last of the figures presented can be appreciated the final shape assumed by the droplet once the solidification process has come to the end, with the characteristic protrusion, visible in Figure 5.18.

The *IBM layer* shown in the third image has initially caused some issues because its presence was an obstacle for the vertical motion of the liquid still present inside the droplet which, according to the experience, is supposed to form the tip. In fact, in the actual process the thin layer of ice is easily broken by the pressure generated by the underlying water expanding during the liquid to solid transition. Numerically, this phenomenon cannot happen but it has been bypassed by imposing that the ice cannot be moved only once it is completely formed, that is to say only when the solid fraction function is equal to the unit and not less.

In Figure 5.20 is shown an intermediate step of the solidification process and the correspondent velocity vectors. First of all, it can be appreciated how inside the ice, which is identified by the red color corresponding to the higher value of the solid fraction, there are no velocity vectors, as expected being the ice completely formed. Secondly, as stated before in the previous equations, velocity is calculated only in the interface region and applied to the surrounding fluid perpendicularly to the freezing front. Being the fluid incompressible, the prevalent direction of the motion inside the droplet in along the symmetry axis which is located in correspondence of the south wall. However, it is thanks to the component perpendicular to it, which pushes the fluid towards the axis, that the final protrusion can be formed.



Figure 5.20: Velocity vectors in correspondence of an intermediate solidification step

5.2.2. The freezing front

The successive analysis performed is about the evolution of the freezing front inside the droplet with time. While the Stefan problem predicts a square root tendency for the problem studied in one dimension and the present code has verified it, experimental

results suggest a linear trend for the freezing process inside the droplet along the symmetry axis.

One of the aims of the present work is to verify which option is more adherent to the numerical results, the linear one, the square root or even a third one. To investigate this topic a series of tests have been performed and then compared to the experimental results and to other numerical works.





Figure 5.21: Position of the freezing front normalised versus normalised time



In Figure 5.21 is shown the result of the analysis on a droplet of $13 \cdot 10^{-14} [m^3]$ of volume, which is clearly not physical in its dimension but it required a reasonable computational time. The first portion of the figure shows a trend close to the linear one, while the last instants present a remarkable acceleration of the freezing process. This fact, which has not been observed experimentally, can be explained looking at Figure 5.22: the frozen layer of ice on the outer surface is not dynamically treated as ice as explained in the previous section but from a thermal point of view, given the way the global thermal diffusivity is calculated, has not negligible influence on the heat transfer. In fact, being the thermal diffusivity of ice an order of magnitude higher than the water's one, the presence of a solid fraction, even a small amount, contributes to enhance the thermal transfer, causing an acceleration of the freezing process, explaining the behaviour in the image.

However the ice accretion on the surface is influenced by the thermal inertia of the air outside the droplet, that is to say the dimension of the domain, which for the case previously presented it was too small, causing this phenomenon to be stronger than the actual one. For this reason a larger domain has been studied, giving as a result an incremented adherence to the experimental result and a slower solidification process, shown in Figure 5.23.

The first difference that stands out is a significant increase in the total solidification time, which for the extended domain is doubled. However, the two trends appear to assume close values in the first phase, while they distance one from the other from the point in which the one with the smaller domain accelerates its solidification, as explained above. Avoiding this phenomenon the behaviour of the solidification process found in this work is more adherent to the experimental and other numerical results,



Figure 5.23: Position of the freezing front, comparison between the extended domain and the previous one

shown in Figure 5.24 and Figure 5.25.



0.8

Figure 5.24: Position of the freezing according to Ablonet's experiment [12]

Figure 5.25: Numerical results for the freezing front position [24]

This simulation has shown a linear tendency for the entire temporal length of the freezing process, except for a certain acceleration surpassed the half of the solidification time. This behaviour of a slightly non linear tendency can be found also in the experimental work even if it appears later in the process.

5.2.3. The effects of the contact angle

In this section the influence of the below surface on which the solidification of the water occurs is investigated: *different* surfaces are tested not considering different physical properties (ex. thermal conductivity...) but from the point of view of the coupling between the cooled wall and the droplet, that is to say imposing different contact angles. It is well known that a surface can be hydrophilic or hydrophobic, causing a different reaction towards the deposition of the droplet on them: on a hydrophilic one the water tends to spread and assume flatter shapes while on a hydrophobic one, the droplet is *rejected*, showing high values for the contact angle between its surface and the cold plate, resulting in more spherical shapes.

The influence of the contact angle will be studied as regard as the total solidification time and the freezing front evolution with respect to time. Experience suggests that hydrophobic surfaces tends to slow down the solidification rate and for this present reason the current tendency is to adopt this kind of materials (or applying surface coatings in order to vary the wetting property) to avoid or delay the ice accretion on the plane surfaces (icing problem).

The objective is to verify if the code employed, with the modification introduced in this work, confirms the described tendencies by investigating the behaviour of droplets characterised by different contact angles. In order to make different droplet's configuration comparable, the fixed parameters are:

- Wall temperature
- Initial temperature
- Droplet's volume
- Mesh size

In Figure 5.26 can be seen the effect of the contact angle on the solidification time: it is clear how hydrophobic surfaces tend to slow down the freezing process. The points on the present figure have been adimensionalised using as reference the droplet with a contact angle of 90° because it is the theoretical limit to distinguish an hydrophobic surface from an hydrophilic one. This operation has been made because total time of phase change is not relevant and comparable to experimental results, giving the small volume of water involved due to computational time.

These results indicate an increasing of the total time of solidification with the contact angle, which present a 40% growth comparing the 120 degrees case with the reference one. This phenomenon can be explained considering the thermal transfer process: the droplet is cooled both by the surrounding air and the cold plate below. Compared to the ice and the water, air has a greater thermal diffusivity which causes thermal waves to move faster inside it but it is commonly known to be an insulator, on the other hand the thermal exchange through the cold plate is way more effective. Consequently the wider the contact area between the droplet and the plate is, compared to the droplet's surface (heat flux through the air), the more the heat transfer is effective and the solidification process fast.

In Figure 5.27 is presented the effect of the contact angle on the freezing front evolution through time which shows similar tendencies independently from the contact angle imposed and it is coherent with the results already presented in Figure 5.25.

Another relevant result which has been found is a physical threshold for the pointy tip to appear: the different simulations performed considering various contact angle values have shown that below a certain value positioned at about $\Theta = 25 - 35^{\circ}$, the protrusion on the top of the droplet does not develop, and the final shape assumed



Figure 5.26: Total time of solidification vs contact angle

by the droplet is smoother, as can be observed in Figure 5.28 for a 20 degrees contact angle.

5.2.4. An elliptical droplet

Physically, for the dimension considered above, the droplets of water have always a spherical cap shape due to Bond numbers much smaller than the unity. Consequently, the effect of gravity is negligible and the surface tension's action is predominant. The effect of gravity in bigger droplets results in flattered shapes which from spherical cap tends to become quasi-elliptical. The curve simulating the real shape is not really an ellipse but it resemble to it in first approximation.

In this paragraph some elliptical droplets have been analysed: it is important to remark that the dimensions involved are, as order of magnitude, the same as for the spherical cases, so this shape of the drop is not a physical consequence of the chosen length but only a study with the aim to comprehend if different dynamics emerge in such cases. As a consequence, the results obtained in this simulation should not be compared with those presented before given the non-physical sense of the initial shape considered but they are interesting as regard as the behaviour of the numerical tool approaching this new shape, which is the one most of the laboratory experiences considers.

In Figure 5.29 and 5.30 are shown two different steps of the freezing evolution, in particular in the second one can be appreciated the pointy protrusion on the top of the droplet.

This result is adherent to laboratory experiences and indicates how the tip formation should be not dependent from the initial shape of the droplet but the precedent results suggest that the main influence can be conferred to the the contact angle and so to the solid surface properties.



Figure 5.27: Position of the freezing front vs time



Figure 5.28: 20° contact angle solidified droplet



Figure 5.29: Intermediate step of the solidification process in a elliptical drop



Figure 5.30: Final shape of the solidified droplet

6. Conclusions

The main result achieved in this thesis work has been the coupling of the Immersed Boundary Method (IBM) with the Volume of Fluid (VoF) approach and the thermal computation. In particular, an IBM whose movement is linked to the temperature and not to an externally imposed velocity (as is usually done) has been implemented in order to simulated the ice accretion inside a droplet of water. This coupling is an original result which, to our knowledge, is yet to be reported in the literature.

This new code development has been implemented in the JADIM research code of the *Institut de Méchanique des Fluides de Toulouse* and validated using as reference the Stefan problem in a one dimensional formulation considering a semi-infinite domain full of fluid. The equations for the Stefan problem have been solved considering the fluid temporal variation in density due to the phase change, in order to validate the velocity computation. In fact, the expansion considered gives as a result the fluid motion which is imposed by exploiting the Immersed Boundary Formulation, driven by the resolution of the thermal field.

The immersed boundary technique has been adopted to simulate the solid phase, it has a double purpose: firstly, to impose a zero velocity field inside the ice part which is solid and fixed in time and space and, secondly, to generate a motion from the solidification front towards the fluid, pushing it as a natural consequence of the change in density.

A grid dependency analysis has been performed of the above formulation and this method is found to require fine grids to maintain accuracy, mainly because the most delicate part of the calculation is in the interface region, which is thin and so the more refined is the grid, the more the results are adherent to the analytical ones; in fact, physically water presents an isothermal phase change while in this work the solidification is considered to happen in a range of temperatures.

Once the numerical tool has been tested on the Stefan problem, several simulations have been performed on a droplet of water, introducing the air as third phase and analysing an axi-symmetric domain. The results obtained are not completely comparable to the experimental ones because a much smaller droplet of water has been chosen in order to satisfy the grid refinement requirements and not to handle too expensive computations.

The simulated droplets have shown the characteristic pointy tip observed in many laboratory experiments which was one of the main purposes at the beginning of this work. Moreover, the fact that this typical protrusion can be simulated by the updated code, thanks to the implementation of the velocity computation due to the fluid expansion, indicates that this is the leading cause of this phenomenon. As a consequence, the so called *Marangoni effect* does not appear to be essential in the formation of the final tip on the top of the solidified droplet, considering that the present code does not include routines with the aim to take account of it.

One of the objectives of the work was to investigate the evolution of the freezing front through time: in the Stefan problem, which considers a one-dimensional domain, the analytical solution gives a square root tendency for the advancement of the solidification process, while some experimental works as well as numerical ones, carried out on water droplets, suggest a more linear behaviour. The obtained results appear to confirm this second trend with a quasi-linear global tendency except for an acceleration after the middle of the process which can be attributed to the local solidification involving the outer layer of the drop.

The last part of the work concerned a parametric study on the influence of the contact angle between the water droplet and the cold substrate. The simulations have been performed keeping the volume of water constant and varying the shape of the droplets by imposing different contact angles and considering spherical cap configurations. The analysed results have concerned the total solidification time, the evolution of the freezing interface and the final shape assumed by the droplet.

The numerical results obtained, with respect to the total time of solidification, highlight the fact that to greater contact angles correspond longer freezing times. This solution is adherent to the actual physical behaviour and confirms the trend to adopt hydrophobic materials or coatings in order to prevent or delay ice accretion on critical plane's surfaces.

The second analysis, concerning the evolution of the solidification front with time, shows no significant influence of the contact angle on the obtained tendency, which always has limited deviations with respect to the linear trend taken as reference and found in experimental studies.

The last result obtained with this parametric study involves the final shape assumed by the droplet and, in particular, the formation of the pointy tip. The characteristic protrusion is found to be linked to the initial shape of the droplet, that is to say that the numerical simulations suggest the existence of a critical angle. Below this value, which is located at about 30 degrees, the typical formation on the top of the droplet cannot be observed: this result should be verified by some experimental campaigns.

Some simulations, in the end, have been performed with the aim to study the possible influence of an elliptical initial shape of the droplet over the spherical cap one. This shape is not adherent to physical reality due to the dimensions of the droplet considered in order to reduce the computational time but can be useful to investigate if substantial differences occur with respect to the previous simulations. This analysis confirms the appearance of the pointy protrusion at the top of the solidified droplet with no strong dependency on the chosen shape.

6.1. Future developments

The main issue which has to be solved regards the calculation of the phase change latent heat, which has been underestimated according to the preliminary analysis performed on the Stefan problem. Starting from the considered methods, adopting the latent heat source term, some additional iterations may be required in order to guarantee numerical stability, which is critical for this method. On the other hand, if the apparent heat capacity method is chosen, a solution could be the adoption of a dynamic mesh in order to track the freezing front and operate with a refined grid in the interface region. Other numerical studies suggest that, for the apparent heat capacity method, some correction loops can be introduced with the aim to perform a more accurate computation of the latent heat. Otherwise, different numerical methods could be employed, looking for a better alternative to those presented in this thesis.

Another possible development consists in using a different approach towards the velocity computation. This means that, instead of calculating the velocity of the freezing front employing the chain rule, which doubles the errors considering two derivatives (and the consequent approximations), it might be advisable to track the front and compute the velocity with respect to the actual motion of the interface. A similar approach could permit to employ less refined grids, avoiding the issue related to the cost of the calculations and imposition of the velocity in the interface region and could also reduce the cited underestimation of the phase change heat.

As mentioned before, an experimental campaign on freezing water droplets on different substrates and their consequent different contact angles should be performed, in order to investigate the actual influence of this parameter concerning the formation of the pointy tip protrusion and to verify the effectiveness of the implemented code.

A. Derivation of the analytical solution of Stefan problem

An analytical solution to the Stefan problem can be obtained also for the case where a velocity is imposed on the fluid. The equation to be solved for the monodimensional case (direction x) are the following:

$$\frac{\partial T_s}{\partial t} = \alpha_s \frac{\partial^2 T_s}{\partial x^2} \qquad 0 < x < s\left(t\right) \tag{A.1}$$

$$\frac{\partial T_l}{\partial t} + V_{liq} \frac{\partial T_l}{\partial x} = \alpha_l \frac{\partial^2 T_l}{\partial x^2} \qquad x > s\left(t\right) \tag{A.2}$$

$$V_{liq}(t) = \left(1 - \frac{\rho_s}{\rho_l}\right) \frac{ds}{dt}$$
(A.3)

with the correspondent initial and boundary condition:

$$\begin{cases} T_s \left(x = 0, \forall t \right) = T_w & \text{imposed wall temperature} \\ T_s \left(x = s \left(t \right), \forall t \right) = T_l \left(x = s \left(t \right), \forall t \right) = T_m & \text{isothermal phase change} \\ T_l \left(x \to \infty, \forall t \right) = T_0 & \text{imposed temperature at infinity} \\ T_s \left(\forall x, t = 0 \right) = T_l \left(\forall x, t = 0 \right) = T_0 & \text{initial temperature} \\ k_s \frac{\partial T_s}{\partial x} - k_l \frac{\partial T_l}{\partial x} = \rho_s L \frac{ds}{dt} & x = s \left(t \right) & \text{heat fluxes equilibrium at the interface} \\ s \left(0 \right) = 0 & \end{cases}$$

(A.4)

In order to obtain a solution it is necessary to operate a variable change, with the aim of converting the partial differential equation into an ordinary differential equation by combining the two independent variables x and t into the single similarity variable η :

$$\eta = \frac{x}{2\delta\sqrt{\alpha_s}} \tag{A.5}$$

Operation some substitutions and simplifications, expressions for the derivative and other quantities can be obtained:

$$\begin{cases} \frac{\partial T}{\partial t} = \frac{\partial T}{\partial \eta} \frac{\partial \eta}{\partial t} = \frac{dT}{d\eta} \left(-\frac{x}{4t\delta\sqrt{\alpha_s t}} \right) \\ \frac{\partial T}{\partial x} = \frac{\partial T}{\partial \eta} \frac{\partial \eta}{\partial x} = \frac{dT}{d\eta} \left(\frac{1}{2\delta\sqrt{\alpha_s t}} \right) \\ \frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x} \left(\frac{\partial T}{\partial x} \right) = \frac{\partial}{\partial \eta} \left(\frac{\partial T}{\partial x} \right) \frac{\partial \eta}{\partial x} = \frac{d^2 T}{d\eta^2} \left(\frac{1}{4\delta^2 \alpha_s t} \right) \end{cases}$$
(A.6)

and

$$s = 2\delta\sqrt{\alpha_s t} \tag{A.7}$$

$$\frac{ds}{dt} = \delta \sqrt{\frac{\alpha_s}{t}} = \frac{2\eta \delta^2 \alpha_s}{x} \tag{A.8}$$

Substituting (A.6) in (A.1) and (A.2) and defining the following constant parameters:

$$\begin{cases} \alpha = \frac{\alpha_s}{\alpha_l} \\ r = \left(1 - \frac{\rho_s}{\rho_l}\right) \end{cases}$$
(A.9)

the PDEs have been transformed into ODEs:

$$\frac{d^2 T_s}{d\eta^2} + 2\delta^2 \eta \frac{dT_s}{d\eta} \qquad 0 < \eta < 1 \tag{A.10}$$

$$\frac{d^2 T_l}{d\eta^2} + \frac{dT_l}{d\eta} \left(2\eta\alpha\delta^2 - 2r\alpha\delta^2\right) \qquad \eta > 1 \tag{A.11}$$

Also the boundary and initial conditions (A.4) have to be manipulate in agreement with the variable change operated and give the following set of equation:

$$\begin{cases} T_s (\eta = 0) = T_w & \text{imposed wall temperature} \\ T_s (\eta = 1) = T_l (\eta = 1) = T_m & \text{isothermal phase change} \\ T_l (\eta \to \infty) = T_0 & \text{initial and infinity temperatures} \\ k_s \frac{dT_s}{d\eta} - k_l \frac{dT_l}{d\eta} = \rho_s L2\delta^2 \alpha_s & \text{heat fluxes equilibrium at the interface} \end{cases}$$
(A.12)

The successive step now consists in solving the two ODEs for solid and liquid phase, with the respective boundary conditions. Firstly will be solved Eq. (A.1) by the mean of substitution assuming $w = \frac{dT_s}{d\eta}$ which gives:

$$\frac{dw}{d\eta} + 2\delta^2 \eta w = 0 \tag{A.13}$$

$$\frac{dw}{w} = -2\delta^2 \eta d\eta \tag{A.14}$$

$$ln\left(w\right) = -\delta^2 \eta^2 + C_0 \tag{A.15}$$

with C_0 integration constant which can be rearranged as:

$$w = C_1 e^{-(\delta\eta)^2} \tag{A.16}$$

and operation another integration step gives:

$$T_s = \frac{\sqrt{\pi}}{2} \frac{C_1}{\delta} erf(\delta\eta) + C_2 \tag{A.17}$$

The boundary conditions (A.12) have to be used in order to define the constants C_1 and C_2 and finally the following expression for the temperature and its derivative can be deducted:

$$T_s = T_w + (T_m - T_w) \frac{erf\left(\delta \frac{x}{2\delta\sqrt{\alpha_s t}}\right)}{erf\left(\delta\right)}$$
(A.18)

$$\frac{dT_s}{d\eta} = \frac{(T_m - T_w)}{erf(\delta)} \frac{2\delta}{\sqrt{\pi}} e^{-(\delta\eta)^2}$$
(A.19)

Analogously, Eq. (A.2) can be dealt with, even if it is a bit more difficult due to the expansion term, the substitution variable is now called $y = \frac{dT_l}{d\eta}$:

$$\frac{dy}{d\eta} = 2yr\alpha\delta^2 - 2\eta\alpha\delta^2 y \tag{A.20}$$

integrating it can be obtained:

$$y = C_3 e^{-\alpha(\delta\eta)^2} e^{2r\alpha\delta^2\eta} \tag{A.21}$$

and

$$T_{l} = C_{3} \frac{\sqrt{\pi}}{2} \frac{e^{\alpha(r\delta)^{2}}}{\sqrt{\alpha\delta}} erf\left[\sqrt{\alpha\delta}\left(\eta - r\right)\right] + C_{4}$$
(A.22)

Finally the constants are obtained using the unused conditions of (A.12) and it gives:

$$T_{l} = T_{0} + (T_{m} - T_{0}) \frac{erfc\left[\sqrt{\alpha}\delta\left(\frac{x}{2\delta\sqrt{\alpha_{s}t}} - r\right)\right]}{erfc\left[\sqrt{\alpha}\delta\left(1 - r\right)\right]}$$
(A.23)

$$\frac{dT_l}{d\eta} = (T_m - T_0) \frac{2}{\sqrt{\pi}} \frac{\sqrt{\pi}\delta}{e^{\alpha(r\delta)^2}} \frac{e^{-\alpha(\delta\eta)^2} e^{2r\alpha\delta^2\eta}}{-erfc \left[\sqrt{\alpha\delta}\left(1 - r\right)\right]}$$
(A.24)

The last parameter to be computed in order to obtain a solution is δ , which requires the solution of the transcendental equation given by the heat fluxes equilibrium (A.12), where the value of the two derivative of temperature have been written in Eq. (A.19) and (A.24):

$$k_s \frac{(T_m - T_w)}{erf(\delta)} \frac{2\delta}{\sqrt{\pi}} e^{-\delta^2} + k_l \frac{(T_m - T_0)}{erfc\left[\sqrt{\alpha\delta}\left(1 - r\right)\right]} \frac{2\delta}{\sqrt{\pi}} \frac{\sqrt{\alpha}}{e^{\alpha(r\delta)^2}} e^{-\alpha\delta^2} e^{2r\alpha\delta^2} = \rho_s L 2\delta^2 \alpha_s \quad (A.25)$$

This equation can be rearranged, obtaining:

$$\frac{e^{-\delta^2}}{erf(\delta)} - \frac{\phi}{\sqrt{\alpha}} \frac{e^{-\alpha\delta^2}}{erfc\left[\sqrt{\alpha}\delta\left(1-r\right)\right]} \frac{e^{2r\alpha\delta^2}}{e^{\alpha(r\delta)^2}} = \frac{\delta\sqrt{\pi}}{Ste}$$
(A.26)

being the two parameters ϕ and *Ste* as defined in chapter 2:

$$\phi = \frac{\rho_l c_{p,l} \left(T_0 - T_m \right)}{\rho_s c_{p,s} \left(T_m - T_w \right)}$$
(A.27)

$$Ste = \frac{\rho_s c_{p,s} \left(T_m - T_w \right)}{\rho_s L} \tag{A.28}$$

It is important to remark that here in Appendix A the parameter α has been defined as $\alpha = \frac{\alpha_s}{\alpha_l}$ while in Chapter 2 the same parameter is slightly different, being $\alpha = \sqrt{\frac{\alpha_s}{\alpha_l}}$ This explain the difference between the equation that has been demonstated here and the shown in Chapter 2 (as to say Eq. 2.36).

Bibliography

- [1] M. B. Bragg et al. "Effect of Ice Accretion on Aircraft Flight Dynamics". In: American Institute of Aeronautics and Astronautics (2000).
- [2] B. Borrell. "How does ice cause a plane to crash?" In: Scientific American 300 (2009).
- [3] J. S. Yong. "Evaluation of the Environmental Impacts and Alternative Technologies of Deicing/Anti-icing Operations at Airports". MA thesis. Massachusetts Institute of Technology, 2001.
- [4] Z. Jin and H. Hu. "Ice process of small water droplets impinging onto a frozen cold plate". In: Journal of Thermophysics and heat transfer 24 (2010), p. 841.
- [5] V. Alexiades and A. D. Solomon. Mathematical Modeling of Melting and Freezing Processes. Hemisphere Publishing Corporation, 1993.
- [6] J. A. Dean. Lange's Handbook of Chemistry. McGraw-Hill, Inc., 1999.
- [7] W. M. Rohsenow, J. P. Hartnett, and Y. I. Cho. Handbook of Heat Transfer. McGraw-Hill, 1998.
- [8] S. Fukusako. "Thermophysical Properties of Ice, Snow and Sea Ice". In: International Journal of Thermophysics 11 (1990), p. 353.
- [9] T. L. Bergman et al. Fundamental of Heat and Mass Transfer. John Wiley and Sons, 2011.
- [10] W. H. Hager. "Wilfrid Noel Bond and the Bond number". In: Journal of Hydraulic Research 50 (2012), pp. 3–9.
- [11] J. C. Batsale D. Lecomte. "A suitable approximate solution of Neumann's problem". In: International Journal Heat Mass Transfer 34 (1991), p. 894.
- [12] E. Ablonet. "Solidification d'une goutte sur une plaque plane". MA thesis. Institut de Mecanique des Fluides de Toulouse, 2016.
- [13] L. Huanga et al. "Effect of contact angle on water droplet freezing process on a cold flat surface". In: Experimental Thermal and Fluid Science 40 (2012), pp. 74– 80.
- [14] W. Jieteng et al. "Deformation of freezing water droplets on a cold copper surface ". In: Science in China Series E: Technological Sciences 49 (2006), pp. 590–600.
- [15] F. Moukalled, L. Mangani, and M. Darwish. *The Finite Volume Method in Computational Fluid Dynamics*. Springer International Publishing Switzerland, 2016.

- [16] A. Pedrono. User manual for JADIM parallel version. IMFT interface. 2015.
- [17] M. T. Abadie. "Hydrodynamics of Gas-Liquid Taylor Flow in Microchannels". PhD thesis. Institut National Polytechnique de Toulouse, 2013.
- [18] B. Bigot et al. "A simple immersed-boundary method for solid-fluid interaction in constant- and stratified-density flows." In: Computers and Fluids 97 (2014), pp. 126-142.
- [19] R. Mittal and G. Iaccarino. "Immersed Boundary Methods." In: Annu. Rev. Fluid Mech. 37 (2005), pp. 239–261.
- [20] Z. Zhentong. "Étude numerique de la solidification d'une goutte sur une surface froide". MA thesis. Institut de Mecanique des Fluides de Toulouse, 2016.
- [21] J. D. Anderson Jr. Fundamentals of Aerodynamics. McGraw-Hill, 2010.
- [22] V. R. Voller, C. R. Swaminathan, and B. G. Thomas. "Fixed Grid Techniques for Phase Change Problems: a Review". In: International Journal for Numerical Methods in Engineering 30 (1990), pp. 875–898.
- [23] V. R. Voller and C. R. Swaminathan. "General Source-Based method for solidification phase change". In: Numerical Heat Transfer 19 (1991), pp. 175–189.
- [24] G. Chaudhary and R. Li. "Freezing of water droplets on solid surfaces: An experimental and numerical study". In: Experimental Thermal and Fluid Science 57 (2014), pp. 86–93.