

### Modélisation du couplage fluide solide avec l'analyse et l'optimisation des contraintes résiduelles et thermo-elasto-plastiques

Joe Khalil

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### THÈSE DE DOCTORAT DE L'UNIVERSITÉ PSL

Préparée à MINES Paris

# Modeling fluid solid coupling with residual and thermo-elasto-plastic stresses analysis and optimization.

Modélisation du couplage fluide solide avec l'analyse et l'optimisation des contraintes résiduelles et thermo-elasto-plastiques.

#### Soutenue par

Joe KHALIL Le 22 Novembre 2022

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#### Composition du jury :

Prof. Łukasz MADEJ AGH University of Science and Technology	Président
Prof. Julien BRUCHON École des Mines de Saint-Étienne	Rapporteur
Prof. Chady GHNATIOS École nationale supérieure d'arts et métiers	Rapporteur
Dr. Chantal DAVID Sciences Computers Consultants	Examinateur
Prof. Elisabeth Massoni Mines Paris - PSL	Co-directrice de thèse
Prof. Elie HACHEM Mines Paris - PSI	Directeur de thèse





For my parents

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# Chapter 1

## Introduction

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#### **1.1** Industrial context of quenching

Quenching is a very important industrial application in particular in automotive, aerospace, and nuclear industries. It is the fast cooling of a solid in the quenchant which could be water, oil, air, or any other fluid. The importance of this process comes with its ability to control the microtructure and the properties of the material. In addition, it precedes all the other processes as forging, rolling, etc. Therefore, a lack of controlling this process will impact the manufacturing chain and results in low quality products. For that reason, it is important to understand the physics behind this process to be able to control it. Numerical and experimental studies of physical processes, with the help of mathematical equations, gave a better understanding of complex problems and decreased the development costs [1–4]. In the history of quenching, the optimization and testing were only done by large companies that can afford large experimental tests and have the needed advanced tools or powerful computers for large amount of calculations. Nowadays, the numerical simulations became more accessible and enough accurate to simulate such a process.

The quenching process belongs to the family of thermal treatment of the material. The purpose is to enhance the hardness of materials and control the microstructure as stated before. This process prevents some low-temperature transformation to happens, by reducing their time-window which makes the microstructure with smaller grain and better hardness. This process also involves many physical phenomena in the solid as well as the surrounding fluid. Moreover, different parameters can be controlled during this process as agitation, piece orientation, quenchant properties, tank size, etc. Figure (1.1) shows real industrial applications of quenching.



Figure 1.1: Industrial quenching [5, 6]

This project is a part of the INFINITY industrial ANR chair that involves important industries in aeronautics, nuclear, and automotive fields. Their interest is a full control of the process, to better understand and easily apply changes to their application. To have a full control, it is important to understand and take into account all the physical phenomena happening in both the solid and the fluid mediums.

#### **1.2** Importance of computational analysis of quenching

Because of the importance of this process in the industrial world, many studies exist in the literature that works on the quenching process, in particular the fluid behavior at the interface [4, 7–9]. These studies concentrate on the parameters that affects the quenching process (e.g. agitation rate, fluid viscosity,...). Additionally, it is a very complex process since it includes several physical phenomena on both the fluid (quenchant) and the solid as mentioned before. Although these studies are interesting and help to understand the heat transfer phenomenon, however most of them are experimental and are still limited to some scenarios that can not be controlled. For that reason, computational analysis became more interesting for such an application to have a better control of the process. Numerically speaking, this kind of application has a Computational Fluid Dynamics (CFD) problem on the outside of the solid, and a Computational Solid Mechanics (CSM) in the solid part.

#### **1.3** Physics behind quenching and thesis objective

This process has two main physical events: boiling and evaporation in the quenchnat, and changes in the solid. First, one must understand what happens when a liquid is in contact with a hot surface. Nukiayama, studied the heat flux between a metal surface and boiling water [10]. Figure (1.2) shows the different stages of heat flux, and it could be divided into four stages:

- 1. From the beginning to point "e" is the free convection stage. Bubbles do not exist yet, but the density of the fluid is decreasing with an increasing temperature.
- 2. Between point "e" and "b" is the nucleate boiling stage. The bubbles starts to appear and form columns. Point "b" is called the critical heat flux; at this point it is the most efficient heat transfer.
- 3. Between point "b" and "c" is the transition boiling. At this stage the vapor layer starts to develop and surround the material. Point "c" is called the Leidenfrost point.
- 4. From point c an beyond is the film boiling. Finally the vapor film is is created and covers the material.



Figure 1.2: Surface heat flux evolution as function of the excess temperature [10].

In the quenching process, the heat transfer passes through all the stages presented but in the other direction (from right to left). It is clear that the cooling process is not continuous and simple, which makes it important to simulate the whole boiling and evaporation process.

On the other side, it is important also to understand what changes the solid passes through. Three main phenomenon occurs in the material while quenching: heat transfer, phase transformation, and mechanical response. These three fields interact with each other during the process as seen in figure (1.3).



Figure 1.3: Link between heat transfer, phase transformation and mechanical response

Since it is a cooling process with a high temperature difference, different phases are created and their volume fraction changes during the process. In parallel, cooling rate is affected by these phases due to the latent heat they generate during the transformation. At the same time, temperature change and phase transformation have a significant impact on the deformation and the stresses in the part. A coupling between phase transformation and mechanical response also exist, since new phases cause stresses, and the stresses can trigger some new phases to appear. These three connected fields are also dependent on the chemical composition of the alloy.

To be able to have a full understanding of the process, one must remove as many assumptions as possible. For that reason, the main objective of this thesis, is to achieve a full framework of the process that includes all the physics happening in both mediums: the solid and the fluid. To summarize the physics explained in this section, figure (1.4) is an illustration of all the different phenomena happening in this process.



Figure 1.4: Full framework illustration

Figure (1.4) gives us the structure of this thesis where the objectives are as follows:

- 1. Achieve the full coupling between the fluid and the solid.
- 2. Solve both systems simultaneously; phase change of the fluid at the interface, and phase transformation with mechanical response in the material.

- 3. Look for quality of the part in terms of residual stresses and deformation.
- 4. Describe numerically the full quenching mechanism, in order to control the process.

In the following section, a global literature review on the quenching process is presented that highlights the most important contributions on this process.

#### **1.4** Summary of the quenching in the literature

In the literature, various efforts were proposed to deal with this process. They can be gathered into two groups: one fluid flow model with boiling transfer coefficients, or two-fluid flow model with heat transfer coefficients for the solid part. In the latter case, the classical approach is to combine the fluid motion with interface tracking technique such as LevelSet [11], Phase Field [12], Volume of Fluid [13]...For example, Garwood et al. [1] have characterized a quench tank for the heat treatment of superalloys forging via simplified finite difference methods and heat transfer coefficients. Srinivasan et al. [14] developed a specific CFD modeling procedure to simulate particular immersion quench cooling process using boiling transfer coefficients in [15].

As expected, computational fluid dynamics is now being used increasingly for multiphase flows and in quench design. However there still considerable uncertainties due to assumptions that must be made in particular: (i) the use of simple geometries, (ii) the use of decoupled fluid solid resolution and finally, (iii) the use of transfer coefficients that approximate the complex quenching environments. Moreover, the consequences of the numerical method limitations are the set of physical model assumptions, e.g.: incompressibility, low density ratio between phases, omission of heat conduction in one of the phases, low fidelity for boiling phenomena, laminar flows, etc. Most of these assumptions are justifiable for their intended applications; however, their use remains generally limited and suffers from systematic revalidation when facing new materials, new geometries or new thermo-mechanical conditions.

One of the good idea is to remove all assumptions which will remove all the limitation that previous models were facing. Khalloufi et al. [16], developed a high fidelity phase change model. This model, includes all the physical phenomena that exist on the interface during quenching. In the context, he worked on level set to be able to capture well the interface. In addition, he worked on an anisotropic mesh adaptation to achieve a high-fidelity spatial resolution. Moreover, the immersed volume method is used for two fluid modeling in the context of multiphase flows [17] and for fluid structure interactions in the context of heat and mass transfer [18]. The coupling of both was a major enhancement of the model. Furthermore, it is

important to mention the study on the Navier Stokes equations to better understand the multi phase flow and the interactive of the two phases. Finally, the thermal behavior on the surface of the material was added to include the heat transfer that is causing boiling for a better accuracy.

This model was tested on several industrial cases with 3D modeling. First, a test was done on a small part to compare with experimental data. Figure (1.5) shows the boiling process during quenching, while the water is in blue and the solid is in red. It is clear the importance of this model, specially when we can visualise the adaptive mesh over time. As a reminder, the work in [16] used the anisotropic mesh adaptation. In addition, it represents the comparison between the experiment and the simulations. It is clear that a larger number of elements give more accurate results. As a matter of fact, for 2e5 elements, the numerical solution shows a good agreement with the experimental data.



Figure 1.5: Numerical results with visible adaptive mesh in comparison with experiments [16]

Several other studies were conducted to investigate the quenchant behavior on the interface. In [19] they worked also on the boiling process adding some experimental observation to validate the numerical model. These studies are important and help to understand the heat transfer that occurs at the interface and the fluid behaviour. On the other hand, another phenomenon is happening in the solid that is also affecting the process in particular phase transformation, stresses and deformations.

Several studies in literature worked on coupling both the fluid and the solid parts. I the work of [20], they did a simulation approach for quenching automotive parts. The model consists of using AVL  $FIRE^{(\mathbb{R})}$  for CFD coupled with  $DANTE^{(\mathbb{R})}$  for CSM with phase transformation. This study works on two different materials: Aluminum which does not have phase transformation, and steel with phase trans-

formation. Figure (1.6) shows the computational domain of the steel gear tested in this study, which consist of having two different codes for fluid and solid.



Figure 1.6: Computational domain for a steel gear study [20].

Subsequently, other studies can be found that work on the phase change at the interface coupled with a partial solid study. In [21], [14], and [22] they worked on a CFD code using AVL  $FIRE^{(\mathbb{R})}$ . Moreover, another study was done in [23], which also considers coupling of the fluid and the solid on two different softwares.

This bibliography is dedicated to contrast between the different fields that exist during the quenching process. In table 1.1, all the studies presented previously are summarized.

However, through all these years, the full coupling and the interaction between the fluid and solid have never been done properly. It exist in the literature several studies that deal with this coupling, but they study particular cases and do not cover the full process. The last row represents the main objective of this thesis. The aim is to create a full Eulerian framework for heat-fluid-solid treatment. This is crucial for the control of the process where different scenario need to be studied and have immediate impact: agitation (form, position, orientation), solid part (position, orientation, and geometry), and many other scenarios.

Since there exist many physical phenomena in this application, in this thesis all the physical phenomena will be presented in different chapters. The boiling and evaporation part is already well developed in the team which will be used as a tool in my project. The main focus will be on the changes happening in the solid,

Model	Numerical simulation	Fluid Solid Coupling
Done by Khalloufi [16]	Studies the boiling effect	No coupling
and ElKosseifi et al. [19]	with phase change	
Done by Aliaga [24],	Studies the behavior in	No coupling
Kang et al. $[25]$ , and	the material including	
Simsir [26]	phase transformation	
Done by Srinivasan et al.	Studies the phase change	Coupling exist but only
[21] $[14]$ , Kopun et al.	at the interface and the	with the thermal
[22], and Bahbah et al.	solid part	behavior (without phase
[23]		$\operatorname{transformation})$
Done by Greif et al. [20]	Studies the CFD on the	Coupling exist with
	interface with the solid	phase transformation,
	part	but the CFD part does
		not include High fidelity
		phase change model
To be done in this thesis	Studies the phase change	High fidelity phase
	at the interface and the	change model coupled
	phase transformation	with phase
	with the mechanical	transformation and
	response in the material	mechanical response

Table 1.1: Summary of all studies presented in this report

and the coupling between the solid and the fluid part. For that reason, chapter 2 will describe the phase transformation process in the steel, and its numerical interpretation. Chapter 3 focuses the geometrical changes in the solid because of the thermo-elasto-plastic stresses and strains. Since the elasticity was already developed in the team, chapter 3 will an extension of the elasticity with the development of the thermal and plastic parts of the deformation. Chapter 4 will be a recall of the phase change model, with the description of the new framework and the fluid-solid coupling. Finally, chapter 5 will be the application of the global model to industrial applications.

#### 1.5 Résumé en français

La trempe est un processus de refroidissement très important adopté de nos jours par la plupart des industries, en particulier les industries automobile, aérospatiale et nucléaire. L'importance de ce procédé vient de sa capacité à contrôler la microstructure, à avoir de meilleures propriétés thermiques comme la dureté et la limite d'élasticité, et à relâcher les contraintes résiduelles. Néanmoins, il s'agit d'un processus très complexe puisqu'il comprend plusieurs phénomènes physiques à la fois sur le fluide et sur le solide. Au niveau du liquide, du fait du contact direct avec une surface chaude, le liquide va s'évaporer et atteindre le point d'ébullition. Au niveau du solide, il existe des contraintes, des déformations qui modifient la forme de la pièce et des transformations de phase qui génèrent de la chaleur latente. Un modèle d'ébullition d'évaporation est été utilisé pour simuler ce qui se passe dans l'environnement du solide. L'importance de ce modèle vient de sa capacité à donner une description réelle du transfert de chaleur qui se produit entre le solide et le fluide. Le changement de température dans le solide affectera à la fois la transformation de phase et la réponse mécanique de la pièce. Une partie bibliographique est introduite dans ce chapitre qui résume les travaux existant dans la litérature sur l'étude numérique de la trempe. Finalement, l'objective de la thèse est de simuler le processus de trempe en prenant compte de toute les physiques existant dans le soliide et dans le fluide.

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## Chapter 2

# Thermal analysis with phase transformation

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#### 2.1 Introduction

First physical phenomena to study is phase transformation, which is one part of the solid study as highlighted in figure (2.1). This is a thermal process that is responsible of the microstructure of the material



Figure 2.1: Phase transformation part of the full framework

For a solid undergoing high temperature gradients and different cooling rates in its thickness, phase transformation is a major physical phenomena that could happen. In general, there are different types of phase transformation in metals. Following table (2.1), these metals could be divided into three main categories: No phase transformation, steel phase transformation, and other alloys phase transformation. Steel was differentiated from other alloys, because it has the most complicated procedure, and it will be a main focus in this thesis.

#### 2.2 Phase transformation in steel

#### 2.2.1 Iron-carbon phase diagrams

Generally, the iron-carbon phase diagrams describe the phases with respect to temperature and carbon percentage as seen in figure (2.2). Each phase can exist de-

No phase transformation	Steel phase	Other alloys phase
	transformation	transformation
No latent heat	Latent heat due to	Latent heat due to other
generation	transformation from	type of transformation
	Austenite to another	
	phase	
<b>Example:</b> aluminum	<b>Example:</b> steel	<b>Example:</b> nickel,
		titanium based alloys

Table 2.1: Metals Types

pending on the chemical composition and the temperature of the alloy. For example for a 0.77% of carbon, the steel will be eutectoid and for a temperature above  $727^{\circ}C$ the phase will be austenite. When cooling this alloy, the austenite will transform directly to pearlite phase.

In this work, steel will be the main interest because of the complication of its phases and it is the most alloy used in industrial applications, which means the left part of the graph in figure (2.2) where the carbon percentage is less than two. Steels, in particular stainless steel, has several phases: pearlite phase which is a mixture of ferrite and cementite phases, mastensite phase, and the austenite phase. During quenching, the steel is subjected to phase transformation, and can have different phases through time. Moreover, phases can transform depending on the cooling rate and the chemical composition of the steel. As a matter of fact, austenite appears at high temperatures. With a slow cooling rate, the alloy will have the same microstructure before heating (same phases); mainly, the phases for slow cooling are pearlite, ferrite or cementite. With a rapid cooling rate, the microstructure will most probably be martensite [1].

#### 2.2.2 Austenite $\gamma$ to $\alpha$ transformations in equilibrium conditions

For a better understanding of the transformations, one must know about the  $\gamma \rightarrow \alpha$  transformations in the equilibrium conditions. As figure (2.2) shows, we can divide the transformations into four categories: eutectoid, hypo-eutectoid, hyper-eutectoid, and low carbon percentage transformations [3].



Figure 2.2: Iron-Carbon phase diagram [2]

#### 2.2.2.1 Low carbon percentage transformation; C % < 0.0218

This transformation begins at  $912^{\circ}C$  approximately, it can varies depending on the carbon precentage. The first stage of transformation, some ferrite grains will appear next to the austenite ones with a low carbon percentage. The ferrite phase continues to grow while cooling until  $727^{\circ}C$  is reached, below that a precipitation of cementite ( $Fe_3C$ ) begins. When the ambiant temperature is reached, the equilibrium structure will be a mix of ferrite with low carbon and  $Fe_3C$  precipitate [2].

#### 2.2.2.2 Eutectoid transformation; C % = 0.77

All this transformation happens on  $727^{\circ}C$ , which is point 3 on the graph, with the following reaction:

$$Fe\gamma(0.77\%C) \rightarrow Fe\alpha(0.0218\%C) + Fe_3C$$
 (2.1)

This reaction is responsible of the creation of the pearlite phase, which is a mixture of ferrite and cementite. Below  $727^{\circ}C$ , the ferrite phase will be almost saturated because of its low percentage of carbon. Thus, the precipitation will

continue on the form of  $Fe_3C$  basically on the cementite grains already developed. At the ambient temperature the pearlite phase will be divided as follows:

% mass of ferrite = 100 - 14.95 x C% = 88.5 % mass

% mass of cementite = 14.95 x C% = 11.5 % mass

Figure (2.3) illustrate the distribution of the pearlite phase during transformation.



Figure 2.3: Pearlite phase formation [2]

#### 2.2.2.3 Hypo-eutectoid transformation; 0.0218 < C % < 0.77

As figure (2.2) shows, the eutectoid transformation comes after a ferritic formation. The transformation begins between  $910^{\circ}C$  and  $727^{\circ}C$  (depending on the carbon percentage); it generates ferrite grains with low carbon and keeps precipitating until  $727^{\circ}C$ .

Below that temperature, an eutoctoid reaction happens as described in reaction (2.1). At the ambient temperature, the material will be composed of eutectoid aggregate with a hypo-eutectoid ferrite. The left side of figure (2.4) describes the distribution of the phases at a  $20^{\circ}C$  temperature in function of the carbon percentage.

#### 2.2.2.4 Hyper-eutectoid transformation; $0.77 < C \ \% < 2.11$

Identically to the hypo-eutectoid, this category has a cementic formation before the eutectoid reaction. the transformation begins between  $1148^{\circ}C$  and  $727^{\circ}C$  (depending on the carbon percentage).

At the ambient temperature, the structure will be an aggregate of eutectoid with  $Fe_3C$  or cementite precipitates. The right side of figure (2.4) describes the structure of the material at the ambient temprature.

Finally, figure (2.5) show the evolution of the microstructure during cooling in the equilibrium conditions. The hypo-eutectoid described in figure (2.5.a) shows ferritic phases with colonies of pearlite. Same for figure (2.5.b) with cementite phase. In addition, figure (2.2) and (2.5) summarizes the three main types of steel:

- 1. The steel only with the eutectoid aggregate and is called "eutectoid steel"
- 2. The steel that has a ferrite precipitate with the eutectoid aggregate is called "hypo-eutectoid steel"
- 3. The steel with a cementite precipitate with the eutectoid aggregate which is called "hyper-eutectoid steel"



Figure 2.4: Different phases variation with respect to carbon percentage at  $20^{\circ}C$  [2]


Figure 2.5: Microstructure evolution during cooling in equilibrium conditions for the a) hypo-eutectoid and b) hyper-eutectoid [4]

# 2.2.3 Austenite $\gamma$ to $\alpha$ transformations out of equilibrium conditions

### 2.2.3.1 Introducing TTT diagrams

One may ask what are the equilibrium conditions in phase transformation. It mostly means that all phases are in a chemical, mechanical and thermal equilibrium. In real life, specifically in industrial applications, the latter case is not common. A solid could undergo at the same time rapid cooling (on the surface) and slow cooling (in the core). On this basis a study called "continuous cooling" is done. The experience shows that the results found in this study could sometimes be complex and difficult to analyse.

For a clearer decomposition of each phenomena and for a better distinction the effect of time from one side and the effect of temperature from the other side, another study was done on the materials. This study analyses the transformations with isothermal conditions on temperatures lower than the limit of the austenite stability zone. This study is called "isothermal conditions" and described by the temperature time transformation (TTT) diagrams.

The kinetics of phase transformation  $\gamma \rightarrow \alpha$  is decribed using TTT diagrams. Figure (2.6) is an example of a hypo-eutectoid steel of type C55. This kind of diagram can be generated using the JMAT pro software; given any chemical composition of steel, the graph could be done with all the information needed. This graph has a logarithmic time as horizontal axis and temperature as vertical axis. The lines in blue corresponds to the transformation level as follows:

• The  $\gamma \to \alpha$  transformation begins with only ferrite phase (I)

- The eutectoid aggregate starts to form after a small fraction of ferrite (II)
- 50% of austenite transformed (III)
- The transformation is finished (IV)



Figure 2.6: TTT diagram of a hypo-eutectoid steel of type C55 [2]

#### 2.2.3.2 Transformations types in steel

The examination of the graph in figure (2.6) shows that the  $\gamma \to \alpha$  transformation could happen with different conditions depending on the maintained temperatures:

- In the temperature domain between  $Ac_3 \approx 775^{\circ}C$  and  $Ms \approx 310^{\circ}C$ , the transformation happens in function of time
- However, below the Ms limit the time has no effect on the transformation, the evolution continues with respect to temperature.

In the temperature domain between the stability limit of ferrite  $(Ac_3)$  and the ambient temperature, the experience shows that the transformation depends on whether we put the material on the higher or the lower temperatures of the interval. We can take the C55 example to elaborate more:

- a) Between the stability limit of ferrite  $Ac_3$  and approximately  $500 550^{\circ}C$ , the transformation happens with a similar procedure of the one with the equilibrium conditions. As a matter of fact, that ferrite grains start to appear and grow until the second limit  $Ac_1$  is reached. After that, a phase that is similar to the eutectoid aggregate starts to appear and it is called pearlite phase. So the first stages of transformation the austenite transform to properlitic ferrite, and pearlite phases.
- b) In a lower temperature domain, between approximately  $500 550^{\circ}C$  and Ms, the  $\gamma \rightarrow \alpha$  transformation is different than the high temperatures domain. The transformation still includes ferrite with saturated carbon and cementite crystals, however, the proeutectoid and eutectoid no longer exist. A new phase here is created and called bainite that comes into two forms upper bainite and lower bainite.
- c) Finally, below the Ms limit which is the starting temperature of the martensite phase. At this stage, the austenite transformation does not depend on time anymore.

In the following section, more details on the temperature limits and phase fraction will be discussed, in addition to the numerical procedure to calculate the phase fractions and their effect on the cooling process.

## 2.3 Numerical interpretation of phase transformation

## 2.3.1 Thermal behaviour

As described before, the phase transformation is a phenomena that highly depends on temperature and the cooling time. In parallel, cooling rate is affected by these phases due to the latent heat they generate during the transformation. The coupling between heat treatment and the phase transformation was done using finite element analysis (FEM) and can be found in [5]. This phenomenon can be mathematically described using the convection diffusion reaction equation,

$$\rho c \frac{\partial T}{\partial t} = \nabla . (\lambda \nabla T) - \nabla . (vT) + R + Q \qquad (2.2)$$

where  $\rho$ , c and  $\lambda$ , are the density, specific heat, and the thermal conductivity respectively.  $\nabla .(\lambda \nabla T)$  represents the diffusion,  $\nabla .(vT)$  the convection and R the reaction. Q is the internal heat source (source term) caused by the latent heat generated from the phase transformation. In this case, the reaction term is considered zero, and the convection term is removed since the velocity is zero inside the part. Equation (2.2) reduces to:

$$\rho c \frac{\partial T}{\partial t} = \nabla . (\lambda \nabla T) + Q \tag{2.3}$$

 $\rho$ , c and  $\lambda$  are dependent on both the temperature and the phase in the material. They are expressed by the linear rule of mixture which is the addition of each phase properties times the phase fraction,

$$P(T,\xi_i) = \sum_{1}^{N} P_i F_i \tag{2.4}$$

where P is the total  $\rho$ , c or  $\lambda$ ,  $P_i$  is the thermal property of the  $i^{th}$  phase, and  $F_i$  is the volume fraction of the  $i^{th}$  phase. The latent heat rate is expressed as function of the enthalpy change of each phase,

$$\dot{Q} = \sum_{i} \Delta H_i \dot{F}_i \tag{2.5}$$

where  $\Delta H_i$  is the enthalpy change of the  $i^{ith}$  phase. Q will be discussed in details in the following section.

Equation (2.3) describes the heat transfer of the process, with some updated thermal coefficients that fits with this application. In fact, if the assumption of the heat transfer coefficient is to be hold, one must use equation (2.3). However, since we are dealing with boiling and evaporation, the equation will change accordingly in the following sections.

## 2.3.2 Temperature limits of phases

Before going into the kinetics of the phase transformation, an important step must be done. One of the conditions for each phase to appear is to be in the corresponding temperature range. Hence, the limits of these ranges are called the critical temperatures and can be extracted from the TTT diagrams or calculated analytically. There are several ways in the literature to determine these temperatures based on the chemical composition of the material. Some of these methods uses the thermodynamics, and some others are based on regression analyses [5].

#### 2.3.2.1 Calculation of the ferrite critical temperature

This critical temperature has two variants, one in the equilibrium conditions  $Ae_3$ , and one out of the equilibrium conditions  $Ac_3$  ("c" stands for continuous cooling and "e" stands for equilibrium conditions). Generally these two values are approximately

equal. The  $Ac_3$  is given by a regression analysis on almost 4000 steel grades, and proposed by Lusk et al. [6],

$$Ac_{3}(^{o}C) = 883.49 - 275.89C + 90.91C^{2} - 12.26Cr + 16.45CCr - 29.96CMn + 8.49Mo - 10.80CMo - 25.56Ni + 1.45MnNi + 0.76Ni^{2} + 13.53Si - 3.47MnSi$$
(2.6)

Moreover, Kirkaldy and Barganis [7], worked on the same expression with the addition of many other alloying elements that is not included in the previous expression,

$$Ae_{3}(^{o}C) = 912 - 203C^{0.5} + 15.2Ni + 44.7Si - 104V + 31.5Mo + 13.1W - 30Mn - 11Cr - 20Cu + 700P + 400Al + 120As + 400Ti$$
(2.7)

#### 2.3.2.2 Calculation of the cementite critical temperature

Subsequently, the calculation of  $A_{Fe_3C}$  is relatively the same as  $Ac_3$ . Lusk et al. [6] also obtained an expression for the cementite critical temperature by a regression analysis on 20,000 steel grades,

$$A_{Fe_{3}C}(^{o}C) = 217.5 + 977.65C - 417.57C^{2} - 35.29Cr + 21.36CCr - 1.50Cr^{2} - 0.95Mn - 1.37CMn - 2.76Mo - .377CNi + 30.36Si - 8.10CSi + 2.58CrSi$$
(2.8)

One must note that this temperature is in out of equilibrium assumption which approximately equal to the one in equilibrium conditions.

#### 2.3.2.3 Calculation of the eutectoid critical temperature

This critical temperature also called  $Ae_1$  is the most complicated to describe. The experimental value of this temperature comes between the temperature in the equilibrium conditions and the one out of the equilibrium conditions. For that reason, Lusk et al. [6] derived three different equations based on different alloying elements:

$$Ae_{1} = \begin{cases} 726.16 + 17.27Cr - 0.39CCr - 1.97Cr^{2} \\ -11.79Mn + 3.95CrMn + 3.76Si \\ -7.46CrSi - 4.64MnSi + 18.61Si^{2} ; Ni=Mn=0 \\ 729.00 - 15.67Mn + 1.33CMn - 1.46Mn^{2} \\ -18.56Ni - 2.13MnNi + 1.65Ni^{2} + 9.15Si \\ -1.85MnSi + 6.63Si^{2} ; Cr=Mo=0 \\ 727.37 + 13.40Cr - 1.03CCr - 16.72Mn \\ +0.91CMn + 6.18CrMn - 0.64Mn^{2} \\ +3.14Mo + 1.86CrMo - 0.73MnMo \\ -13.66Ni + 0.53CNi + 1.11CrNi \\ -2.28MnNi - 0.24Ni^{2} + 6.34Si - 8.88CrSi \\ -2.34MnSi + 11.98Si^{2} ; Mn \neq 0 \end{cases}$$
(2.9)

#### 2.3.2.4 Calculation of the bainite and martensite critical temperatures

Steven and Haynes [8] proposed a formulation for the bainite starting temperature:

$$B_s(^{\circ}C) = 656 - 58C - 35Mn - 75Si - 15Ni - 34Cr - 41Mo$$
(2.10)

Furthermore, an equation was proposed by Andrews [9] to martensite starting temperature:

$$M_s(^{\circ}C) = 561 - 474C - 35Mn - 17Ni - 17Cr - 21Mo$$
(2.11)

Another formulation was proposed by Kirkaldy and Venugoplan [7] for the martensite temperature:

$$M_s(^{\circ}C) = 512 - 453C - 16.9Ni + 15Cr - 9.5Mo + 217C^2 - 71.5CMn - 67.6CCrx$$
(2.12)

## 2.3.3 Isothermal phase transformation models

Several models have been developed to study the isothermal transformation mathematically. Most of the model describe the kinetics with same basis but with some modifications. The equation on which most of the models are based is the following:

$$F_i = A_i t_j^{B_i} \tag{2.13}$$

where  $F_i$  is the fraction of he  $i^{th}$  phase, A and B are phase transformation parameters that depends on the time, and will be defined later. A more general equation is introduced to take into account the decrease in the transformation rate because of the lack of availability in the volume of nucleation:

$$\dot{F}_{i} = (1 - F_{i})^{r_{i}} B_{i} A_{i} \left(A_{i} t_{j}\right)^{n_{i}-1}$$
(2.14)

where r is the saturation parameter that depends on the temperature and the growth of the grains. This parameter can take different number that leads to different equations. The fraction of each phase is given for example by Avrami r = 1 [10] and Austin-Rickett r = 2 [11].

$$F_{i} = \begin{cases} 1 - exp\left(-A_{i}t_{j}^{B_{i}}\right) & ; r=1 \text{ (Avrami)} \\ 1 - \left(1 + A_{i}t_{j}^{B_{i}}\right)^{-1} & ; r=2 \text{ (Austin-Ricket)} \\ 1 - \left(1 + (r_{i} - 1)A_{i}t_{j}\right)^{\frac{r_{i} - 1}{B_{i}}} & ; r \neq 1 \end{cases}$$
(2.15)

If the initial conditions are not a 100% stable austenite, the equation is corrected:

$$F_{i}(t) = F_{i}^{0} + \left(F_{i}^{max} - F_{i}^{0}\right)\left(-A_{i}t_{j}^{B_{i}}\right)$$
(2.16)

where  $F_i^0$  and  $F_i^{max}$  are the initial and the equilibrium fractions.

In addition, a mathematical model of non-isothermal transformation is required to simulate the phase transformation during quenching, where each point in the sample has a different thermal history. For thermally activated transformations, the thermal history of the sample determines the state of transformation. Consider the three different thermal pathways in figure 2.7. Each path yields a different amount of product phase, even if the paths start and end at the same temperature and time.

Therefore, both temperature and time cannot be used as state variables. For that reason, a new state variable  $\beta$  that depends on the thermal path needs to be defined for the non-isothermal process. Next, an unspecified kinetic function  $G(\beta)$  is defined and the transformed part is associated with the thermal path.

$$F_i = G_i\left(\beta\right) \tag{2.17}$$

 $G(\beta)$  can be in any form of the isothermal equation of motion shown above. If the transformation mechanism is fixed for the region of interest, the new state variable can be considered proportional to the number of atomic hops. Temperature determines the mobility of atoms, and time defines the duration of the process [13].



Figure 2.7: Different thermal passes for the same start and end [12]

$$\beta = \int_0^t c_i(T)dt \tag{2.18}$$

where  $c_i(T)$  is a rate constant that depends on temperature and can be describes as,

$$c_i(T) = c_i^0 exp\left(-\frac{E_i}{RT}\right) \tag{2.19}$$

where  $c_i^0$  is an exponantial factor, E is the activation energy, and R is the gas contant. Using these equations, the rate of the transformation in terms of  $\beta$  can be written as,

$$\dot{F}_i = \frac{dG}{d\beta}\frac{d\beta}{dt} = c(T)\frac{dG}{d\beta}$$
(2.20)

Therefore,  $\beta$ , F, and T are variables of the transformation rate. This discovery introduces the concept of "additivity" first proposed by Scheil [14]. This concept was later extended to solid phase transformations by Chan [15] and then Christians [16] proposed a generalized model.

The principle of additivity has long been discussed and studied by many authors [17–21]. The general conclusion that can be drawn from these studies is that the traditional Scheil-Cahn-Christian additivity principle is not completely accurate in calculating non-isothermal kinetics from isothermal kinetics data. However, some of the cited works have improved the principle of additivity to achieve a better fit to experimental data. Most of these methods require additional experimentation. Alternatively, Lusk et al. [6] has developed a global non-additive motion model that is also integrated into the  $DANTE^{(R)}$  software.

From this point forward, the rest of the work will be using the Johnson-Mehl-Avrami-Kolmogrov (JMAK) equations to describe the kinetics of the phase transformation with the additivity principle.

#### 2.3.4 Kinetics of phase transformation

As described in the previous sections, the phase transformation must be studied out of the equilibrium conditions. Thus, the TTT diagrams are the graphs that can provide every information regarding the phases and their volume fraction. Also, there exist in the literature many mathematical equations that describes the physics of phase transformation; the most common equations used to determine the phase fraction during diffusion-controlled transformation is described by Johnson–Mehl–Avrami–Kolmogorov (JMAK) and given as follows:

$$F_i = 1 - exp(-At_i^B) \tag{2.21}$$

Where  $F_i$  is the volume fraction of the diffusion controlled phases, A, B, and  $t_j$  are determined with the help of the TTT diagrams.

$$A = -\frac{\ln(1 - F_{\theta})}{\theta^B} \tag{2.22}$$

$$B = \frac{\ln \{ \ln(1 - F_{\theta}) / \ln(1 - F_{\phi}) \}}{\ln(\theta/\phi)}$$
(2.23)

Where  $F_{\theta}$  (=0.005) and  $F_{\phi}$  (= 0.995) are the fraction at the beginning (time= $\theta$ ) and the end (time= $\phi$ ) of the transformation.  $F_{\theta}$  and  $F_{\phi}$  are calculated at each temperature, which means A and B are dependent on the temperature.

$$t_j = \Delta t_j + \left\{ -\frac{\ln(1 - F^{1-j})}{A} \right\}^{1/B}$$
(2.24)

Where  $\Delta t_j$  is the time step, and  $F^{j-1}$  is the fraction at the previous time step.

As discussed before, each phase has a range of temperature where the transformation could happen. Figure 2.8 shows an example of an eutectoid alloy, where  $T_{Ps}$  is the same as  $Ae_1$ ,  $T_{Pf}$  is the final pearlite temperature,  $T_{Ms}$ , and  $T_{Mf}$  are the start and finish temperature of martensite respectively. However, another condition must be satisfied in order to the transformation begins. As seen in figure (2.8), the cooling curve is divided into time steps, and the transformation begins when the following condition is satisfied:

$$\sum_{j=1}^{m} \frac{\Delta t_j}{\tau_j} = 1 \tag{2.25}$$



Figure 2.8: TTT diagram for eutectoid steel.

Numerically speaking, at each time step  $\theta$  is calculated which is the transformation starting time at a given temperature. If  $\theta$  is equal to the current time of the simulation, the transformation will begin which is known by the incubation time. This explains the condition in equation (2.25).

In addition, the diffusion-less transformation is described by Koistinen and Marburger (KM) [22] which calculates the volume fraction of the martensitic phase.

$$F_m = [1 - exp \{-0.011 (M_s - T_i)\}] \left(1 - \sum F_i\right)$$
(2.26)

Where  $F_m$  is the martensite volume fraction,  $M_s$  is the temperature of the beginning of the martensite phase. Equation (2.21) and (2.26), are mainly used in the model to predict the volume fraction during phase transformation, as most of the studies in literature use [4, 12, 23, 24].

Having the fraction of each phase, now we can calculate the latent heat generated by the phase transformation. Q is described as follows,

$$Q = \sum_{i} \Delta H_i \frac{\Delta F_i}{\Delta t} \tag{2.27}$$

Where  $\Delta H_i$  is the enthalpy change of the  $i^{th}$  phase. At each time step,  $\Delta F_i$  is calculated and multiplied by its corresponding enthalpy change. This will give us the latent heat at each time step.

Finally, since the latent heat is calculated, it will be added to equation (2.3) as a source term, and in addition the fraction of each phase is calculated.

## 2.3.5 Algorithm for phases calculations

The flowchart below, represents the algorithm for the phase transformation calculations. As a start, the model requires a temperature field for the solid, in addition to the updated material properties based on the temperature. The first decision the model makes, is to make sure if it is a eutectoid steel where we only have pearlite, bainite, and martensite phase, or not eutectoid where we have in addition a ferrite or a cementite phase. Moreover, we have two types of cooling: fast and slow cooling. The fast cooling means that the temperature drops very fast that it does not reach any starting point of pearlite, ferrite, or bainite phase. In this case we will only have martensite phase. The slow cooling is when the cooling curve intersects with the TTT diagram. In fact the model will check if the temperature is within the pearlite/ferrite range, and then the incubation time. If the temperature is in the good range and did not reach the incubation time, (or the cooling curve did not intersect with the TTT diagram) the pearlite or ferrite phases will not appear. Finally when the phases are calculated, the associated latent heat will be calculated, and added as a source term to the equation (2.3).

#### Algorithm 1 Phase transformation in the solid

- A. Get the temperature **T** distribution from the Fluid-Solid domain.
- B. Phase fractions calculation:

1: if 
$$T < T_{ps}$$
 then  
2: if  $\sum_{j=1}^{m} \frac{\Delta t_j}{\tau_j} = 1$  then  
3: Calculate  $F_p$   
4: else  
5: No pearlitic transformation  
6: end if  
7: else if  $T_{mf} < T < T_{ms}$  then  
8: Calculate  $F_m$   
9: end if

- C. Calculate  $\rho$ ,  $C_p$ ,  $\lambda$ , E, and  $\beta$  with respect to the temperature and phase fractions.
- D. Calculate the latent heat generated from each transformation
- E. End of time-step

## 2.4 Numerical validation

## 2.4.1 Test case 1: 1.8-m-diameter steel 2D cylinder

First test case is a 2D cylinder of 1.8 m diameter and 3 m in length tested in [25]. The cylinder is made of 28NCD6 steel with an initial temperature of 865°C. The surroundings is approximated by a constant heat transfer coefficient  $h = 1,500W.m^{-2}.K^{-1}$  with temperature of 20°C. The real quenching time is 90,000 seconds with a time-step of 1 second. An unstructured mesh is used with approximately 5,700 elements and 3,000 nodes.

Figure (2.9) shows the cooling curve of the cylinder in the core and at the surface. It is clear that in the core the cooling rate decreases at some point because of the latent heat generated from the Austenite/Ferrite transformation. The simulation have a good agreement with the reference. In addition, figure (2.10) shows the final microstructure of the material from the core to the surface. The Ferrite phase appears in a small fraction in the core, while the Bainite phase dominates between the core and the surface. The Martensite phase appears on the surface with a residual of the Austenite phase.



Figure 2.9: Temperature history in the core of the cylinder.

### 2.4.2 Test case 2: 380-mm-diameter steel 3D cylinder

In this section, a 380-mm-diameter steel cylinder as seen in figure (2.11) was simulated based on the test case found in [26]. In this work, the algorithm used



Figure 2.10: Phase distribution of the fractions along the cylinder radius.

is similar to the one introduced in the flowchart. The 1080 steel cylinder has a 750-mm-height and a mesh of 46,128 elements and 9,038 nodes, and has an initial temperature of  $850^{\circ}C$ . Figure (2.11) shows the results of the simulation at different point in the cylinder.



Figure 2.11: Temperature history of the 380-mm-cylinder.

It is clear that the pearlite phase appears as well as the latent heat generated. This could be seen in the core of the cylinder between 1,000 and 1,500 seconds of cooling where the latent heat affected the temperature. In addition, the simulation seems to be in coherence with the reference, noting that the reference is a simulation and not an experimentation.

#### 2.4.3 Test case 3: 38-mm-diameter steel 3D cylinder

This geometry is similar to the previous but with smaller dimensions. It refers to the same reference [26], and it has the same conditions as the previous one. The mesh has 43,979 elements and 8,695 nodes. Figure (2.12) shows results of the 38-mm-Cylinder quenching simulation, with a temperature history in the core and at the surface.



Figure 2.12: Temperature history of the 38-mm-cylinder.

Certainly the cooling of this work-piece is faster, it took 100 seconds approximately to reach the ambient temperature. The results are in good accordance with the reference unless at some point where we could see some difference in the cooling rate. This could be a result of some approximations done for the material properties, since in the reference article not all the information were included. One must also note that the thermal properties as the heat capacity, thermal conductivity and the density depends on both the temperature, and the phase fraction. This makes the model more complicated. The most important point is that the phase fractions are well calculated, in addition to the latent heat generation. And one final reason is that the solver used could have a different approach of the one used in the reference article. This makes the diffusion process for example different, but the most important part is that the steady-state temperature is the same for both cases.

Figure (2.13) shows each fraction distribution at the end of the quenching process. Since the cooling is very fast at the surface, most of the phase will be martensite with a residual of austenite. Figure (2.13a) shows a maximum of 0.74 as martensite



Figure 2.13: Phases fraction distribution at the end of the quenching process.

phase fraction while the remaining 0.26 are residual austenite. This is not the case in the core, the cooling rate is slower which will cause a pearlite transformation as it is clear in figure (2.13c). The intermediate phase, bainite, can be barely seen in figure (2.13b) between the martensite and the pearlite phases.

These results confirm that the model is well calculating the phases and the latent heat. The model also can handle different types of steel. In other words, if the steel is not eutectoid, a ferrite fraction may appear. The generalized model was tested on this same test case, using different material that includes ferrite in its microstructure. This could be shown in figure (2.14) where the pearlite phase is mixed with ferrite in the core. To note that the martensite and bainite distributions are almost the same.



Figure 2.14: Phases fraction distribution at the end of the quenching process with ferrite.

## 2.5 Conclusion

The phase transformation in steels was presented in this section. It was shown the importance of this process in quenching, and its effect on the cooling process. In addition, a numerical model was presented to simulate the transformation of each phase during the quenching based on mathematical equations. Finally, 2D and 3D numerical test cases were presented to validate this model. Indeed the phase transformation has a major effect on the cooling rate, it also affects the mechanical response which another phenomena happening in the solid. In the following section the thermo-elasto-plastic model is presented that decribes the mechanical behaviour of the solid during quenching.

## 2.6 Résumé en français

Le chapitre 2, portant sur l'analyse thermique avec transformation de phase, en particulier dans les aciers inoxydables, est composé de trois parties. Les différentes transformations de phases possibles sont d'abord décrites, en fonction du cycle thermique et de la teneur en carbone. Ensuite, partant d'une formulation en température de la loi de conservation de l'énergie, la chaleur latente dégagée par une transformations thermiquement activées (ce qui est le cas durant la trempe), ce terme source dépend de la fraction volumique de chaque phase impliquée dans la transformation, évaluée le long du chemin thermique considéré. Cette cinétique de transformation est décrite ici par un modèle de type JMAK. Enfin, trois cas tests (1 en 2D, 2 en 3D) de simulation du refroidissement d'un cylindre avec transformation de phase sont présentés et comparés à des simulations équivalentes de la littérature. Des profiles de température comparables sont trouvés, ainsi qu'une répartition des phases en cohérence avec les températures critiques établies pour chaque transformation.

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## Chapter 3

## Thermo-elasto-plastic treatment

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## 3.1 Introduction

The second physical phenomena happening in the solid is the mechanical response as seen in figure (3.1). Although the quenching process does not require applying forces on the solid, the high temperature gradients cause many geometrical changes in the solid [1]. Here comes the importance of developing a solid solver that can handle complex industrial geometries. The deformation vector in this application can be partitioned into different types of deformations: elastic, plastic, thermal, and phase transformation deformations. During quenching, the solid passes through different stages of cooling, the solid can reach very low temperatures at the surface while still at high temperature in the core. This difference in temperature can cause a significant thermal deformation; in addition, the plasticity limit changes with temperature, which makes the solid in a plastic regime. Since the temperature change, the phase transformation, and the mechanical response are all connected as described in figure (1.3), the appearance of new phases due to temperature change can cause in a local deformation due to that change.



Figure 3.1: Mechanical response part of the full framework

At the macroscopic scale, we assimilate quenched metals, occupying a finite domain, to a continuous and homogeneous medium. The mathematical model of the problem is therefore based on the fundamental equations of the mechanics of continuous mediums, namely the mass conservation equation and the dynamic equilibrium equation. For the problem to be correctly posed, equations relating to the boundary conditions are introduced. Finally, in order to model the mechanisms governing the thermo-elasto-plastic strain along with the phase transformation in the material, constitutive law equations are also added. These allow for example to link the stresses to the deformation rates during the flow of the material.

In the following sections we will introduce first the elastic model, and then we introduce the plasticity to this model. Afterwards, the thermal and the phase transformation deformations will be added to the model. Numerical examples and benchmarks will be added to validate every step of the model.

### 3.2 Elasticity

A solid under a deforming force, passes through different stages of deformation. The first stage is the elastic deformation, where the solid is not permanently deformed, if the force is removed then it will go back to its initial state. Such solver is important for many applications as the electrical wire behavior [2], the dynamics of the elastic shock in materials [3], or bio-medical applications that usually include complex shapes.

A general solid solver with the displacement as an unknown field, and all other quantities as stress, strain, pressure ... are calculated with post-processing approach [4, 5]. However, this model has a poor performance for material near the incompressibility limit. Some problems appears when dealing with such method as locking, unstable pressure fields, and weak performance in bending applications [6].

This subject has seen a significant portion of development aimed at relaxing or removing the above restrictions. For ease of implementation, selective and reduced integral methods such as B-bar [6-8], F-bar [9-12], and mean expansion finite element method [13] are used. These methods avoid the numerical instability of the inf-sup or Ladyzhenskaya-Babuska-Brezzi (LBB) conditions by reducing the incompressible order at the quadrature point [14]. These proposed solutions are accurate for structured quadrilateral and hexahedral meshes that requires a two times higher computing time than the unstructured tetrahedral elements [15].

Considering the case of static and incompressible elasticity, we get an elliptic equation similar to the Stokes problem of fluid mechanics, but in the transient case, that is, elastic dynamics is a hyperbolic equation. Given the similarity of the equations, it is common to extend the velocitiy/pressure mixed/coupled formulation of the Stokes problem [16], to the displacement/pressure mixed formulation of the

static elasticity [17]. This development acts as a link between the various methods already implemented in fluid mechanics and the field of solids mechanics.

A steady-state incompressible linear elastic solid was modeled in [18] using a displacement/pressure mixed formulation with the Orthogonal Sub Scale approach (OSS) [19], showed high capabilities in the incompressible limit. In [20, 21], inconpressible non-linear materials were also modeled using the OSS method. This work shows the potential of a strain/displacement or stress/displacement mixed formulation. However, there is an agreement between the accuracy and the computational cost. Also, a three unknown formulation (displacement/strain/pressure) was tested in [22] and found to be accurate and effective in the region near the incompressible limit.

Most of the previous formulations were established for a steady-state problems, and it was mentioned that the transient elasto-dynamics is an elliptic problem instead of a parabolic one because of the second order displacement derivative of the momentum equations. This issue was focused on in different works in the literature.

Part of this work involves [23–26], where the finite strain non-linear solid dynamics solver is based on a new form of linear equations in the Lagrange framework. This procedure consists of introducing a new variable **F** that stands for the deformation gradient, and Lagrange multiplier for the angular momentum conservation if needed. The results shows a second order accuracy in stress. Furthermore, a new variable J was introduced in the bending related and in the incompressibility problems, which represents the Jacobian determinant of the deformation gradient [27, 28]. In recent studies [29–31],  $\mathbf{H} = cof$  : **F** is added, which is a nodel co-factor tensor. This method, like the other methods in the F node interpolation-based method family, is inherently unstable. Therefore, a streamline Upwind/Petrov-Galerkin (SUPG) stabilization method with penalties on the deformation gradient was used. Testing demonstrates the ability of this methodology to solve the problem of incompressible limits, but it is expensive because of the number of unknown per node.

Subsequently, a velocity/pressure mixed formulation is presented in [15, 32] where the displacement field is calculated from the velocity discretization. The authors argue that the Variational Multi-Scale (VMS) method is inadequate to stabilize the transient part of the problem. They solved the problem using a pressure rate equation, which they called the Dynamic Variational Multi-Scale (D-VMS). The tests have also proven to be robust and accurate. In [33], a mixed displacement/pressure formulation in a total Lagragian framework was presented in several variations of the VMS approach. This method has also proven to be accurate and robust.

The work in [34] presents the displacement/pressure finite elements formulation for nearly incompressible materials. Variational Multi-scale with two types of error estimators were used, and the formula was examined in various numerical convergence tests.

In the following sections, a new non-linear elastodynamic model developed in [35] will be presented and used for the advancement of this work. This model can solve elasticity for unstructured terahedral mesh with complex shapes and an acceptable computational cost. This proposed displacement/pressure mixed formulation is used with the split of the stress tensor into a deviatoric and a volumetric parts [36]. The momentum equation is supplemented by the constitutive pressure equation. Also this model proposes a fully implicit mixed displacement/pressure formulation in an updated Lagrangian framework. The resulting set of equations is susceptible to unstable pressure fields. The variational Multi-Scale (VMS) stabilization method was implemented to this model to ensure a high fidelity solver. The framework is combined with the moving mesh method, so the mesh follows the body of the updated Lagrange framework. In addition, this model will be extended to solve plastic, thermal, and phase transformation deformation and stresses.

More details on the governing equations and the stabilization method with numerical validation will be presented in the following sections of this chapter.

#### 3.2.1 Solid dynamics in Lagrange space

The Lagrangian solid dynamics equations governs the changing rate of density and the displacement of solid. The initial and current domains  $\Omega_0$  and  $\Omega$  respectively are two open sets in  $\mathbb{R}^d$  with Lipshitz boundaries, where d is the spatial dimension.  $\Gamma$  denotes the boundary of the problem, and split into two sets  $\Gamma = \overline{\partial \Omega_u \cup \partial \Omega_t}$  and  $\partial \Omega_u \cap \partial \Omega_t = \emptyset$ , where  $\Omega$  is the Dirichlet boundary condition for the displacement, and  $\Omega_t$  is the Nuemann boundary condition for the traction force. The motion of a body under deformation is given by:

$$\boldsymbol{\phi}: \Omega_0 \to \Omega = \boldsymbol{\phi}\left(\Omega_0\right),\tag{3.1}$$

$$\boldsymbol{\phi}: \Gamma_0 \to \Gamma = \boldsymbol{\phi} \left( \Gamma_0 \right), \tag{3.2}$$

$$\mathbf{X} \mapsto \mathbf{x} = \boldsymbol{\phi} \left( \mathbf{X}, t \right). \tag{3.3}$$

This represents a material coordinate mapping  $\mathbf{X}$  in the total Lagrangian framework of the infinitesimal solid particle, to  $\mathbf{x}$ , the same particle coordinate but in updated Lagragian framework.  $\boldsymbol{\phi}$  is considered invertible and smooth.  $J = det \mathbf{F}$ and  $\mathbf{F} = \nabla_{\mathbf{X}} \boldsymbol{\phi}$  are the Jacobian and the deformation gradient respectively, and the solid displacement is given by:  $\mathbf{u} = \mathbf{x} - \mathbf{X}$ .

The governing are given by:

$$\rho \ddot{\mathbf{u}} - \nabla \boldsymbol{\sigma} = \boldsymbol{f} \quad in \ \Omega, \tag{3.4}$$

$$\rho J = \rho_0 \quad on \ \partial \Omega_u \tag{3.5}$$

where  $\rho_0$  and  $\rho$  are the initial and current body density respectively, f is the forcing term,  $\sigma$  is the symmetric Cauchy-stress tensor,  $\ddot{\mathbf{u}}$  is the material second derivative for the displacement, and also the acceleration.

This mixed formulation of displacement/pressure with the decomposition of the stress tensor into a deviatoric and a volumetric part describe how the model works. The decomposition of the stress tensor is essential especially when we are working with nearly incompressible or fully incompressible materials. Also, this decomposition is done only because the material is considered isotropic. Hence, the stress tensor is given by:

$$\boldsymbol{\sigma} = p\boldsymbol{I} + dev\left[\boldsymbol{\sigma}\right] \tag{3.6}$$

where  $\boldsymbol{I}$  is the identity matrix.

To complete the system of equations, initial and boundary conditions are necessary. We assume first that the body had no displacement at the beginning of the simulation which makes  $\mathbf{u}(\mathbf{X}, 0) = \mathbf{u}_0 = 0$ . This leads to  $\boldsymbol{\phi}(\mathbf{X}, 0) = \mathbf{X}, \mathbf{F}|_{t=0} = \mathbf{I}$ , and  $J|_{t=0} = 1$ . A stress free assumption is considered at t = 0. Below are the boundary conditions:

$$\mathbf{u}|_{\Gamma_{\mathbf{u}}} = \boldsymbol{u}_d\left(\boldsymbol{x}, t\right), \tag{3.7}$$

$$\boldsymbol{\sigma}\boldsymbol{n}|_{\Gamma_t} = \boldsymbol{t}\left(\boldsymbol{x}, t\right) \tag{3.8}$$

where  $\boldsymbol{n}$  is the outward normal on  $\Gamma$ .

#### 3.2.2 Linear elastic equations

Assuming very small body displacement, Hook's law can be applied to describe the elastic behavior. The solid is considered as a spring with a linear correlation between the stress and strain while the slope is the Young's modulus of the material. First, the steady-state interpretation will be presented, and then the transient one is developed.

#### 3.2.2.1 Steady-state interpretation

The steady-state formulation is a development of the Stokes equations with **u** as a leading variable instead of the velocity. This change in equations will be a better explanation to the stabilization technique that will be used. For a linear elastic problem,  $\mathbf{x} \approx \mathbf{X}$ ,  $\Omega_0 \approx \Omega$ ,  $\nabla_{\mathbf{X}} \approx \nabla_{\mathbf{x}}$ , and  $\rho_0 = \rho$ . As mentioned before this model is based on the decomposition of the stress tensor, and this was done using the two unknown variable of the problem: the displacement  $\mathbf{u}$  and the hydro-static pressure p. So the stress tensor becomes:

$$\boldsymbol{\sigma} = p\boldsymbol{I} + 2\mu dev \left[\nabla^s \mathbf{u}\right],\tag{3.9}$$

$$p = K\epsilon_v, \tag{3.10}$$

$$\epsilon_v = \nabla.\mathbf{u}.\tag{3.11}$$

Where  $\epsilon_v$  is the volumetric strain, and  $\nabla^s$  is the symmetrical gradient operator given by:

$$\nabla^s = \frac{1}{2} \left( \nabla + \nabla^T \right) \tag{3.12}$$

Also  $\mu$  is one of the Lamé constants, which is also called shear modulus of the material and K is the bulk modulus which is also called modulus of volumetric compressibility and they both are expressed by:

$$\mu = \frac{E}{2(1+\nu)},$$
(3.13)

$$K = \frac{1}{3} \frac{E}{(1 - 2\nu)}.$$
(3.14)

Having all the expression needed as the stress tensor and the boundary conditions, the system of equations for the steady-state problem can be written as follows:

$$\begin{cases} -\nabla p - 2\mu \nabla .dev \left[\nabla^{s} \mathbf{u}\right] = \boldsymbol{f} & \text{in } \Omega, \\ \nabla \mathbf{u} - \frac{1}{K} p = 0 & \text{in } \Omega, \\ \boldsymbol{\sigma}. \boldsymbol{n} = \boldsymbol{t} & \text{on } \partial \Omega_{t}, \\ \mathbf{u} = 0 & \text{on } \partial \Omega_{u}, \\ \rho J = \rho_{0} & \text{in } \Omega. \end{cases}$$
(3.15)

This set of equation can interpret both compressible and incompressible materials. With  $K \to \infty$  and a constant density, the material will be incompressible, and the second equation in 3.15 becomes:

$$\nabla \mathbf{u} = 0 \quad in \ \Omega. \tag{3.16}$$

It can also be interpreted as an isohoric phenomena by implying  $\epsilon_v = 0$  which gives the same results.

The variational form of these equations is given by:

$$a\left(\mathbf{u},\mathbf{w}\right) + \left(p,\nabla,\mathbf{w}\right) = L\left(\mathbf{w}\right) \forall \mathbf{w} \in W_0 \subset \left[H_0^1\right]^d, \qquad (3.17)$$

$$(\nabla \mathbf{.u}, q) - \left(\frac{1}{K}p, q\right) = 0 \forall q \in \mathcal{Q} \subset L^2_{\int = 0}$$
(3.18)

where  $a(\mathbf{u}, \mathbf{w})$  and  $L(\mathbf{w})$  are given by:

$$a\left(\mathbf{u},\mathbf{w}\right) = \int_{\Omega} 2\mu dev\left[\nabla^{s}\mathbf{u}\right] : \nabla^{s}\mathbf{w}d\Omega, \qquad (3.19)$$

$$L(\mathbf{w}) = \int_{\Omega} \boldsymbol{f} \cdot \boldsymbol{w} d\Omega + \int_{\partial \Omega_t} \boldsymbol{w} \cdot \boldsymbol{t} d\Gamma, \qquad (3.20)$$

Where (.,.) is the  $L^2$  inner product. Thus, the discrete formulation of the equations is:

$$a\left(\mathbf{u}_{h},\mathbf{w}_{h}\right)+\left(p_{h},\nabla.\mathbf{w}_{h}\right)=L\left(\mathbf{w}_{h}\right)\forall\boldsymbol{w}_{h}\in W_{h,0},$$
(3.21)

$$\left(\nabla \cdot \mathbf{u}_h, q_h\right) - \left(\frac{1}{K}p_h, q_h\right) = 0 \forall q_h \in \mathcal{Q}_h, \qquad (3.22)$$

where the subscript h indicate the discrete form of the variable.

When using the Babuska-Brezzi stability, which is also called inf-sup [14], the interpolation relation between the two fields is constrained, hence compelling different interpolations for p and u. For that reason, having equal order of interpolation for both fields shows a poor performance since the condition is not respected. Since in this application P1/P1 elements were used, various stabilization types exists. The Variational Multi-Scale method (VMS) is one of stabilization method that enables the same order interpolation. Some of the works in the literature used the VMS with equal order interpolation and they showed a proof of convergence with stability, as in [16] the VMS was applied to the Stokes equations. Later it was used for Navier-Stokes equation as in [37], as well as in linear elastic model as in [17, 38]. The VMS approach consists of applying an orthogonal decomposition of the fields (pressure and displacement) which gives a natural stabilization. This decomposition of the solution spaces is described below:

$$W_0 = W_{h,0} + W'_0, (3.23)$$

$$W = W_h + W', (3.24)$$

$$\mathcal{Q} = \mathcal{Q}_h + \mathcal{Q}',\tag{3.25}$$

As described in [19] there are two scale components: fine and coarse scale for the pressure and the displacement and they are given by:

$$\mathbf{u} = \mathbf{u}_h + \mathbf{u}',\tag{3.26}$$

$$p = p_h + p'. \tag{3.27}$$

The same decomposition is also applied on the weighing functions:

$$\mathbf{w} = \mathbf{w}_h + \mathbf{w}',\tag{3.28}$$

$$q = q_h + q'. \tag{3.29}$$

Two sets division was made on equations (3.21) and (3.22): the course and the fine scale. The unresolved fine scales are modeled with respect to the residual based terms. they are solved in an approximate matter with static condensation, and re-added in the coarse scale equations. Hence, additional terms will appear which they are corrected by a local stabilization parameter. The enhancement of stability, the reduction of oscillation in the pressure field, and the increase in accuracy of the standard Galerkin formulation come from these additional terms. The fine scale problem is solved and it is represented on the sum of the interior of the elements [39], with a formulation with respect to the transient coarse scale variables. The fine scale variables are given by:

$$\mathbf{u}' = \sum_{T_h} \left( \tau_{\mathbf{u}} P'_{\mathbf{u}} \left( R_{\mathbf{u}} \right) \right), \qquad (3.30)$$

$$p' = \sum_{T_c} \left( \tau_c P'_c(R_c) \right),$$
 (3.31)

where  $R_{\mathbf{u}}$  and  $R_c$  are the residuals from the finite element resolution,  $P'_{\mathbf{u}}$  and  $P'_c$  are the projection operators, and  $\tau_{\mathbf{u}}$  and  $\tau_c$  the tuning parameters.

As mentioned before, the fine scale parameters will be added to the coarse scale problem, which gives us a new variational form of the problem with the coarse scale:

$$a\left(\left(\mathbf{u}_{h}+\mathbf{u}'\right),\mathbf{w}_{h}\right)+\left(\left(p_{h}+p'\right),\nabla.\mathbf{w}_{h}\right)=L\left(\mathbf{w}_{h}\right)\forall\boldsymbol{w}_{h}\in W_{h,0},\qquad(3.32)$$

$$\left(\nabla \left(\mathbf{u}_{h}+\mathbf{u}'\right),q_{h}\right)-\left(\frac{1}{K}\left(p_{h}+p'\right),q_{h}\right)=0\forall q_{h}\in\mathcal{Q}_{h},$$
(3.33)

and the variational form of the fine scale:

$$a\left(\left(\mathbf{u}_{h}+\mathbf{u}'\right),\mathbf{w}'\right)+\left(p',\nabla,\mathbf{w}'\right)=L\left(\mathbf{w}'\right)\forall\boldsymbol{w}'\in W_{0}',$$
(3.34)

$$\left(\nabla \cdot \left(\mathbf{u}_{h} + \mathbf{u}'\right), q'\right) - \left(\frac{1}{K}p_{h}, q'\right) = 0 \forall q' \in \mathcal{Q}'.$$
(3.35)

Assuming that the sub-scale are quasi static, and solving the fine scale equation with respect to the initial residual, and re-integrating in the coarse scale equation, we can finally get the set of coarse scale equations with the stabilization term for the pressure in the linear elastic problem. The equations are described below:

$$a\left(\mathbf{u}_{h},\mathbf{w}_{h}\right)+\left(p_{h},\nabla.\mathbf{w}_{h}\right)+\sum_{K\in T_{h}}\left(\tau_{\mathbf{c}}R_{c},\nabla_{x}.\mathbf{w}_{h}\right)=L\left(\mathbf{w}_{h}\right)\forall\boldsymbol{w}_{h}\in W_{h,0},\qquad(3.36)$$

$$\left(\nabla \mathbf{u}_{h}, q_{h}\right) - \left(\frac{1}{K}p_{h}, q_{h}\right) - \sum_{K \in T_{h}}\left(\tau_{\mathbf{u}}R\left(\mathbf{u}_{h}\right), \nabla q_{h}\right) = 0 \forall q_{h} \in \mathcal{Q}_{h}, \quad (3.37)$$

$$R(\mathbf{u}_{h}) = \mathbf{f} + \nabla p_{h} + 2\mu \nabla .dev \left[\nabla^{s} \mathbf{u}_{h}\right].$$
(3.38)

$$R_c = \frac{1}{K} p_h - \nabla_x \mathbf{u}. \tag{3.39}$$

where  $R(\mathbf{u}_h)$  is the finite elements residual, and  $\tau_{\mathbf{u}}$  is a parameter coming from the study of stabilization parameters response that come from Fourier study of the problem for the sub-scales [20].

If we compare the standard equations with the stabilized ones we can see additional integrals that are evaluated element-wise. These integrals are the sub-grid scales representation, and they help to get a more stable solution, and less oscillations in the pressure field.

#### 3.2.2.2 Transient interpretation

At this point, we can see the first difference between the transient linear elasticity equations and the Stokes equations. As a matter of fact, in Stokes equations the velocity is the primary unknown which requires a first order derivative to get the inertia term. However, the primary unknown for transient linear elastic equation is the displacement  $\mathbf{u}$  which requires a double derivative to solve the transient problem. The transient form of the Stokes equation is parabolic, while in the linear elastic equation is parabolic, while in the linear elastic equation is parabolic.

the case when we deal with solids near the incompressibility limit. In addition, the pressure is considered a Lagrange multiplier and it is essential for the divergence-free constraint of  $\mathbf{u}$ . The governing equations for the transient linear elasticity is expressed as follows:

$$\begin{cases} \rho \ddot{\mathbf{u}} - \nabla p - 2\mu \nabla .dev \left[\nabla^{s} \mathbf{u}\right] = \boldsymbol{f} & \text{in } \Omega, \\ \nabla \mathbf{u} - \frac{1}{K} p = 0 & \text{in } \Omega, \\ \boldsymbol{\sigma} . \boldsymbol{n} = \boldsymbol{t} & \text{on } \partial \Omega_{t}, \\ \mathbf{u} = 0 & \text{on } \partial \Omega_{u}. \end{cases}$$
(3.40)

Because of the Courant-Friedrichs-Lewy (CFL) condition, the time-step should have a small value for better results, especially for explicit time integrator. Consider  $t \in [0, T]$  which is the time interval, and a division into N time-steps of equal intervals  $\Delta t$ . This work adopted a Backward differential formula (BDF). The first and second order accurate BDFs are adopted and given by:

$$\boldsymbol{a}^{n+1} \approx \frac{1}{\Delta t^2} \left( \mathbf{u}^{n+1} - 2\mathbf{u}^n + \mathbf{u}^{n-1} \right) + O\left(\Delta t\right), \qquad (3.41)$$

$$a^{n+1} \approx \frac{1}{\Delta t^2} \left( 2\mathbf{u}^{n+1} - 5\mathbf{u}^n + 4\mathbf{u}^{n-1} - \mathbf{u}^{n-2} \right) + O\left(\Delta t^2\right).$$
 (3.42)

where a is the acceleration. The BDFs are common for high frequency dissipation, which is responsible of removing oscillations.

Finally the discrete-stabilized-variational formulation of the transient linear elastic equations, following the same procedure in the previous section [16, 38], is given by:

$$(\rho \ddot{\mathbf{u}}, \mathbf{w}_h) + a\left(\mathbf{u}_h, \mathbf{w}_h\right) + (p_h, \nabla \cdot \mathbf{w}_h) + \sum_{K \in T_h} \left(\tau_{\mathbf{c}} R_c, \nabla_x \cdot \mathbf{w}_h\right) = L\left(\mathbf{w}_h\right) \forall \boldsymbol{w}_h \in W_{h,0},$$
(3.43)

$$\left(\nabla \mathbf{u}_{h}, q_{h}\right) - \left(\frac{1}{K}p_{h}, q_{h}\right) - \sum_{K \in T_{h}}\left(\tau_{\mathbf{u}}R\left(\mathbf{u}_{h}\right), \nabla q_{h}\right) = 0 \forall q_{h} \in \mathcal{Q}_{h}, \quad (3.44)$$

$$R(\mathbf{u}_{h}) = \boldsymbol{f} - \rho \ddot{\mathbf{u}} + \nabla p_{h} + 2\mu \nabla .dev \left[\nabla^{s} \mathbf{u}_{h}\right].$$
(3.45)

Where  $R(\mathbf{u}_h)$  is the updated finite element residual. The additional parameters that damp out the oscillation are the same as the previous equations.

## 3.2.3 Lagrange formulation for non-linear transient elasticity

#### 3.2.3.1 Hyper-elastic model

For a near real life behavior, it is better to model the elasticity with a non-linear formulation. Considering a non-linear solid with the Helmholtz free or the strain energy  $\Psi(\mathbf{C})$  function, with  $\mathbf{C}$  being the right Cauchy-Green strain tensor given by:  $\mathbf{C} = \mathbf{F}^T \mathbf{F}$ .  $\mathbf{F}$  is the gradient of deformation:  $\mathbf{F}_{ij} = x_{i,j} = \frac{\partial x_i}{\partial X_j}$ . We also have the Piola-Kirchhoff stress tensor given by:  $\mathbf{S} = J \mathbf{F}^{-1} \boldsymbol{\sigma} \mathbf{F}^{-T}$  with J the Jacobian determinant of  $\mathbf{F}$ , which is a derivative of  $\Psi(\mathbf{C})$  with respect to  $\mathbf{C}$ :

$$\boldsymbol{S} = 2\partial_{\boldsymbol{C}}\boldsymbol{\Psi}\left(\boldsymbol{C}\right). \tag{3.46}$$

As it is done before,  $\Psi(C)$  will be decomposed into a volumetric and a deviatoric part to take into account the compressibility and the incompressibility:

$$\Psi(\boldsymbol{C}) = \mathrm{U}(J) + \mathrm{W}(\bar{\boldsymbol{C}}). \qquad (3.47)$$

with  $\overline{C}$  being the deviatoric-volume-preserving part of C, and  $J = \sqrt{detC}$ .

The Helmholtz free energy for isotropic hyper-elastic models is given with respect to the strain invariant. If we consider a Neo-Hookean elastic solid, with a Simo-Taylor volumetric model [40]:

$$U(J) = \frac{1}{4}\kappa \left(J^2 - 1\right) - \frac{1}{2}\kappa lnJ,$$
(3.48)

W 
$$(\bar{C}) = \frac{1}{2}\mu (tr\bar{C} - 3) = \frac{1}{2}\mu (\bar{I}_1 - 3).$$
 (3.49)

where  $\kappa$  and  $\mu$  are material properties, and  $I_1 = tr\bar{C}$ . If we consider small displacement,  $\mu$  and  $\kappa$  are the shear and bulk modulus of the material, and the model will be linear. We can also split the stress tensor into a volumetric and deviatoric part:

$$p = 2J^{-1} \boldsymbol{F} \frac{\partial U(J)}{\partial \boldsymbol{C}} \boldsymbol{F}^{T} = U'(J) = \frac{1}{2} \kappa \left( J + J^{-1} \right), \qquad (3.50)$$

$$dev\left[\boldsymbol{\sigma}\right] = 2J^{-1}\boldsymbol{F}\frac{\partial W\left(\bar{\boldsymbol{C}}\right)}{\partial \boldsymbol{C}}\boldsymbol{F}^{T} = \mu J^{-\frac{5}{3}}dev\left[\boldsymbol{F}\boldsymbol{F}^{T}\right].$$
(3.51)

We recall that F is the gradient of deformation and given by  $F = \nabla_{\mathbf{X}} \mathbf{u} + I$ , hence:

$$\boldsymbol{F}\boldsymbol{F}^{T} = \nabla_{\mathbf{X}}\mathbf{u} + \nabla_{\mathbf{X}}^{T}\mathbf{u} + \nabla_{\mathbf{X}}\mathbf{u}\nabla_{\mathbf{X}}^{T}\mathbf{u} + \boldsymbol{I}.$$
(3.52)

As a reminder, all the previously presented equation were solved in an updated Lagrangian regime, while these equation are in the Total Lagragian framework. If we consider the following relation:

$$\nabla_{\mathbf{X}}\mathbf{u} = (\boldsymbol{I} - \nabla \mathbf{u})^{-1} - \boldsymbol{I}, \qquad (3.53)$$

and we also consider a very small increment in the deformation field noted as  $\delta \mathbf{u}$ , we can assume that  $(\mathbf{I} - \nabla \mathbf{u})^{-1} = \mathbf{I} + \nabla \mathbf{u}$ , and we get:

Finally, the system of equations is given by:

$$\begin{cases} \rho \ddot{\mathbf{u}} - \nabla_x p - \nabla_x . dev \left[\boldsymbol{\sigma}\right] = \boldsymbol{f} & \text{in } \Omega, \\ \nabla_x \mathbf{u} - \frac{1}{K} p = g & \text{in } \Omega, \\ \boldsymbol{\sigma} . \boldsymbol{n} = \boldsymbol{t} & \text{on } \partial \Omega_t, \\ \mathbf{u} = 0 & \text{on } \partial \Omega_u. \\ \rho J = \rho_0 & \text{in } \Omega. \end{cases}$$
(3.55)

Where  $\ddot{\mathbf{u}}$  is acceleration and also called the material derivative of  $\mathbf{u}$ , and given by:

$$a = \dot{\mathbf{v}} = \ddot{\mathbf{u}} = \frac{\partial \mathbf{v}}{\partial t} + \nabla_x \left( \mathbf{v} \right) \cdot \left( \mathbf{v} - \mathbf{v}_{domain} \right) = \frac{\partial^2 \mathbf{u}}{\partial t^2} + \nabla_x \left( \frac{\mathbf{u} - \mathbf{u}^-}{\Delta t} \right) \cdot \left( \mathbf{v} - \mathbf{v}_{domain} \right) .$$
(3.56)

If we substitute in the first equation in (3.55), we get:

$$\rho\left(\frac{\partial^2 \mathbf{u}}{\partial t^2} + \nabla_x \left(\frac{\mathbf{u} - \mathbf{u}^-}{\Delta t}\right) \cdot \left(\mathbf{v} - \mathbf{v}_{domain}\right)\right) - \nabla_x p - \nabla_x dev\left[\boldsymbol{\sigma}\right] = \boldsymbol{f} \quad in \ \Omega. \quad (3.57)$$

#### 3.2.3.2 Variational Multi-scale stabilization method

For the hyper-elastic equations, the VMS stabilization method was also applied with the same Orthogonal Sub-Scale decomposition of spaces as done in (3.23) (3.24) (3.25). Also, the resovable coarse and the unresolved fine scale decomposition was made as in (3.26) (3.27), and the same for the weighing functions as in (3.28) (3.29). Hence, the transient mixed formulation of the hyper-elastic solution is described in the following equations:

Coarse Scale

$$\left(\rho \frac{\partial^2 \left(\mathbf{u} + \mathbf{u}'\right)}{\partial t^2}, \mathbf{w}_h\right) + a\left(\left(\mathbf{u} + \mathbf{u}'\right), \mathbf{w}_h\right) + \left(p_h + p', \nabla_x \cdot \mathbf{w}_h\right) = L\left(\mathbf{w}_h\right) \forall \mathbf{w}_h \in W_{h,0},$$
(3.58)

$$\left(\nabla_{x}.\left(\mathbf{u}_{h}+\mathbf{u}'\right),q_{h}\right)-\left(\frac{1}{K}\left(p_{h}+p'\right),q_{h}\right)=\left(g,q_{h}\right)\forall q_{h}\in\mathcal{Q}_{h},\qquad(3.59)$$

Fine Scale

$$\left(\rho \frac{\partial^2 \left(\mathbf{u} + \mathbf{u}'\right)}{\partial t^2}, \mathbf{w}'\right) + a\left(\left(\mathbf{u} + \mathbf{u}'\right), \mathbf{w}'\right) + \left(p_h + p', \nabla_x \cdot \mathbf{w}'\right) = L\left(\mathbf{w}'\right) \forall \mathbf{w}' \in W', \quad (3.60)$$

$$\left(\nabla_{x}.\left(\mathbf{u}_{h}+\mathbf{u}'\right),q'\right)-\left(\frac{1}{K}\left(p_{h}+p'\right),q'\right)=\left(g,q'\right)\forall q'\in\mathcal{Q}',$$
(3.61)

The same procedure done before, where the fine scale are resolved and re-injected in the coarse scale equation, is also done here. An essential remark to take into consideration is that the sub-scales are not followed in time, this interpretation is detailed in [41]. Besides, there is a quasi-dependence on time for the sub-scales because of the time dependency of the large scale residual. More information can be found in [42]. Thus, the coarse scale equations are as follows:

$$\left(\rho \frac{\partial^2 \mathbf{u}}{\partial t^2}, \mathbf{w}_h\right) + a'\left(\mathbf{u}, \mathbf{w}_h\right) + \left(p_h, \nabla_x \cdot \mathbf{w}_h\right) + \sum_{K \in T_h} \left(p', \nabla_x \cdot \mathbf{w}_h\right) = L\left(\mathbf{w}_h\right) \forall \mathbf{w}_h \in W_{h,0},$$
(3.62)

$$\left(\nabla_{x}.\mathbf{u}_{h},q_{h}\right) - \left(\frac{1}{K}p_{h},q_{h}\right) - \sum_{K\in T_{h}}\left(\frac{1}{K}p',q_{h}\right) - \sum_{K\in T_{h}}\left(u',\nabla_{x}q_{h}\right) = (g,q_{h})\,\forall q_{h}\in\mathcal{Q}_{h}.$$
(3.63)

The residual from the finite elements is given by:

$$R\left(\mathbf{u}\right) = \boldsymbol{f} - \rho \ddot{\mathbf{u}} + \nabla_x p_h + \nabla_x dev \left[\boldsymbol{\sigma}\right], \qquad (3.64)$$

$$R(p_h) = g - \nabla_x \mathbf{u} + \frac{1}{K} p_h. \tag{3.65}$$

Finally, as in equations (3.34) (3.34), the fine scales are modeled and we get:

$$\begin{pmatrix} \rho \frac{\partial^2 \mathbf{u}}{\partial t^2}, \mathbf{w}_h \end{pmatrix} + a \left( \mathbf{u}, \mathbf{w}_h \right) + \left( p_h, \nabla_x \cdot \mathbf{w}_h \right) + \sum_{K \in T_h} \left( \tau_c \left( g - \nabla_x \cdot \mathbf{u}_h + \frac{1}{K} p_h \right), \nabla_x \cdot \mathbf{w}_h \right)$$
  
=  $L \left( \mathbf{w}_h \right) \forall \mathbf{w}_h \in W_{h,0},$ (3.66)

$$(\nabla_{x}.\mathbf{u}_{h},q_{h}) - \left(\frac{1}{K}p_{h},q_{h}\right) + \sum_{K\in T_{h}} \left(\frac{\tau_{c}}{K}\left(\nabla_{x}.\mathbf{u}_{h} - \frac{1}{K}p_{h} - g\right),q_{h}\right) + \sum_{K\in T_{h}} \left(\tau_{u}\left(\rho\ddot{\mathbf{u}}_{h} - \nabla_{x}p_{h} - \nabla_{x}.dev\left[\boldsymbol{\sigma}\right] - \boldsymbol{f}\right),\nabla_{x}q_{h}\right) = (g,q_{h})\,\forall q_{h}\in\mathcal{Q}_{h}.$$
(3.67)

If we compare the standard equations (Galerkin), and the previous stabilized equation, with the ones above, we can see additional integrals that are evaluated element-wise. These integrals are the sub-grid scales representation, and they also help to get a more stable solution, and less oscillations in the pressure field. In addition, they take into account both incompressible and compressible problems. In [43, 44] a general definition of these parameters is presented, and they are given by:

$$\tau_u(K) = \left( \left( \frac{\rho}{(c_0 \Delta t)^2} \right)^2 + \left( \frac{2\mu}{c_1 h_k^2} \right)^2 \right)^{-\frac{1}{2}}, \qquad (3.68)$$

$$\tau_c(K) = \left( (2c_2\mu)^2 \right)^{-\frac{1}{2}},$$
(3.69)

where  $h_k$  is the characteristic length of the elements, and  $c_0$ ,  $c_1$ , and  $c_2$  are parameters to be determined.

#### 3.3 Plasticity

Unlike elasticity, plasticity is the state in the material where the deformation becomes permanent with a irreversible change of shape. Normally, plasticity is achieved when a load is constantly added to a material until it reaches its plasticity limit or what we call the yield strength. However, when it comes to high changes in temperature and phases transformation in the material, the yield strength changes accordingly. Numerically speaking, it is a complicated non-linear process, and it is found in the literature with several variations. In general, the return mapping algorithm is adopted in most of the works with some differences. In this section, we will understand the physics behind plasticity and explain the return mapping algorithm in details. But first, it is important to present an overview on the development of elasto-plasticity in the last decades. In fact, the linear elasticity has had more interest in community than the plasticity in the last three decades.

As discussed in the previous section, in [16, 38] a stabilized stokes equations were developed, where later in [17] it was extended to incompressible elasticity equations. In [45-49] these ideas were extended to a visco-elasto-plasticity with non linear equations. Yet, the equations were not robust in terms of stabilization over all elastic/plastic spectrum.

In a recent works [50–52], a bubble function stabilization was used to avoid stabiliation tuning, which later in [12] the work was extended to a VMS hyper-elasticity.

Besides, in [18, 53, 54] incomressible hyper-elasticity and elasto-plasticity were studied using the orthogonal sub-scale (OSS) decomposition method. This work was later extended in [55] to a nearly incompresible plasticity with large deformation. An interesting feature of this work is the modification of the stabilization operator with subgrid-scale shear modulus. In [56], a nodal finite element spaces were added for the strains and the displacement, in both static and dynamic cases. This was done using the Drucker-Prager and Mohr-Coulomb models for plasticity. All these works only presented static computations except for the work in [56].

The works presented above and in the previous section, brings this field into the current state of practice. In the previous section, the elasticity and hyperelasticity were presented and showed accurate and stable results with a simple linear tetrahedral elements for transient and static cases [35]. As a recall, in this work the OSS decomposition with the VMS stabilization method were used. For that reason, the plasticity will be added to this work to have an elasto-plastic and hyper-elastoplastic models . In the rest of this section, we will see what are the governing equations and the specification of plasticity, and how it will be added to the elastic model using the return mapping algorithm.

## 3.3.1 Elasto-plasticity criterion

#### 3.3.1.1 Total strain tensor decomposition

Since the we are dealing with a small increment of displacement, one can decompose the total strain using the Pradtl-Reus definition:

$$\varepsilon = \varepsilon^{el} + \varepsilon^{pl}, \tag{3.70}$$

where  $\varepsilon$ ,  $\varepsilon^{el}$ , and  $\varepsilon^{pl}$  are the total strain, elastic strain, and the plastic strain tensors respectively. The elastic strain tensor can be written using the symmetric gradient operator as described in the previous section  $\varepsilon^{el} = \frac{1}{2} (\nabla u + \nabla u^T)$ . And equation (3.70) can be written as:
$$\varepsilon^{el} = \varepsilon - \varepsilon^{pl}.\tag{3.71}$$

#### 3.3.1.2 Stress tensor definition

Using the Hook's law, and equation (3.71) we can write the stress response as follow:

$$\boldsymbol{\sigma} = C : \left(\varepsilon - \varepsilon^{pl}\right),\tag{3.72}$$

Where C is a fourth-order tensor that describe the elastic moduli. As mentioned before, we are working with isotropic materials, so the stress tensor can be split into a deviatoric and a volumetric part:

$$\sigma = \tilde{\sigma} + p\mathbf{I},\tag{3.73}$$

$$\tilde{\boldsymbol{\sigma}} = \boldsymbol{C}^{\text{dev}} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^p) = 2\mu \left( \tilde{\boldsymbol{\epsilon}} - \tilde{\boldsymbol{\epsilon}}^p \right)$$
(3.74)

$$p = \kappa \operatorname{tr} \left( \epsilon - \epsilon^p \right) \tag{3.75}$$

where  $\tilde{\sigma}$  is the deviatoric part of  $\sigma$ , and  $C^{\text{dev}}$  is the deviatoric part of the elastic moduli. For simplicity, strating from this section the diacritic tilde designate the deviatoric part.

#### 3.3.1.3 Yield function

#### General properties definition

We seek to generalize the notion of flow threshold plastic observed in the onedimensional case of the test of traction. In this case, the set of possible uniaxial stresses  $\sigma$  checks the scalar relation:

$$\boldsymbol{\sigma} - \boldsymbol{\sigma}_0 \leqslant 0 \tag{3.76}$$

The stresses  $\boldsymbol{\sigma} \leq \boldsymbol{\sigma}_0$  correspond to those where the material remains elastic and the case where  $\boldsymbol{\sigma} = \boldsymbol{\sigma}_0$  defines the stress allowing the plastic deformation.

We must therefore define all the states of stress likely to cause plastic deformation. For this we introduce a scalar function f of the stress tensor components  $\sigma$ and having the following properties:

$$\begin{cases} f(\boldsymbol{\sigma}) \leqslant 0 & \text{Elastic Domain} \\ f(\boldsymbol{\sigma}) > 0 & \text{Not allowed (Plastic Domain)} \end{cases}$$
(3.77)

For a general case and to fit in the elasto-plastic model, the function f called the Yield function, is expressed with respect to the deviatoric stress tensor, and the hardening rule that will be discussed in the following section.

In the principal stress space, the plastic domain f = 0 defines a surface. The assumptions made previously make it possible to specify the characteristics of this surface called "yield surface":

The assumption of invariance of the plastic behavior, when the hydrostatic pressure varies, means that:

$$\forall \boldsymbol{\sigma} \quad f(\boldsymbol{\sigma}_{I} + \boldsymbol{\sigma}_{,\boldsymbol{\sigma}_{II}} + \boldsymbol{\sigma}_{,\boldsymbol{\sigma}_{III}} + \boldsymbol{\sigma}) = f(\boldsymbol{\sigma}_{I}, \boldsymbol{\sigma}_{II}, \boldsymbol{\sigma}_{III})$$
(3.78)

Geometrically, this implies that the surface is invariant in any vector translation parallel to  $I(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$ . It is therefore a cylinder of generatrices that are parallel to I and its shape is characterized by its cross section C through the plane  $(\pi)$  normal to I, passing through the origin and with equation  $\boldsymbol{\sigma}_I + \boldsymbol{\sigma}_{II} + \boldsymbol{\sigma}_{III} = 0$ : on this plane, the three coordinate axes project along three axes at  $120^{\circ} \ 0\boldsymbol{\sigma}'_I, 0\boldsymbol{\sigma}'_{II}, 0\boldsymbol{\sigma}'_{III}$ and it contains the coordinate vectors  $(s_I, s_{II}, s_{III})$  (figure (3.2))

The isotropy hypothesis makes it possible to assert that f is invariant when any permutation of the principal stresses happen: the surface is therefore invariant in a symmetry with respect to the planes bisectors of those containing the principal axes and its section line admits  $0\sigma'_{I}, 0\sigma'_{II}, 0\sigma'_{II}$  as axes of symmetry.

The assumption of behavioral invariance, when we change the sign of  $\sigma$ , implies that C also admits as axes of symmetry the bisectors A1, A2 and A3 of the axes  $0\sigma'_{I}, 0\sigma'_{II}, 0\sigma'_{II}$  (figure (3.2)).

A simple geometric calculation shows that the six points  $Q_i i (i = 1 - 6)$  of C, located on the axes  $0\boldsymbol{\sigma}'_I, 0\boldsymbol{\sigma}'_{II}, 0\boldsymbol{\sigma}'_{III}$  and which all represent the equivalent loads (within a hydrostatic pressure) to a uni-axial loading, are at a distance from the point O.

Finally, the hypothesis of obedience to Hill's principle [57] implies that the flow boundary and C are convex, which means they are located above any chord and below any tangent (or the opposite). We deduce that C is between the two regular hexagons  $H_1$  and  $H_T$  admitting respectively for midpoints sides, or vertices, the points  $Q_i i (i = 1 - 6)$  (figure (3.2)).

We can therefore see that the hypotheses made considerably restrict the choice of possible criteria. The hexagon  $H_T$  and the circle passing through the points  $Q_i$  are two possible cases corresponding, respectively, to the Tresca and von Mises criteria, as we shall see.



The axes  $0\sigma'_{I}, 0\sigma'_{II}, 0\sigma'_{III}$ , are the projections of the coordinate axes. Under the assumptions of isotropy, invariance behavior when  $\sigma \to -\sigma$ and maximum work, the section line C is located in the hatched area between the two regular hexagons  $H_1$  and  $H_T$  (Tresca criterion) and is symmetrical with respect to the three axes  $0\sigma'_{I}, 0\sigma'_{II}, 0\sigma'_{III}$  and with respect to their bisectors  $A_1, A_2$  and  $A_3$ . The circle passing through the points  $Q_i$ , equidistant from the center 0, corresponds to the von Mises criterion.

Figure 3.2: Cross section by the plane  $(\pi) \sigma_I + \sigma_{II} + \sigma_{III} = 0$  of the flow boundary [58]



Figure 3.3: Mohr representation of the state of stress in one point M (when the facet describes all the orientations of space, the end of the stress vector T describes the hatched area between the three semicircles) [58]

### Tresca plasticity criterion

This is, historically, the first criterion of plasticity proposed. He assumes that

plastic deformation is possible at point M when that the maximum fission at M reaches a critical value k. Given the representation of Mohr in figure (3.3), this condition is easily expressed by introducing the principal stresses  $\sigma_I$ , I = 1 - 3:

$$f = Max_{J,K} \left(\sigma_J - \sigma_K\right) - 2k \tag{3.79}$$

It is the equation of a prism with six faces of generatrices parallel to I as seen in figure (3.4) and admitting the regular hexagon  $H_T$  for cross section by the plane  $\pi$  (figure (3.2)).

By considering the uniaxial traction, one deduces from figure (3.3) that, for the Tresca criterion, the maximum shear is equal to:

$$k = \frac{\sigma_0}{2}$$
 Tresca criterion (3.80)

The section of the flow surface by the plane  $\sigma_{III} = 0$  corresponds to the case of the plane stress where the boundary flow area is a non-regular hexagon with parallel sides to the axes, in the 1st and 3rd sectors, and on sides parallel to the first bisector, in the other two (figure (3.4b)).

#### von Mises plasticity criterion

It corresponds to the cylinder of revolution of axis I (figure (3.5a)) in which the prism of the Tresca criterion fits and whose cross section is the circle passing through the points  $Q_i$  (figure (3.2)).

As the plane  $\pi$  contains the vectors  $(s_I, s_{II}, s_{III})$ , we deduce that in principal axes, f is written:

$$f = 3\left(s_I^2 + s_{II}^2 + s_{III}^2\right) - 2\sigma_0^2 \tag{3.81}$$

It is easy to show that an equivalent form is:

$$f = (\sigma_I - \sigma_{II})^2 + (\sigma_{II} - \sigma_{III})^2 + (\sigma_{III} - \sigma_I)^2 - 2\sigma_0^2$$
(3.82)

We deduce that in plane stress and main axes where  $\sigma_{III} = 0$ , the criterion is written:

$$f = 2\left(\sigma_I^2 - \sigma_I \sigma_{II} + \sigma_{II} - \sigma_0^2\right) \tag{3.83}$$

In the plane  $(\sigma, \sigma_{II})$ , it is the equation of an ellipse where is inscribed the hexagon of the Tresca criterion (figure (3.5b)).

It is shown that it can then be expressed in the two equivalent forms:

$$f = (\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6\sigma_{12}^2 + 6\sigma_{23}^2 + \sigma_{13}^2 - 2\sigma_0^2 \quad (3.84)$$

$$f = 3\left(s_{11}^2 + s_{22}^2 + s_{33}^2 + 2s_{12}^2 + 2s_{23}^2 + s_{13}^2\right) - 2\sigma_0^2 = 3\boldsymbol{s} : \boldsymbol{s} - 2\sigma_0^2$$
(3.85)

From a physical point of view, the material being assumed to be isotropic, the relevance of these expressions corresponds to the mathematical fact that the two previous expressions are invariants of the tensors  $\sigma$  and  $\tilde{\sigma}$ , which means that they keep the same value, regardless of the choice of reference frame.

From equation (3.84), we deduce that, for the von Mises criterion, the maximum split is equal to:

$$k = \frac{\sigma_0}{\sqrt{3}}$$
 von Mises criterion (3.86)

which gives a value approximately 15% greater than the value according to the Tresca criterion.

One of the major interests of the von Mises criterion is that, contrary to the Tresca criterion, it has a simple analytical form with arbitrary axes. For that reason, we will adopt the von Mises criterion for the rest of the work.



b) Plane Stress Case

Figure 3.4: Geometrical representation of the Tresca plasticity criterion [58]



Figure 3.5: Geometrical representation of the von Mises plasticity criterion [58]

## 3.3.1.4 Hardening law

The work hardening of the material is induced by the multiplication in the material of the dislocations generated by the stress field to accommodate the plastic deformation and which modify the flow boundary, that is to say the stress states allowing the continuation of the plastic deformation. In the yield function, two main terms exist, the yield surface and the hardening rule:

$$f\left(\tilde{\boldsymbol{\sigma}}, \bar{\varepsilon}\right) = \left|\left|\tilde{\boldsymbol{\sigma}}\right|\right| + H\left(\bar{\varepsilon}\right),\tag{3.87}$$

where  $||\tilde{\boldsymbol{\sigma}}||$  is the equivalent von Mises stress given by  $||\tilde{\boldsymbol{\sigma}}|| = \sqrt{\frac{3}{2}}\tilde{\boldsymbol{\sigma}}:\tilde{\boldsymbol{\sigma}}$ , and  $H(\bar{\varepsilon})$  the hardening rule. In tension, this leads at least, initially, to an increase in the plastic yield stress. We are going to specify the two main classes of models used to describe this evolution and generalize relation (3.87) relating to a very specific history of deformation.

## **Isotropic Hardening**

The state of hardening of the material evolving only because of its plastic deformation, one naturally generalizes the definition of the speed of generalized deformation, by allocating it to the plastic component of the speeds of deformation, and we then define the generalized deformation as its integral, throughout the history of the element of matter between the initial moment  $\mathbf{u} = 0$  and the current moment  $\mathbf{u} = t$ :

$$\dot{\bar{\varepsilon}} = \left(\frac{2}{3}\dot{\varepsilon}_{ij}^{pl}\dot{\varepsilon}_{ij}^{p}l\right)^{\frac{1}{2}} \qquad \text{and} \qquad \bar{\varepsilon} = \int_{0}^{t}\dot{\bar{\varepsilon}}\left(\mathbf{u}\right)d\mathbf{u} \tag{3.88}$$

The integral is done throughout the trajectory of the material element and the generalized strain rate is therefore the particle derivative of the generalized strain. One thus obtains, at any point of the flow, a positive and non-decreasing scalar, independent of the choice of the reference and which extends to any history of deformation the concept of plastic deformation  $\varepsilon^{pl}$  define in the tensile test.

The simplest generalization of the tensile results is to assume that the plastic yield stress  $\sigma_0$  evolves like the tensile stress and depends only on  $\bar{\varepsilon}$ . As an example, the equation (3.87) with  $H(\bar{\varepsilon}) = -2\sigma_0^2(\bar{\varepsilon})$ .

Geometrically, this means that at each point of the flow, the flow boundary undergoes homothety and therefore expands isotropically in all directions: the cross section remains a circle centered on the origin and of proportionally increasing radius to  $\sigma_0(\bar{\varepsilon})$  (figure (3.6a)). Thus, for example, for the forming of sheets in plane stress, the flow boundary of the main stresses remains an ellipse centered on the origin of the stresses and whose axes expand, the ratio of their length remaining constant (figure (3.7)).

A direct consequence of this assumption of behavior is that, if the metal passes from a traction to a compression, the stress threshold in compression is the opposite of the final tensile stress. The material is said to have no Bauschinger effect.



Figure 3.6: Representation of the isotropic hardening with a von Mises criterion. [58]



Figure 3.7: Evolution of the yield surface in isotropic hardening. [58]

## General Hardening: including the kinemtic hardening

The hypothesis of isotropic work hardening is not always completely satisfactory, in particular in the case where the strain rate strongly changes direction.

A simple case is that of a mechanical test where the sign of the stress is changed: traction-compression, for example. It is then observed that, after returning to the elastic range, the elastic limit in compression is lower in absolute value than the final stress observed just before unloading: this is one of the Bauschinger effects as seen in figure (3.8a).

Physically, this phenomenon corresponds to the fact that the deformation orients the population of dislocations stored in the material, this orientation being mainly opposed to the continuation of the deformation in the same direction.

From a mechanical point of view, the simplest modeling of this phenomenon, due to Prager [59], consists in assuming that, at each point of the flow and at each instant, the flow boundary tends to move in a direction determined by the strain rate. So that after a finite deformation, the border is no longer symmetrical with respect to the origin of the stresses: its center is translated by the vector X as illustrated in figure (3.8b). This displacement is called "kinematic work hardening".

Prager developed a purely kinematic work hardening model, that is to say that the flow boundary, at each point of the flow, undergoes only one translation without changing shape.

A more general and relatively simple model has been proposed by Hughes [60]. It consists in assuming, at the same time, an isotropic expansion of the flow boundary and a displacement of its center (figure (3.8b))

This model thus supposes that the total hardening is a linear combination of kinematic hardening and isotropic hardening. It is used by Aliaga [61] in the context of the numerical simulation of quenching operations of steel forgings. The tensor  $\mathbf{X}$ , whose trace is zero, is called "kinematic tensor". One then generalizes the criterion of plasticity of von Mises and the generalized constraint in the form:

$$f\left(\tilde{\boldsymbol{\sigma}},\bar{\varepsilon}\right) = \sqrt{\frac{3}{2}\left(\tilde{\boldsymbol{\sigma}}-\mathbf{X}\right):\left(\tilde{\boldsymbol{\sigma}}-\mathbf{X}\right)} - 2\sigma_{0}^{2}\left(\bar{\varepsilon}\right), \qquad (3.89)$$

The plastic strain rate is obtained by derivation from f or  $||\tilde{\sigma}||$  with respect to  $\tilde{\sigma}$ . In such a formulation, one dissociates the concept of stress from plastic flow  $\sigma_0(\bar{\varepsilon})$ , defining the radius of the cross section of the cylinder of flow from the tensile stress  $\sigma(\bar{\varepsilon})$  which one supposes of the form:

$$\sigma\left(\bar{\varepsilon}\right) = \mathbf{R}_e + H\left(\bar{\varepsilon}\right) \tag{3.90}$$

The equations governing the evolution of the kinematic vector and of the isotropic component of work hardening, starting from the evolution of the tensile stress are the following ones:

This model depends on a scalar and dimensionless coefficient  $\beta$  between 0 and 1, which is the weighting coefficient of the "kinematic work hardening". For 0 or 1, work hardening is purely isotropic or kinematic; in between, it is mixed.

One can simply visualize the effect of the parameter  $\beta$  by applying equations (3.89)-(3.91) to the case of a tensile test until deformation  $\bar{\varepsilon}_1$  followed by compression. Simple calculations then show that the stress  $\sigma(\bar{\varepsilon})$  and the non-zero components of X are worth:

$$\begin{cases} \sigma = R_e + H(\bar{\varepsilon}) & 0 < \bar{\varepsilon} < \bar{\varepsilon}_1(\text{Traction}) \\ X_{11} = -2X_{22} = -2X_{33} = \frac{2\beta}{3}H(\bar{\varepsilon}) & 0 < \bar{\varepsilon} < \bar{\varepsilon}_1(\text{Traction}) \\ \sigma = -R_e - H(\bar{\varepsilon}) + 2\beta H(\bar{\varepsilon}_1) & \bar{\varepsilon} > \bar{\varepsilon}_1(\text{Compression}) \\ X_{11} = -2X_{22} = -2X_{33} = \frac{2\beta}{3}(2H(\bar{\varepsilon}_1) - H(\bar{\varepsilon})) & \bar{\varepsilon} > \bar{\varepsilon}_1(\text{Compression}) \end{cases}$$
(3.92)



Figure 3.8: Representation of the kinematic work hardening with a general von Mises criterion. [58]



Figure 3.9: Uni-axial tension/compression hardening curves, according to the Hughes mixed hardening model for different values of the coefficient  $\beta$  [58]

Figure (3.9) clearly illustrates the effect of the choice of the parameter  $\beta$  which can only be identified by reversing the direction of the deformation. Thus, microbending-unfolding tests on sheets for stamping, where the maximum deformation after bending reaches 40%, show that the behavior of steel and aluminum alloy sheets can be represented with  $\beta \sim 0, 13$  and 0.18 respectively [62], which shows that the isotropic component of hardening is dominant.

Nevertheless, taking this component into account seems essential to obtain a good stress forecast residual after shaping. For that reason, and for the nature of our application, only the isotropic hardening will be taken into account. Several types of isotropic hardening exists, first we have the **perfect plasticity** where there is no hardening, and then we can have **linear isotropic hardening**, and the general case **non-linear isotropic hardening**. In the following sections we will see several types of hardening depending on the application.

#### 3.3.1.5 Flow rule

It is assumed that, at any time and at any point in the material, the strain rate is the sum of an elastic strain rate and a plastic strain rate, according to equation (3.70).

Expressing in the deformation rate poses some problems, since it requires writing the derivative of the stress tensor or the deviatoric stress tensor and this derivative must be objective, that is to say independent the choice of reference frame [63]. This difficulty is discussed in detail, for example in [64].

We will give here a possible formulation [64]. To the velocity field, we associate the tensor of the velocities of rotation  $\dot{R}_{ij}$  of the element of the material by the formula:

$$\dot{R}_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right) = -\dot{R}_{ji} \quad i = 1 - 3; j = 1 - 3$$
(3.93)

By construction, this tensor is antisymmetric (its transposed matrix is equal to its opposite  $-\dot{R}_{ij}$ ) and the terms of the diagonal are zero. One defines, in all generality, the elastic component of the deformation by the relations in speed [58]:

$$\begin{cases} \dot{\theta}^{e} = -\frac{\dot{p}}{K^{e}} \\ \dot{e}^{e} = \frac{1}{2G} \frac{\mathrm{d}_{J}s}{\mathrm{d}t} \\ \dot{e}^{i} = \frac{1}{2G} \frac{\mathrm{d}_{J}s}{\mathrm{d}t} \end{cases} \text{ ou } \dot{\varepsilon}^{e} = \frac{1+v}{E} \frac{\mathrm{d}_{J}\sigma}{\mathrm{d}t} - \frac{v}{E} \left(\dot{\sigma}_{ii}\right) 1 \qquad (3.94)$$
$$= \dot{s} - \mathbf{R} \cdot s + s \cdot \dot{R} \quad \frac{\mathrm{d}_{J}\sigma}{\mathrm{d}t} = \dot{\sigma} - \mathbf{R} \cdot \sigma + \sigma \cdot \dot{R}$$

with

 $\frac{\mathrm{d}_{j}s}{\mathrm{d}t}$ 

The derivative of s, thus introduced, is called the "derivative of Jauman". The elastic domain is defined by the plasticity criterion  $f(\tilde{\sigma}) < 0$ . The plastic strain rate then verifies:

$$\dot{\varepsilon}^{p} = \begin{cases} 0 & \text{if } \begin{cases} f(\tilde{\boldsymbol{\sigma}}) < 0 \\ f(\tilde{\boldsymbol{\sigma}}) = 0 \end{cases} & \text{and } \frac{\partial f}{\partial \tilde{\boldsymbol{\sigma}}} : \dot{\tilde{\boldsymbol{\sigma}}} < 0 \\ \gamma \frac{\partial f}{\partial \tilde{\boldsymbol{\sigma}}} & \gamma \ge 0 & \text{if } f(\tilde{\boldsymbol{\sigma}}) = 0 & \text{and } \frac{\partial f}{\partial \tilde{\boldsymbol{\sigma}}} : \dot{\tilde{\boldsymbol{\sigma}}} \ge 0 \end{cases}$$
(3.95)

where  $\gamma$  is a positive consistency parameter. It can only occur if the criterion is satisfied:  $f(\tilde{\boldsymbol{\sigma}}) = 0$  and if the stress velocity is directed towards the outside of the elastic domain.

# 3.3.2 Return mapping algorithm

The general idea of the return mapping algorithm is to correct the deviatoric stress tensor. At the beginning of the increment, it is considered as only elastic behavior, where the elastic predictor  $\tilde{\sigma}^{trial}$  is computed. Using this predictor, we can identify if the behavior is plastic or elastic by computing the yield function  $f^{trial}$ . The deviatoric stress tensor is then corrected only if the material is in the plastic zone. In this section, the return mapping algorithm is decribed in details.

First, Having the data on the previous time-step: the displacement  $\mathbf{u}_n$ , the strain rate  $\dot{\varepsilon}_n$ , the plastic strain  $\dot{\varepsilon}_n^{pl}$ , the deviatoric stress tensor  $\tilde{\boldsymbol{\sigma}}_n$  and and the hardening parameter  $\alpha_n$ . A linear hardening rule is considered in this section, and the extension to more complicated hardening rules is straightforward [65]. The hardening rule is given by  $\sqrt{\frac{2}{3}} (\sigma_Y + K\alpha)$ , where  $\sigma_Y$  is the yield strength, and K is the hardening modulus.

The second step is to solve the elasticity equations, and update the parameters as there is no plasticity. We get the new displacement vector  $\mathbf{u}_{n+1}$  and strain tensor  $\varepsilon_{n+1}$ . Afterwards, we compute the deviatoric trial stress given by:

$$\tilde{\boldsymbol{\sigma}}_{n+1}^{trial} = 2\mu \left(\varepsilon_{n+1} - \varepsilon_n^{pl}\right). \tag{3.96}$$

This form of the stress tensor, is as it is called a trial form, where the plastic strain is preserved from the previous time-step and subtracted from the total strain on the current time-step. This is only used to check the elastic/plastic regime of the element in the solid. Having this parameter we can now compute the yield function that defines the state of the material as described in (3.77). f is given by:

$$f_{n+1}^{trial} = \left\| \tilde{\boldsymbol{\sigma}}_{n+1}^{trial} \right\| - \sqrt{\frac{2}{3}} \left( \sigma_Y + K\alpha \right)$$
(3.97)

If  $f_{n+1}^{trial} \leq 0$  the material is still in the elastic state which means that every trial parameter is the actual parameter:  $(\bullet)_{n+1} = (\bullet)_{n+1}^{trial}$ . However, f is not allowed to be positive because it means that we are outside the yield surface which is not physical. Accordingly, the deviatoric trial stress should be corrected to return back to the yield surface (here comes the name of the **return mapping** algorithm). To return to the allowed conditions,  $f(\tilde{\sigma}_{n+1}, \bar{\varepsilon}_{n+1})$  should be zero. Thus, we get:

$$f(\tilde{\boldsymbol{\sigma}}_{n+1}, \alpha_{n+1}) = \|\tilde{\boldsymbol{\sigma}}_{n+1}\| - \sqrt{\frac{2}{3}} \left(\sigma_Y + k(\alpha_{n+1})\right) = 0$$

$$\frac{\tilde{\boldsymbol{\sigma}}_{n+1}}{n} - \sqrt{\frac{2}{3}} \left(\sigma_Y + K\alpha_{n+1}\right) = 0$$

$$\frac{\tilde{\boldsymbol{\sigma}}_{n+1}^{trial} - 2\mu\Delta\gamma\mathbf{n}}{n} - \sqrt{\frac{2}{3}} \left(\sigma_Y + K\left(\alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma\right)\right) = 0 \qquad (3.98)$$

$$2\mu\Delta\gamma \left(1 + K/3\mu\right) = f_{n+1}^{trial}$$

$$\Delta\gamma = \frac{f_{n+1}^{trial}/2\mu}{1 + K/3\mu},$$

where n is the direction tensor found from the flow rule in (3.95) and given by:

$$\boldsymbol{n} = \frac{\tilde{\boldsymbol{\sigma}}}{\|\tilde{\boldsymbol{\sigma}}\|}.\tag{3.99}$$

In addition, the hardening parameter  $\alpha$  is updated as follows:

$$\alpha_{n+1} = \alpha_n + \sqrt{\frac{2}{3}} \Delta \gamma, \qquad (3.100)$$

where  $\Delta \gamma$  is the equivalent plastic strain increment. Finally we can correct the deviatoric trial stress and update the plastic strain:

$$\tilde{\boldsymbol{\sigma}}_{n+1} = \tilde{\boldsymbol{\sigma}}_{n+1}^{trial} - 2\mu\Delta\gamma\boldsymbol{n}$$
(3.101)

$$\varepsilon_{n+1}^{pl} = \varepsilon_n^{pl} + \Delta \gamma \boldsymbol{n}. \tag{3.102}$$

The described algorithm is summarized in the following chart:

## Algorithm 2 Return mapping algorithm

- A. Data at the increment n are known:  $\dot{\varepsilon}_n, \dot{\varepsilon}_n^{pl}, \tilde{\sigma}_n, and\alpha_n$ .
- B. Update  $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_n$
- C. Calculate the elastic predictor:  $\tilde{\sigma}_{n+1}^{trial} = 2\mu(\varepsilon_{n+1} \varepsilon_n^{pl})$
- D. Compute the yield function:  $f_{n+1}^{trial} = \left\| \tilde{\boldsymbol{\sigma}}_{n+1}^{trial} \right\| \sqrt{\frac{2}{3}} \left( \sigma_Y + K \alpha \right)$ 
  - 1: if  $f_{n+1}^{trial} \leq 0$  then
  - 2: Purely elastic behavior,
  - 3: Set  $(\bullet)_{n+1} = (\bullet)_{n+1}^{trial}$
  - 4: else if  $f_{n+1}^{trial} > 0$  then
  - 5: Elasto-plastic behavior,

6: Compute 
$$\Delta \gamma = \frac{f_{n+1}^{trial}/2\mu}{1+K/3\mu}$$

7: and 
$$\mathbf{n} = \frac{\tilde{\sigma}_{n+1}^{trial}}{\left\|\tilde{\sigma}_{n+1}^{trial}\right\|}$$

- 8: Correct the deviatoric tensor:
- 9:  $\tilde{\boldsymbol{\sigma}}_{n+1} = \tilde{\boldsymbol{\sigma}}_{n+1}^{trial} 2\mu\Delta\gamma\mathbf{n}$
- 10: Update the hardening parameter:

11: 
$$\alpha_{n+1} = \alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma$$

- 12: Update the plastic strain:
- 13:  $\varepsilon_{n+1}^{pl} = \varepsilon_n^{pl} + \Delta \gamma \mathbf{n}$
- 14: end if

### Remark

For a non-linear hardening rule as  $k(\alpha) = K\alpha + (K_{\infty} - \sigma_Y)(1 - e^{-\delta\alpha})$ , the solution becomes as seen in equation (3.103):

In that case, the equation must be linearized or solved by a numerical approach as Newton-Raphson method.

$$f(\tilde{\sigma}_{n+1}, \alpha_{n+1}) = \|\tilde{\sigma}_{n+1}\| - \sqrt{\frac{2}{3}} \left(\sigma_Y + k(\alpha_{n+1})\right) = 0$$

$$\frac{\tilde{\sigma}_{n+1}}{n} - \sqrt{\frac{2}{3}} \left(\sigma_Y + K\alpha_{n+1} + \left(K_{\infty} - \sigma_Y\right) \left(1 - e^{-\delta\alpha_{n+1}}\right)\right) = 0$$

$$\frac{\tilde{\sigma}_{n+1}^{trial} - 2\mu\Delta\gamma \mathbf{n}}{n} - \sqrt{\frac{2}{3}} \left(\sigma_Y + K\left(\alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma\right) + \left(K_{\infty} - \sigma_Y\right) \left(1 - e^{-\delta\left(\alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma\right)}\right)\right) = 0$$

$$2\mu\Delta\gamma + \sqrt{\frac{2}{3}} \left(\sigma_Y + K\left(\alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma\right) + \left(K_{\infty} - \sigma_Y\right) \left(1 - e^{-\delta\left(\alpha_n + \sqrt{\frac{2}{3}}\Delta\gamma\right)}\right)\right) - \|\tilde{\sigma}_{n+1}^{trial}\| = 0$$

$$(3.103)$$

## 3.3.3 Return mapping algorithm for large displacement

In this section the return mapping algorithm will be explained for large displacement, or the hyper-elasto plasticity. As stated before, the first step is to get the data at the previous time-step: the displacement  $\mathbf{u}_n$ , the strain rate  $\dot{\varepsilon}_n$ , the plastic strain  $\dot{\varepsilon}_n^{pl}$ , the deviatoric stress tensor  $\tilde{\boldsymbol{\sigma}}_n$  and and the hardening parameter  $\alpha_n$ . Note that also in this section, the same linear hardening rule is used. Elasticity is then solved without taking plasticity into account to get the new displacement vector  $\mathbf{u}_{n+1}$  and strain tensor  $\varepsilon_{n+1}$ . The deviatoric trial stress is expressed differently in that case. As explained in the hyper-elasticity the deviatoric part of the stress tensor is expressed as follow:

$$dev\left[\boldsymbol{\sigma}\right] = \mu J^{-\frac{5}{3}} dev\left[\boldsymbol{F}\boldsymbol{F}^{T}\right].$$
(3.104)

With  $\boldsymbol{F}\boldsymbol{F}^{T}$  is given by equation (3.52). The diviatoric trial stress is given by:

$$\tilde{\boldsymbol{\sigma}}_{n+1}^{trial} = \mu J^{-\frac{5}{3}} \left[ (\boldsymbol{F}_e)_{n+1}^{trial} \right] \left[ (\boldsymbol{F}_e)_{n+1}^{trial} \right]^T, \qquad (3.105)$$

where  $(\mathbf{F}_e)_{n+1}^{trial}$  is given by:

$$(\mathbf{F}_{e})_{n+1}^{trial} = (\mathbf{F}_{n+1}) (\mathbf{F}_{n}^{p})^{-1},$$
 (3.106)

where  $F_n^p$  is the plastic deformation gradient and is updated at each time step using the equation below:

$$\boldsymbol{F}_{n+1}^p = \exp\left(\Delta\gamma\boldsymbol{n}\right)\boldsymbol{F}_n^p. \tag{3.107}$$

From this step, the procedure stays the same as before. For that reason equations (3.97), (3.98), (3.99), (3.100), (3.101), and (3.102) remains the same but with a different deviatoric stress tensor, and the Lame coefficient is multiplied by  $J^{-\frac{5}{3}}$ . Finally the algorithm becomes as follows:

#### Algorithm 3 Return mapping algorithm for large displacement

- A. Data at the increment n are known:  $\dot{\varepsilon}_n, \dot{\varepsilon}_n^{pl}, \tilde{\sigma}_n, and\alpha_n$ .
- B. Update  $\varepsilon_{n+1} = \varepsilon_n + \Delta \varepsilon_n$
- C. Calculate the elastic predictor:  $\tilde{\boldsymbol{\sigma}}_{n+1}^{trial} = \mu J^{-\frac{5}{3}} \left[ (\boldsymbol{F}_e)_{n+1}^{trial} \right] \left[ (\boldsymbol{F}_e)_{n+1}^{trial} \right]^T$ With  $(\boldsymbol{F}_e)_{n+1}^{trial} = (\boldsymbol{F}_{n+1}) (\boldsymbol{F}_n^p)^{-1}$ And  $\boldsymbol{F} = (\boldsymbol{I} - \nabla \mathbf{u})^{-1}$
- D. Compute the yield function:  $f_{n+1}^{trial} = \left\| \tilde{\boldsymbol{\sigma}}_{n+1}^{trial} \right\| \sqrt{\frac{2}{3}} \left( \sigma_Y + K \alpha \right)$ 
  - 1: if  $f_{n+1}^{trial} \leq 0$  then 2: Purely elastic behavior, 3: Set  $(\bullet)_{n+1} = (\bullet)_{n+1}^{trial}$ 4: else if  $f_{n+1}^{trial} > 0$  then 5: Elasto-plastic behavior, 6: Compute  $\Delta \gamma = \frac{f_{n+1}^{trial/2\mu J^{-\frac{5}{3}}}}{1+K/3\mu J^{-\frac{5}{3}}}$ 7: and  $\mathbf{n} = \frac{\tilde{\sigma}_{n+1}^{trial}}{\|\tilde{\sigma}_{n+1}^{trial}\|}$ 8: Correct the deviatoric tensor: 9:  $\tilde{\sigma}_{n+1} = \tilde{\sigma}_{n+1}^{trial} - 2\mu J^{-\frac{5}{3}} \Delta \gamma \mathbf{n}$ 10: Update the hardening parameter: 11:  $\alpha_{n+1} = \alpha_n + \sqrt{\frac{2}{3}} \Delta \gamma$ 12: Update the plastic strain and deformation gradient: 13:  $\varepsilon_{n+1}^{pl} = \varepsilon_n^{pl} + \Delta \gamma \mathbf{n}$ 14:  $\mathbf{F}_{n+1}^p = \exp(\Delta \gamma \mathbf{n}) \mathbf{F}_n^p$ 15: end if

## 3.3.4 Variational form with VMS stabilization

As described in the aforementioned algorithm, the plasticity is sort of correction of the deviatoric stress tensor that exceeds the yield surface. For that reason, the variational formulation does not change compared to the elastic one (3.36)(3.37)(3.38) with some small modification:

$$a''(\mathbf{u}_h, \mathbf{w}_h) + (p_h, \nabla . \mathbf{w}_h) + \sum_{K \in T_h} \left( \tau_{\mathbf{c}} R_c, \nabla_x . \mathbf{w}_h \right) = L(\mathbf{w}_h) \,\forall \mathbf{w}_h \in W_{h,0}, \qquad (3.108)$$

$$\left(\nabla \cdot \mathbf{u}_{h}, q_{h}\right) - \left(\frac{1}{K}p_{h}, q_{h}\right) - \sum_{K \in T_{h}}\left(\tau_{\mathbf{u}}^{\prime}R\left(\mathbf{u}_{h}\right), \nabla q_{h}\right) = 0 \forall q_{h} \in \mathcal{Q}_{h}, \qquad (3.109)$$

$$R(\mathbf{u}_h) = \boldsymbol{f} + \nabla p_h + \nabla . \tilde{\boldsymbol{\sigma}}'. \qquad (3.110)$$

where  $\tilde{\sigma}'$  is the modified deviatoric stress tensor corrected as described in equation (3.101), which makes *a* modified as follows:

$$a''(\mathbf{u}_h, \mathbf{w}_h) = \int_{\Omega} \tilde{\boldsymbol{\sigma}}' : \nabla^s \mathbf{w} d\Omega.$$
(3.111)

In addition,  $\tau'_{\mathbf{u}}$  is the modified stabilization parameter as follows:

$$\tau_u (K)' = \left( \left( \frac{\rho}{(c_0 \Delta t)^2} \right)^2 + \left( \frac{2\mu_e f f}{c_1 h_k^2} \right)^2 \right)^{-\frac{1}{2}}, \qquad (3.112)$$

where  $\mu_{eff} = \beta \mu$ , with  $\beta = \left(1 - \frac{2\mu\Delta\gamma}{\|\tilde{\sigma}^{trial}\|}\right)$ . The idea of having an effective viscosity is that we are considering the plastic area

The idea of having an effective viscosity is that we are considering the plastic area as weaker regions. In other words, when the material is under a plastic behavior, the lame coefficient can be considered as lower than the actual one. This parameter is added to the stabilization term, and it is originated from the corrected deviatoric stress tensor equaition:

$$\tilde{\sigma}_{n+1} = \tilde{\sigma}_{n+1}^{trial} - 2\mu\Delta\gamma\mathbf{n},\tag{3.113}$$

Having  $\mathbf{n} = \tilde{\sigma}_{n+1}^{trial} / \|\tilde{\sigma}_{n+1}^{trial}\|$ , equation (3.113) becomes

$$\tilde{\sigma}_{n+1} = \left(1 - \frac{2\mu\Delta\gamma}{\|\tilde{\sigma}_{n+1}^{trial}\|}\right)\tilde{\sigma}_{n+1}^{trial}.$$
(3.114)

Thus we can define  $\mu_{eff,n+1}$  as

$$\mu_{eff,n+1} = \left(1 - \frac{2\mu\Delta\gamma}{\|\tilde{\boldsymbol{\sigma}}^{trial}\|}\right)\mu,\tag{3.115}$$

# 3.4 The Moving Mesh Method (MMM)

As an adaptive strategy, the R-method is used for  $\mathbf{v}_{domain}$  [66]. This adaptive method is done by the relocation of the nodes making sure the node concentration is in high gradients regions. The procedure is done with a mapping from the domain that is not deformed in a parameter space  $\Omega_c$ , to the deformed one in the physical space  $\Omega$ . This mapping ensures provide the physical domain coverage with a computational mesh. There are three main criterion to take into account:

- 1. Mesh equations
- 2. Monitor Function
- 3. Interpolation

The choice of an appropriate mesh equation for a specific application with an efficient resolution is very important for this method. In this work, the solid dynamics equations are the ones who guide the mesh. To guide the redistribution of the mesh, a monitor function is essential. This functions depends on the arc-length of the solutions in 1D, the curvature, and post-defined errors if needed. In addition, a smoothing is required in practice. The interpolation to the new mesh of the dependent variables is not always needed unless the mesh equations are independent on time and solved apart from the PDE.

In the case where there is no interpolation, as the the moving finite element method proposed in [67, 68], the mesh equations is solved simultaneously with the PDE. The main criterion of this method are:

- 1. Equidistribution principle
- 2. Mesh equations
- 3. The method of lines (MOL) approach.

The first use of the equidistribution principle was to solve Boundary value problems (BVP) for ordinary differential equations (ODE), and it was proposed by [69]. It consists of selecting nodes so that specific measurements that represent the error in the solution are adjusted at each subinterval. The MOL approach is used usually in most of the codes of the moving mesh method, which may give a stiff equation, hence a very small time-step is needed for convergence. In this work, a moving mesh finite elements approach is used, where the mesh equations are dependent on the solid dynamics equation, with the application of the equidistribution principle on the finite element residual of the PDE. This method has various advantages:



Figure 3.10: Illustration of the moving mesh with a varying volume [35].

- 1. Interpolation free method.
- 2. Detects, track and resolve moving boundaries.
- 3. The method of lines (MOL) approach

Subsequently, to overcome the stiffness of the equations, the use of an implicit time scheme is essential. Figure (3.10) shows the displacement of an elements by a displacement vector that can activate a volume change if needed. Therefore, adopting this method, the mesh is moved with the velocity of the solid.  $\mathbf{v} = \mathbf{v}_{domain} \Rightarrow \mathbf{v} - \mathbf{v}_{domain} = 0$ . Finally the variational form the problem becomes:

$$\left(\rho \frac{\partial^2 \mathbf{u}}{\partial t^2}, \mathbf{w}_h\right) + a'\left(\mathbf{u}_h, \mathbf{w}_h\right) + \left(p_h, \nabla \cdot \mathbf{w}_h\right) + \sum_{K \in T_h} \left(\tau_{\mathbf{c}} R_c, \nabla_x \cdot \mathbf{w}_h\right) = L\left(\mathbf{w}_h\right) \forall \mathbf{w}_h \in W_{h,0}$$
$$\left(\nabla \cdot \mathbf{u}_h, q_h\right) - \left(\frac{1}{K} p_h, q_h\right) = (g, q_h) \forall q_h \in Q_h,$$
(3.116)

where a' is given by:

$$a'(\mathbf{u}_h, \mathbf{w}_h) = \int_{\Omega} \mu \operatorname{dev}[\boldsymbol{\sigma}] : \nabla^s \mathbf{w} d\Omega$$
(3.117)

# 3.5 A global thermo-elasto-plastic model

Figure (1.3) explains well the connection between the mechanical behaviour and the other phenomena. It is clear that the mechanical behaviour affects both phase transformation and the temperature, however their effect is negligible. This could

be seen in many research projects in the literature, that they neglect the effect of the mechanical behavior.

On the other side, the mechanical response is highly affected by temperature and phase transformation. This could be seen in figure (3.11) from [1], where throughout the cooling process the shape of the cylinder is changing. This change is due to many stresses caused by the temperature change and the phase transformation.



Figure 3.11: Temperature distribution and deformed shape at 2.0, 5.0, 15.0, and 100.0 seconds [1].

As an extention to the Pradtl-Reuss rule [1] [70], the total strain during the cooling process is given by

$$\varepsilon_{ij} = \varepsilon_{ij}^e + \varepsilon_{ij}^p + \varepsilon_{ij}^{th} + \varepsilon_{ij}^{ph} + \varepsilon_{ij}^{tp}$$
(3.118)

where  $d\varepsilon_{ij}^e$ ,  $d\varepsilon_{ij}^p$ ,  $d\varepsilon_{ij}^{th}$ ,  $d\varepsilon_{ij}^{ph}$ , and  $d\varepsilon_{ij}^{tp}$  are the elastic, plastic, thermal, phase transformation, and transformation-induced plasticity strain increments respectively. The elastic and plastic deformation are described in the previous section, in this section the three additional deformations will be described.

## 3.5.1 Thermal strain

The thermal deformation is only considered a volumetric deformation and expressed by the following expression:

$$\varepsilon^{th} = \beta \left( T - T_{ref} \right) \text{ with } \beta = 3\alpha_L$$
 (3.119)

Where  $\beta$ ,  $\alpha_L$ , T, and  $T_{ref}$  are the volumetric and linear expansion terms, the temperature and the reference temperature respectively.

# 3.5.2 Phase transformation strain

This part of the phase transformation deformation is also considered volumetric. It is caused by the volume fraction change of each phase. This type of strain is similar to the thermal one, it is responsible of local deformation and it is expressed by:

$$\dot{\varepsilon}^{ph} = \sum_{i \to j} \frac{1}{3} \frac{\rho_i - \rho_j}{\rho_j} \dot{F}_{i \to j} I \tag{3.120}$$

where  $\rho_i$  and  $\rho_j$  are the density of the initial and final phase respectively,  $F_{i\to j}$  is the fraction rate change from phase i to phase j.

## 3.5.3 Transformation-induced plasticity

Due to the change of the microstructure, stress is created between transformed regions and neighbor regions. This stress creates a deformation called transformationinduced plasticity strain and it is described as follows:

$$\dot{\varepsilon}^{tp} = \sum_{i \to j} \frac{3}{2} K_{i \to j} f_{i \to j}(F_j) \dot{F}_{i \to j} dev[\sigma] = \langle \kappa \rangle dev[\sigma]$$
(3.121)

where f is a phase transformation function and f(F) = F for pearlite and ferrite, and f(F) = (2 - F)F for martensite and bainite.  $\langle \kappa \rangle$  is a coefficient relates the transformation-induced plasticity strain to the deviatoric stress. To include this strain in the model, a term is added to the Lame equation (3.13) as follows:

$$\mu_{n+1}' = \frac{E_{n+1}}{2\left(1 + \nu_{n+1}\right)\left(1 + 2\mu_n \left\langle \kappa \right\rangle\right)} \tag{3.122}$$

where (n + 1) and (n) are the current and the previous time-step respectively.

## 3.5.4 Hardening rule for quenching

For the quenching application, the general Johnson-Cook hardening model will be used as follows:

$$\sigma_0 = \sigma_{00} + K.\dot{\bar{\varepsilon}}^m + H.\bar{\varepsilon}^{n1}, \qquad (3.123)$$

where  $\sigma_{00}$ , M, N, m, and n1 are plasticity parameters that are given with the material properties. These parameters depends on the temperature and the phase, hence equation (3.123) becomes:

$$\sigma_0 = \sum_i F_i \cdot \left[ \sigma_{00_i} \left( T \right) + K_i \left( T \right) \cdot \dot{\bar{\varepsilon}}^{m_i(T)} + H_i \left( T \right) \cdot \bar{\varepsilon}^{n1_i(T)} \right].$$
(3.124)

# **3.6** Numerical validation

Now that we have presented the equations of the elasticity and elasto-plasticity, with the return mapping algorithm, it is time to present some numerical test cases. First, we will show some elastic and hyper-elastic benchmarks to validate the elasticity model, and then we will proceed with elasto-plastic benchmarks.

# 3.6.1 Elasticity and hyper-elasticity

In this section, a 2D and 3D test cases will be presented to validate the elasticity model presented in section (3.2). These test cases are done in [35].

#### 3.6.1.1 Static Cook's membrane test

The Cook's membrane problem is a common test that normally gives a polluted pressure field [71]. Figure (3.12) shows the structured and unstructured meshes with P1/P1 elements for the displacement and pressure fields. A linear elastic behavior is considered with the material's properties the following: Young's modulus E = 250, poisson's ratio  $\nu = 0.5$ , and the density  $\rho = 1$ . The displacement is imposed as zero in all directions on the left side, and free to move on the top and bottom sides. A vertical traction force of 6.25 is applied on the right side.

The standard Galerkin P1/P1 elements mixed formulation gives oscillations in the pressure field when no stabilization is applied. In this case, the VMS stabilization is used which gives a cleaner and stable pressure field. The pressure field for different meshes is presented in figures (3.14). In addition, the tip displacement shows a good convergence on relatively coarse meshes as seen in figure (3.13). An important note is that the results are similar for unstructured tetrahedral meshes.

## 3.6.1.2 Transient Cook's membrane test

The transient version of the aforementioned Cook's test case is presented here. This test case is considered bending-dominant problem. For this case the hyper-elasticity model is applied, even though the final result converged to the linear elastic results. The simulation time is 7s with a time-step of 0.025s. All the properties presented previously, along with the initial and boundary conditions remain the same. The geometry in this case is the one presented in figure (3.12) with a 0.1 scale factor. The mesh used is a unstructured and fixed one with approximately 6000 elements.

As we can see in figures (3.15) and (3.16), the y displacement of the tip A evolution with time for two different time integration schemes. The solution oscillates around the steady state solution for both cases. Moreover, figure (3.17) shows a clean and stable pressure field at different time steps. We can conclude from figure

(3.15) and (3.16) that the BDF1 time scheme highly dissipating with a first order accuracy, while the second time scheme (BDF2) is less dissipating with a second order accuracy. This can be seen from the higher amplitude in the BDF2 scheme, and the slower energy dissipation with time.

#### 3.6.1.3 3D bending beam

A 3D square cylinder of dimensions of  $1 \times 1 \times 6m$  is tested in this section. A 5.2 degree rotation with respect to the z axis is applied to the beam to avoid symmetry. As initial conditions, the beam is stress free with a zero displacement. The initial velocity is given by:

$$\mathbf{v}(\mathbf{x},0) = \mathbf{v}(x,y,z,0) = \left(\frac{5z}{3},0,0\right)^T \text{ m/s} \quad y \in [0,6]\text{m}.$$
 (3.125)

The coordinates system origin is located at (0.5, 0.5, 0). The material is considered Neo-Hookean with the following properties:  $\rho_0 = 1,100 kg/m^3$ , E = 17 MPa, and  $\nu = 0.5$ .

Zero displacement Dirichlet boundary condition in all direction is imposed on the bottom of the cylinder. All other surfaces are considered traction free. The final time of the simulation is 2 seconds. Three different refined meshes were tested for a mesh convergence study, and to achieve convergence for very fine meshes. Such formulations are more devoted to divergence for refined meshes. Figures (3.18a), (3.18b), and (3.18c) shows the three different levels of refinement with number of elements equal to 1,790, 11,660, and 81,018 respectively.

Figure (3.19) shows the pressure field for three different meshes, while figure (3.20) shows the pressure field at different time-steps. Figure (3.20) also illustrates the MMM method described previously, where the mesh is moved with the domain at each time step, for a consistency with the formulation.

Figure (3.21) shows the x component of the displacement for the three different meshes, along with the reference solution. It is clear that the convergence is fast even with a coarse mesh. This proves the capability of the presented formation for relatively coarse unstructured meshes. Figure (3.22) shows the Z displacement of the tip A with respect to time, it is added to have a complete study.



Figure 3.12: Geometrical presentation, structured and unstructured meshes for the Cook's membrane. [35]



Figure 3.13: Mesh convergence study for the steady state Cook's membrane test and comparison with that from Scovazzi et. al [15]

# 3.6. NUMERICAL VALIDATION



(c) Unstructured mesh pressure field

Figure 3.14: Pressure field for different meshes. [35]



Figure 3.15: Y displacement of tip A versus time for first order time discretization and comparison with that from Castanar et. al [33].



Figure 3.16: Y displacement of tip A versus time for second order time discretization and comparison with that from Castanar et. al [33].



Figure 3.17: Pressure field at 1, 3, 5, and 7 seconds. [35]



Figure 3.18: Three different levels of refinement of unstructured meshes. [35]



Figure 3.19: 3D Bending Beam mesh convergence study. [35]



Figure 3.20: Pressure contours of the beam at 0.5, 1, 1.5, and 2 seconds. [35]



Figure 3.21: X displacement of tip versus time and comparison with that from Scovazzi et. al [15] [35]



Figure 3.22: Z displacement of tip versus time. [35]

# 3.6.2 Elasto-plasticity and hyper-elasto-plasticity

In this section, the return mapping algorithm is applied to 2D and 3D test cases to validate the elasto-plastic model presented in section (3.3).

#### 3.6.2.1 Tensile test on a rectangular plate with perfect plasticity.

Figure (3.23) describe the geometry used for this test case. The lower plane is fixed, and the upper plane is subjected to a total displacement of 0.1 mm, while the other sides are free to move. The material properties are: the Lamé coefficient  $\mu = 76.92 \ GPa$ , the bulk modulus  $\kappa = 166.66 \ GPa$ , and the yield strength  $\sigma_y =$ 200 MPa. For this case, an unstructured uniform mesh that has approximately 22,000 elements and 4,000 nodes has been used. The results will be compared to analytical results of the problem.

This is a perfect plasticity case where there is no hardening. Figure (3.24) shows the load vs displacement of the problem. When the material enters the plastic zone, the load remains constant with the deformation since there is no hardening. In addition, the results are in accordance with the analytical solution. Figures (3.25)and (3.26) shows the equivalent plastic strain and the equivalent Von Mises stress respectively.



Figure 3.23: Geometrical representation of the rectangular block with the boundary conditions.



Figure 3.24: Load displacement curve for the tensile test on the rectangular bar.



Figure 3.25: Equivalent plastic strain distribution.



Figure 3.26: Von Mises stress distribution.

#### 3.6.2.2 Tensile test on a rectangular plate with linear plasticity.

This test case is the same as the previous one represented in figure (3.23). The difference is that instead of prefect plasticity, a linear isotropic hardening rule reduced from the Hansel-Spittel hardening rule is considered and given by:

$$\sigma_0 = \sigma_y \left( \varepsilon_0 + \bar{\varepsilon}^p \right), \tag{3.126}$$

where  $\varepsilon_0 = 0.03$  is a regularization coefficient, and  $\bar{\varepsilon}^p$  is the equivalent plastic strain. The yield strength is given by  $\sigma_y = 700 \ MPa$ , and the Lamé coefficient and the bulk modulus are the same as before.

Unlike the previous case, the hardening rule is linear. For that reason, we can see in figure (3.27) a linear increase in the force with respect to deformation when the material is in the plastic zone. The equivalent Von Mises stress and equivalent strain are presented in figures (3.29) and (3.28) respectively, shows a different distribution from the previous test case because of a different hardening rule.



Figure 3.27: Load displacement curve for the tensile test on the rectangular bar.



Figure 3.28: Equivalent plastic strain distribution.



Figure 3.29: Von Mises stress distribution.

# 3.6.2.3 Tensile test on a rectangular plate with a hole with linear plasticity.

This test case is also similar to the rectangular plates represented before, but with a hole in the middle of the plate. The mesh is fine near the hole, and coarse elsewhere and it consists of approximately 17,000 elements and 8,500 nodes. The geometry and the mesh are represented in figures (3.30) and (3.32) respectively. The hardening rule is given by  $\sqrt{\frac{3}{2}} (\sigma_y + k\alpha)$  which is the same as presented in the return mapping algorithm (2). The material properties are: K = 0.7 MPa,  $\sigma_y = 0.3 MPa$ ,  $\mu = 76.92 MPa$ , and  $\kappa = 166.67 MPa$ . A dirichlet boundary condition is applied on the top of the square with a total displacement of 0.006m, while the bottom is fixed. The right and the left side of the square are free to move. This test case is compared to the one presented in [72]. Figure (3.31) shows the pressure field for the current work and the reference. The results shows a good accordance with the reference.



Figure 3.30: Geometrical representation of the plate with a hole with the boundary conditions.



Figure 3.31: Pressure field for the current work and the reference [72]



Figure 3.32: Mesh representation of the problem.

#### 3.6.2.4 Static Cook's membrane test for large displacement plasticity

This test case is the same as the one describe in figure (3.12). To be able to test the large deformation plasticity, the cook's membrane is one of the best benchmark to compare with. The test has the same boundary conditions as before with a different traction force of 0.3125, and it is tested on different meshes for a mesh convergence study. The lame coefficient is  $\mu = 80.1938$  with the bulk modulus  $\kappa = 164.21$ . A non-linear isotropic hardening rule is used and given by:

$$k(\alpha) = K\alpha + (K_{\infty} - \sigma_Y) [1 - \exp(\delta\alpha)], \qquad (3.127)$$

where K,  $K_{\infty}$ , and  $\delta$ , are material constants given by: K = 0.12924,  $K_{\infty} = 0.715$ , and  $\delta = 16.93$ .

Figure (3.33) represents the mesh convergence study. It is in coherence with the reference especially on larger meshes.


Figure 3.33: Mesh convergence study for the steady state Cook's membrane in the plasticity regime test and comparison with that from Abboud et. al [72].

### 3.7 Conclusion

In this section, the mechanical response was presented. The deformation during quenching comes into different parts: elastic, plastic, thermal, and phase transformation deformation. Each of these types of deformation was described numerically. The contribution of this thesis is the plastic, thermal and phase transformation deformation that were added to the already developed elastic solver. Numerical test cases and benchmarks were presented to validate this model. So far, the major phenomena happening in the solid were presented. It was shown that the phase transformation not only affect the temperature, but also the mechanical response. In addition, the temperature change affects the mechanical properties of the material which lead to stresses and deformations. In the following section, the boiling and evaporation model will be presented. This process will be responsible of the heat transfer between the solid and the fluid, with the mechanical behavior of the fluid.

#### 3.8 Résumé en français

Le chapitre 3 détaille la partie mécanique du solide de ce travail en proposant un modèle élastoplastique dans un formalisme de déformations lagrangien réactualisé. Les équations de la mécanique (traduisant conservation de la quantité de mouvement et de la masse) sont formulées en déplacements – pression, puis résolues par une méthode de type éléments finis sur un maillage simplicial avec une approximation linéaire pour les deux champs. La formulation discrète est enfin stabilisée par une technique de type VMS. Cinq types de déformations sont prises en compte : élastique, plastique, thermique, induite par les transformations de phases, et plastique de transformation. Le comportement élastique choisi est celui d'un matériau hyper-élastique de type néohookéen. Ce choix ainsi que la formulation du problème, sont repris d'un travail récent fait au laboratoire. L'apport de ce travail de thèse. sur ce chapitre, est donc l'introduction du comportement plastique, avec des lois d'écrouissage associées, d'abord dans un cadre petites déformations puis grandes déformations, et son implémentation effective dans un code de calcul (dérivée de Jaumann pour calculer la vitesse de déformation, algorithme du retour radial et stabilisation VMS notamment). Cette implémentation est ensuite validée sur un cas de traction d'une plaque, d'abord sans écrouissage puis avec un écrouissage linéaire. permettant d'avoir une solution analytique, puis, sous cette même condition, sur un cas de traction d'une plaque trouée. Les résultats sont alors comparés à la littérature. Enfin, une étude de convergence en fonction de la taille de maille est menée sur une membrane de Cook avec un écrouissage isotrope non-linéaire.

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BIBLIOGRAPHY

# Chapter 4

# Boiling, evaporation, and general framework

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#### 4.1 Introduction

The previous two chapters described the physical phenomena happening in the solid. This is an important study in the quenching context however the study of the fluid part is also important (figure(4.1)). As expected, computational fluid dynamics is now being used increasingly for multiphase flows and in quench design. However there still considerable uncertainties due to assumptions that must be made in particular: (i) the use of simple geometries, (ii) the use of decoupled fluid solid resolution and finally, (iii) the use of transfer coefficients that approximate the complex quenching environments. Moreover, the consequences of the numerical method limitations are the set of physical model assumptions, e.g.: incompressibility , low density ratio between phases, omission of heat conduction in one of the phases, low fidelity for boiling phenomena, laminar flows, etc. Most of these assumptions are justifiable for their intended applications; however, their use remains generally limited and suffers from systematic revalidation when facing new materials, new geometries or new thermomechanical conditions.



Figure 4.1: Heat transfer, boiling and evaporation parts of the full framework

One of the good idea is to remove all assumptions which will remove all the limitation that previous models were facing. Khalloufi et al. [1], developed a high fidelity phase change model. This model, includes all the physical phenomena that

exist on the interface during quenching. In the context, he worked on level set to be able to capture well the interface. In addition, he worked on an anisotropic mesh adaptation to achieve a high-fidelity spatial resolution. Moreover, the immersed volume method is used for two fluid modeling in the context of multiphase flows [2] and for fluid structure interactions in the context of heat and mass transfer [3]. The coupling of both was a major enhancement of the model. Furthermore, it is important to mention the study on the Navier Stokes equations to better understand the multi phase flow and the interactive of the two phases. Finally, the thermal behavior on the surface of the material was added to include the heat transfer that is causing boiling for a better accuracy.

In the following sections of this chapter, the level-set approach will be explained with the anisotropic mesh adaptation adopted for this work, then the phase change model developed will be presented, and finally the fluid-stucture interaction with the immersed body method will be explained. Numerical test case are also presented to validate this model.

#### 4.2 Level-set approach for interface capturing

The first use of the level-set methods is the computer graphics context to restore images [4]. It was later developed in [5] to apply these methods to incompressible flows. This method is used nowadays in many physical applications as two-fluid flows [6], phase change and boiling [7, 8], fluid-structure interaction [9], and many more applications. One must note that if the solid has simple geometries as a sphere or a square, a simple analytical functions can be solved that defines the solid with their corresponding meshes. However, this is not the case when we deal with complex geometries on an industrial level. In this case, a surface mesh is performed on the solid and then embedded in the main computational domain to have one fluid/solid domain.

#### 4.2.1 Standard level-set approach

Let  $\Omega$  be the global domain,  $\Omega_s$  and  $\Omega_f$  are the solid and the fluid domains respectively. The level-set function is a signed distance function where it is zero on the interface  $\Gamma = \Omega_f \cap \Omega_s$  and defined at each node in the domain as follows:

$$\alpha(X) = \begin{cases} -\operatorname{dist}(X, \Gamma) & \text{if } X \in \Omega_f, \\ 0 & \text{if } X \in \Gamma, \\ \operatorname{dist}(X, \Gamma) & \text{if } X \in \Omega_s. \end{cases}$$
(4.1)

The time evolution of this function is expressed using a transport equation as follows:

$$\frac{d}{dt}\alpha(x,t) = \frac{\partial\alpha}{\partial t} + v \cdot \nabla\alpha = 0 \tag{4.2}$$

Figure (4.2) represents the level set function on a circle solid in a fluid domain. This function satisfies this conditions:  $\|\nabla \alpha\| = 1$ . This condition is lost once the we have a convected interface by a velocity, for that reason this property needs to be reloaded for a recovery. This is done by solving the Hamilton-Jacobi equation [6]:

$$\frac{\partial \alpha}{\partial \tau} + \mathbf{s}(\alpha)(\|\nabla \alpha\| - 1) = 0 \tag{4.3}$$

where  $\tau$  is a ficticious time-step and  $s(\alpha)$  is the sign of  $\alpha$ . When the level set gradient recovers its value, we can say that the steady-state is reached. Hence, the solution of equation (4.3) is a distance function from the interface with the same zero isovalue. By doing this procedure, finding explicitly the zero isovalue is avoided.



Figure 4.2: Level-set representation of a multi-domain problem.

This is a very important property since all the properties at the interface will be distributed using the level-set. To demonstrate this phenomena, a 2D simulation of a rising bubble in a tank of water is performed. Figure (4.3a) shows the level-set at the beginning of the simulation. If the function is not reinitialized with time, the isovalues drift away from the interface as seen in figure (4.3b). That means that it is not a distance function anymore, which will give an inaccuracy in the properties distribution and that will change in the physics of the problem. Besides, figure (4.3c) the level set is properly reinitialized, thus the problem solved remains physically correct. Also, the difference in the height of the bubble in figures (4.3b) and (4.3c) shows the reinitialization effect on the physics of the problem. However, since the Hamiltion-Jacobi procedure is iterative can cause a high computational cost

for larger meshes and more complicated geometries. Another method was proposed in [10] that avoids this problem and it is called the convected level-set method.



Figure 4.3: 2D rising bubble. The zero isovalue is in red, and the levelset isovalues are in black. (a) Initial time, (b) result after 3 seconds with no reinitialization of the levelset, (c) result after 3 seconds with reinitialization of the levelset

#### 4.2.2 Convected Level-set method

To proceed with this method, the level-set function must be truncated as follows:

$$\tilde{\alpha} = Etanh\left(\frac{\alpha}{E}\right) \tag{4.4}$$

where E is the truncation thickness.

An important thing that features this method is that the level-set defined by equation (4.4) is bounded, which makes it possible to impose Dirichlet boundary conditions. Moreover, the gradient of this equation tends to zero far from the interface. This feature reduces the computational time, and avoids singularities on sharp edges and corners, which suits well the mesh adaptation procedure. The condition that the level-set satisfy is now in this form:

$$\|\nabla \tilde{\alpha}\| = 1 - \left(\frac{\tilde{\alpha}}{E}\right)^2 \tag{4.5}$$

For notation simplicity, we remove the tilde and  $\alpha$  will refer to the truncated

level-set. A linearization is applied to the gradient in order to express it with respect to the old level-set (at the previous time-step):

$$\|\nabla \alpha\| \approx \frac{\nabla \alpha^{-}}{\|\nabla \alpha^{-}\|} \nabla \alpha \tag{4.6}$$

Subsequently, the correction of the Hamilton-Jacobi to the convective form gives:

$$\frac{\partial \alpha}{\partial \tau} + \mathbf{s}(\alpha) \frac{\nabla \alpha^{-}}{\|\nabla \alpha^{-}\|} \nabla \alpha = \mathbf{s}(\alpha) \left(1 - \left(\frac{\alpha}{E}\right)^{2}\right)$$
(4.7)

If we define  $V = s(\alpha) \frac{\nabla \alpha^-}{\|\nabla \alpha^-\|}$  as the reinitialization velocity, and we combine it with equation (4.7) as it is done in [10] we get:

$$\frac{\partial \alpha}{\partial t} + v \cdot \nabla \alpha + \lambda \mathbf{s}(\alpha) \left( \|\nabla \alpha\| - \left(1 - \left(\frac{\alpha}{E}\right)^2\right) \right) = 0$$
(4.8)

where  $\lambda$  is a constant proportional to the velocity. This equation ensures the initial nature of the level-set function: a signed distance function. Finally, the equation can be written as follows:

$$\frac{\partial \alpha}{\partial t} + (v + \lambda V) \cdot \nabla \alpha = \lambda \mathbf{s}(\alpha) \left( 1 - \left(\frac{\alpha}{E}\right)^2 \right)$$
(4.9)

This method is proved to reduce the computational time, with an enhanced mass conservation than the conventional level set method [10-12].

#### 4.2.3 Mixing laws

In this work, most of the simulations are done in a single domain, specifically when dealing with boiling and evaporation, different phases are all immersed in one domain. Using the aforementioned level-set method, all the thermal and material properties will be distributed in space. To prevent singularities and to have a smooth distribution near the interface, a mixing law should be introduced. The Heavyside function gives a smooth distribution and is given by:

$$H(\alpha) = \begin{cases} 1 & \text{if } \alpha > \varepsilon \\ \frac{1}{2} \left( 1 + \frac{\alpha}{\varepsilon} + \frac{1}{\pi} \sin\left(\frac{\pi\alpha}{\varepsilon}\right) \right) & \text{if } |\alpha| \le \varepsilon \\ 0 & \text{if } \alpha < -\varepsilon \end{cases}$$
(4.10)

where  $\alpha$  is the level-set function,  $\varepsilon$  is the interface thickness and expressed in function of the mesh size in the normal direction of the interface:  $\varepsilon = O(h_{lim})$ . In the interface proximity, the mesh size can be computed using the following equation:

$$h_{lim} = \max_{j,l \in K} \nabla \alpha. \mathbf{x}^{jl}, \tag{4.11}$$

where  $\mathbf{x}^{jl} = \mathbf{x}^l - \mathbf{x}^j$  and K is the considered mesh element. While solving the PDE's, the whole domain is considered as "one phase", and the set of equations is solved on the whole domain. By the help of the Heavyside function, the properties distribution will be continuous and heterogeneous, and with the help of the anisotropic mesh adaptation the transition thickness will be small. The thermal properties as the density  $\rho$ , the heat capacity  $c_p$ , the dynamic viscosity  $\mu$ , and the temperature at the beginning are expressed using the Heavyside equation as follows:

$$\rho = \rho_f H(\alpha) + \rho_s (1 - H(\alpha))$$

$$\mu = \mu_f H(\alpha) + \mu_s (1 - H(\alpha))$$

$$\rho C_p = (\rho_f C_{pf} H(\alpha) + \rho_s C_{ps} (1 - H(\alpha)))$$

$$\rho C_p T = \rho_f C_{pf} T_f H(\alpha) + \rho_s C_{ps} T_s (1 - H(\alpha))$$
(4.12)

The equations above are linear mixing laws; however, when it comes to linear conductivity  $\lambda$  the linear mixing gives inaccurate results. A harmonic mixing law was proposed in [13] to maintain the heat flux conservation:

$$k = \left(\frac{H(\alpha)}{k_f} + \frac{1 - H(\alpha)}{k_s}\right)^{-1}$$
(4.13)

The proposed method for immersion only needs the material properties without the use of the heat transfer coefficient. By solving the PDE's with the mixed properties the heat transfer will be taken into consideration naturally.

#### 4.3 Anisotropic mesh adaptation

Since we are dealing with immersed solids, one must properly define the object and material properties must be properly dispersed to provide an accurate composition of physical problems. The mesh around the interface needs to be fine for accurate calculations in multiphase framework. In fact, adapting the mesh to physical behavior or the phenomenon under investigation is a way to improve the accuracy of numerical results. However, discontinuities in the properties between the solid and the liquid can cause problems. In fact, if the discontinuities randomly intersect the mesh elements, they will not be detected properly and may reduce the accuracy. Therefore, the goal is to combine the level set approach with a local mesh refinement around the zero isovalue of the level set function to achieve an accurate capture of the fluid-solid interface with little computational effort. The key to these aspects is the anisotropic mesh adaptation. This produces highly stretched, well-positioned elements that allow you to properly capture sharp gradients. This means that the element can be stretched in a particular direction depending on the capabilities of the solution. Several approaches to constructing anisotropic adaptive mesh are described in the literature, often depends on local modifications of the existing mesh [14-16]. These primarily require extension of the length measurement path in the spatial direction and can be done using metric fields to redefine geometric distances. Mesh fitting techniques based on post-error estimation have also been well developed [17], leading to a standardized fitting process. In this project, the mesh adaptation technique developed in [18, 19] will be used, where the the anisotropic mesh adaptation is driven by directional error estimator. The mesh adapts dynamically to the solution depending on interface position and the velocity. The goal is to improve the discretization of the region where the field of the solution is predominantly nonlinear. Improvements affect both the density of the element and its shape. These shapes are anisotropically adjusted and stretched along the direction in which the solution fields considered are linear. The mesh is locally refined around the zero isovalue of the level set function. This allows you to clearly define the interface and reduce a large number of elements compared to traditional isotropic refinements. To do this, first perform an error analysis on the mesh. Next, a metric field is defined to correlate the error with the geometry. The anisotropy error indicator is defined from this metric field and is used as a function of the remeshing optimization problem.

#### 4.3.1 Edge-based error estimator

The P1 element approximation  $u_h$  is obtained by the Lagrange interpolation on the regular function  $u \in C^2(\Omega)$ . Each vertex *i* of the grid has  $V^i = v(x^i) = v_h(x^i)$ (where  $x_i$  is the coordinate of vertex *i*). As shown in Figure (4.4), let  $\Gamma(i)$  be the "patch" associated with the vertex  $x^i$  of the mesh, define it as a set of nodes that share an edge with  $x^i$ , and let  $x^{ij}$  represent the edge connecting  $x^i$  and  $x^j$ . Since the gradient  $\nabla v_h x^{ij}$  on the edge  $x^{ij}$  is continuous, it can be written as:

$$V^{j} = V^{i} + \nabla v^{h} \cdot x^{ij}, \qquad (4.14)$$

which give us

$$\nabla u_h \cdot x^{ij} = V^j - V^i \,. \tag{4.15}$$



Figure 4.4: Patch associated with node  $x^i$ 

Based on the work in [19], post-error estimation based on edge-based error analysis associated with the length distribution tensor approach is defined:

$$||\nabla v^{h} \cdot x^{ij} - \nabla v(x^{i}) \cdot x^{ij}|| \leq \max_{y \in |x^{i}, x^{j}|} |x^{ij} \cdot H_{v}(y) \cdot x^{ij}|, \qquad (4.16)$$

with  $H_v$  is the hessian of v. To calculate the gradient  $g^i$  of v restored on node  $x^i$ , we use the following:

$$\nabla g_h \cdot x^{ij} = g^j - g^i \,. \tag{4.17}$$

The Hessian projection based on the edge gradient at the extremities is obtained as follows:

$$\left(\nabla g_h \cdot x^{ij}\right) \cdot x^{ij} = \left(g^j - g^i\right) \cdot x^{ij},\tag{4.18}$$

$$\left(H_v \cdot x^{ij}\right) \cdot x^{ij} = g^{ij} \cdot x^{ij}, \qquad (4.19)$$

where  $g^{ij} = g^j - g^i$ . The error on the edges is expressed with:

$$e^{ij} = |g^{ij} \cdot x^{ij}|$$
 (4.20)

This error sample is an accurate interpolation error along the edge and can evaluate global L2 errors. Equation (4.20) can only be evaluated if the gradient of u is known and is continuous at the nodes, hence recovery methods need to be considered.

#### 4.3.2 Gradient recovery procedure

In this work the gradient operator used for recovery is expressed as:

$$G^{i} = \arg\min_{G} \left( \sum_{j \in \Gamma(i)} | (G - \nabla v_{h}) \cdot x^{ij} |^{2} \right), \qquad (4.21)$$

Denoting  $X^i$  the length distribution tensor at node i, and using the tensor product we get:

$$X^{i} = \frac{1}{|\Gamma(i)|} \left( \sum_{j \in \Gamma(i)} x^{ij} \otimes x^{ij} \right).$$
(4.22)

The role of  $X^i$  is to represent the average of the edges distribution in the patch. If we combine equations (4.21) and (4.22), we get:

$$G^{i} = (X^{i})^{-1} \sum_{j \in \Gamma(i)} U^{ij} x^{ij} .$$
(4.23)

Hence, the error estimator is written as:

$$e_{ij} = G^{ij} \cdot x^{ij} \tag{4.24}$$

At this stage, it is important to relate  $e_{ij}$  to a metric that fits the mesh adaptation technique.

#### 4.3.3 Metric construction

The neighboring nodes should be considered so that the best average representation is the metric defined for each node [18]. The metric can be considered as a tensor where its eigenvalues are connected to the mesh sizes, and its eigenvectors define the directions of the applied sizes. The metric M is a positive symmetric definite tensor that represents a local base that modifies the computation of the distance from the Euclidean space to the metric space, therefore it is expressed as:

$$\widetilde{M}^i = (\widetilde{X}^i)^{-1}, \tag{4.25}$$

where

$$\widetilde{X}^{i} = \frac{1}{|\Gamma(i)|} \left( \sum_{j \in \Gamma(i)} s^{ij} \otimes s^{ij} \right) .$$
(4.26)

where  $s^{ij}$  is the stretching factor of the  $ij^{th}$  edge. This factor is chosen making sure that global number of nodes stays the same. It is considered as the ratio between the length of the adapted edge and the original edge. More details can be found in [20].

#### 4.3.4 Mesh adaptation criterion

When simulating complex physics with turbulence and heat transfer, such as quenching processes, capturing accurately all the properties of the problem is highly desirable, such as flow fields, temperature changes, and liquid-solid interfaces. Accordingly, various fields can be used as criteria for mesh adaptation: it takes into account the change in velocity direction, its magnitude, the level set function, and the temperature field.

The usual technique for deriving a single metric on each node in the mesh is to consider multiple fields of interest, calculate the metric for each sensor field, and perform a metric crossing operation [21]. This work simplifies this process and uses one metric that describes different variables. Thus, based on the aforementioned theory, the extension to account for different source of errors is possible, and the it is expressed as follows:

$$v\left(x^{i}\right) = \left\{\frac{\mathbf{V}^{i}}{\left|\mathbf{V}^{i}\right|}, \frac{\left|\mathbf{V}^{i}\right|}{\max_{j}\left|\mathbf{V}^{j}\right|}, \frac{\mathbf{T}^{i}}{\mathbf{T}_{\max}}, \frac{\phi}{\max(\phi)}\right\}$$
(4.27)

Since all the fields are normalized (the components of the velocity  $v_x$ ,  $v_y$  and  $v_z$  by the local velocity norm, and the level set function by their respective global maximum), all variables vary fairly with no dominance in a field that is much higher in absolute value. In the framework of the immersed volume method, the goal is to provide a good representation of the fluid/solid interfaces for a fixed number of nodes in the mesh.

#### 4.4 Phase change model

A pseudo-compressible model is described in this section taking into account the mass transfer that happens on the interface. A finite difference method was used to derive this model in [22].

#### 4.4.1 Phase change governing equations

As a reminder here below the Navier-Stokes equations:

$$\rho(\partial_t v + v \cdot \nabla v) - \nabla \cdot (2\mu\varepsilon(v)) + \nabla p = f_{ST} + f, \qquad (4.28)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0, \qquad (4.29)$$

where v is the velocity, p the pressure,  $\rho$  the density,  $\mu$  the dynamic viscosity,  $f_{ST}$  the surface tension, and f an additional source term of the momentum equation.

This model depends on the mixing law and the Heavyside function described in equations (4.12) and (4.10), used for the density distribution in space. The mass conservation in  $\Omega$  is given by:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0. \tag{4.30}$$

The mass transfer rate  $\dot{m}[kg.m^{-2}.s^{-1}]$  between the vapor and liquid phases is given by:

$$\frac{\partial}{\partial t} \left( \rho_{vp} H(\alpha) \right) + \nabla \cdot \left( \rho_{vp} H(\alpha) v \right) = \dot{m} |\nabla \alpha| \delta(\alpha), \qquad (4.31)$$

$$\frac{\partial}{\partial t}\left((1 - H(\alpha))\rho_l\right) + \nabla \cdot \left(\rho_l(1 - H(\alpha))v\right) = -\dot{m}|\nabla\alpha|\delta(\alpha), \qquad (4.32)$$

where  $\delta$  is a Dirac function. By expanding equations (4.31) and (4.32), we will get:

$$\rho_{vp}\frac{\partial H(\alpha)}{\partial t} + \rho_{vp}H(\alpha)\nabla \cdot v + \rho_{vp}v \cdot \nabla H(\alpha) = \dot{m}|\nabla\alpha|\delta(\alpha), \quad (4.33)$$

$$-\rho_l \frac{\partial H(\alpha)}{\partial t} + \rho_l (1 - H(\alpha)) \nabla \cdot v - \rho_l v \cdot \nabla H(\alpha) = -\dot{m} |\nabla \alpha| \delta(\alpha). \quad (4.34)$$

If we divide equations (4.33) and (4.34) by their respective density and we sum them, we obtain the updated mass conservation equation

$$\nabla \cdot v = \dot{m} \left( \frac{1}{\rho_{vp}} - \frac{1}{\rho_l} \right) |\nabla \alpha| \delta(\alpha).$$
(4.35)

Since the mass transfer happens at the vapor/liquid interface, the velocity is not divergence free. Summing equations (4.33) and (4.34) and dividing by  $(\rho_{vp} - \rho_l)$  gives us:

$$\frac{\partial H(\alpha)}{\partial t} + v \cdot \nabla H(\alpha) = \frac{\rho}{\rho_l - \rho_{vp}} \nabla \cdot v.$$
(4.36)

Having the time and space derivative of the Heavyside function  $\frac{\partial H(\alpha)}{\partial t} = \frac{\partial H(\alpha)}{\partial \alpha} \frac{\partial \alpha}{\partial t} = \delta(\alpha) \frac{\partial \alpha}{\partial t}$  and  $\nabla H(\alpha) = \delta(\alpha) \nabla \alpha$ , we get:

$$\delta(\alpha)\frac{\partial\alpha}{\partial t} + \delta(\alpha)v \cdot \nabla\alpha = \frac{\rho}{\rho_l - \rho_{vp}}\nabla \cdot v.$$
(4.37)

Combining equations (4.37) by (4.35) leads to

$$\delta(\alpha)\frac{\partial\alpha}{\partial t} + \delta(\alpha)v \cdot \nabla\alpha = \frac{\rho}{\rho_l - \rho_{vp}}\dot{m}\left(\frac{1}{\rho_{vp}} - \frac{1}{\rho_l}\right)|\nabla\alpha|\delta(\alpha). \tag{4.38}$$

We extend the equation to the whole domain and simplify it leads to

$$\frac{\partial \alpha}{\partial t} + v \cdot \nabla \alpha = \frac{\rho}{\rho_l \rho_{vp}} \dot{m} |\nabla \alpha|. \tag{4.39}$$

The level set equation is now given by:

$$\frac{\partial \alpha}{\partial t} + \left[ v - \frac{\rho}{\rho_l \rho_{vp}} \dot{m} \frac{\nabla \alpha}{|\nabla \alpha|} \right] \cdot \nabla \alpha = 0.$$
(4.40)

Finally, by neglecting the heat from the capillary and the viscosity forces, the energy equation becomes:

$$\rho c_p \left( \frac{\partial T}{\partial t} + v \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = -\left( L + (c_p^{vp} - c_p^l)(T - T_{\text{sat}}) \right) \dot{m} \delta(\alpha) |\nabla \alpha| \frac{\rho^2}{\rho_{vp} \rho_l}.$$
(4.41)

where T,  $T_{\text{sat}}$ ,  $c_p$ ,  $c_p^{vp}$ ,  $c_p^l$ , and k are the temperature, saturation temperature, the global specific heat, the vapor specific heat, the liquid specific heat and k is the thermal conductivity respectively.

This formulation is naturally realted to the interface thickness. In what follows in this section, the mass transfer rate  $\dot{m}$  existing in equation (4.41) will be defined.

#### 4.4.2 Surface mass transfer rate

The vaporized liquid between t and t+dt releases a heat defined by an elementray volume dV as seen in figure (4.5). This heat is used to resolve the mass transfer rate by considering a domain composed of both liquid and vapor (figure 4.5). The interface position at the time t is defined by  $\alpha(t)$  the level set at time t, dS the corresponding elementary surface and n its normal pointing in the vapor direction.



Figure 4.5: Volume dV that has vaporized between t and t + dt

dQ is the heat released by the volume dV the vaporized liquid during the elapsed time between t and t + dt and is given by:

$$dQ = \rho_l L dV \tag{4.42}$$

where L is the vaporization enthalpy  $[J.kg^{-1}]$ . The heat fluxes are respectively defined in the liquid and the vapor by  $\phi_l = -k_l \nabla T_l$  and  $\phi_{vp} = -k_{vp} \nabla T_{vp}$  where  $k_l$  and  $k_{vp}$  are the liquid and vapor thermal conductivity respectively. The condensation and vaporization occurs when the change of fluxes across the interface  $[\![\phi]\!] = [\phi_{vp} - \phi_l]_{|\alpha=0} n$  is negative and positive respectively. Thus dQ is given by:

$$dQ = \int_{t'=t}^{t+dt} \llbracket \phi \rrbracket dS dt'.$$
(4.43)

By differentiating and taking the limit when dt tends to zero we get:

$$\lim_{dt\to 0} \rho_l L \frac{\alpha(t+dt) - \alpha(t)}{dt} = \lim_{dt\to 0} \frac{1}{dt} \int_{t'=t}^{t+dt} (-k_{vp} \nabla T_{vp} + k_l \nabla T_l)_{|\alpha=0} .ndt'.$$
(4.44)

We get the surface mass transfer rate, which is called the Stefan condition,

$$\dot{m} = \rho_l L \frac{d\alpha}{dt} = \left(-k_{vp} \nabla T_{vp} + k_l \nabla T_l\right)_{|\alpha=0} .n \,. \tag{4.45}$$

The fluxes balance evaluation is required at the interface to complete equation (4.45). It is not a straightforward evaluation when an implicit definition is used at the interface. For that reason, a delta formulation is used by approximating integral of the surface by a delta Dirac function on every elementary volume as follows:

$$\int_{S_i} \left( -k_{vp} \nabla T_{vp} + k_l \nabla T_l \right)_{|\alpha=0} .ndS_i = \int_{\Omega_i} \delta(\alpha) \left( -k_{vp} \nabla T_{vp} + k_l \nabla T_l \right) .nd\Omega_i .$$
(4.46)

Finally, we integrate (4.45) on  $\Omega_i$  to get the surface mass transfer expression:

$$\dot{m} = \frac{\int_{\Omega_i} \delta(\alpha) \left( -k_{vp} \nabla T_{vp} + k_l \nabla T_l \right) \cdot n \, d\Omega_i}{\int_{\Omega_i} \delta(\alpha) d\Omega_i} \,. \tag{4.47}$$

#### 4.4.3 Implicit surface tension

The continuum surface force model is used to include the surface tension to the Navier-Stokes equations [23]. First the surface force is written as a volume as follows:

$$f_{\rm ST} = -\gamma \kappa \delta \mathbf{n} \,. \tag{4.48}$$

where  $\gamma$  is the surface tension coefficient,  $\delta$  is a Dirac function,  $\kappa$  is the mean curvature and n is the normal to the interface. Then equation (4.48) is inserted as a source term in equation (4.29). However, an explicit implementation imposes the following severe restriction on the time step [23]:

$$\Delta t < (\Delta x)^{\frac{3}{2}} \sqrt{\frac{\rho_l + \rho_{vp}}{4\pi\gamma}}.$$
(4.49)

On one hand, if we do not respect this restriction, spurious oscillations can happen to the solution that destabilize the interface. On the other hand, it impose a penalty on the computational cost of the simulation because it is lower than the time-step restriction of a CFL condition in almost two order of magnitude. For that reason, a new implicit surface tension implementation is developed in [24] to overcome this restriction, which is also used in [2, 25, 26]. With the use of differential geometry, the Laplacian of the surface  $\Delta_s I_{\Gamma}$  of an identity function is given by  $-\kappa n$ . The time evolution of an interface is given by  $I_{\Gamma}^{n+1} = I_{\Gamma}^n + v^{n+1}\Delta t$ ; on which we apply the Laplacian operator  $\Delta_s$ . In addition, we can decompose the surface Laplacian into a standard Laplacian  $\nabla^2 v - \frac{\partial^2 v}{\partial n^2} - \kappa \frac{\partial v}{\partial n}$ . If we multiply by the surface tension coefficient gives us a new surface tension expression:

$$f_{\rm ST} = -\gamma \kappa \delta n - \gamma \delta \Delta t \left( \frac{\partial^2 v}{\partial n^2} + \kappa \frac{\partial v}{\partial n} - \nabla^2 v^{n+1} \right) \,. \tag{4.50}$$

The initial term of the surface tension force  $-\gamma\kappa\delta n$  comes now with additional terms proportional to the time step. These terms act as an isotropic diffusion with the subtraction of a diffusion term in the normal direction of the interface. More details can be found in [2].

# 4.4.4 Variational MultiScale method for the Navier-Stokes equations

After all the developments done in the previous sections, we can write the Navier-Stokes equations in a general form:

$$\rho(\partial_t v + v \cdot \nabla v) - \nabla \cdot (2\mu\varepsilon(v)) + \nabla p = f_{ST} + f, \qquad (4.51)$$

$$\nabla \cdot v = f_c, \qquad (4.52)$$

The stabilization of the Navier-Stokes formulation depends on the choice of element type in spaces for the pressure and the velocity. The standard Galerkin mixed elements equal order continuous linear/linear interpolation does not give stable discretization and generates uncontrollable oscillations that give poor results. The Variational MultiScale method (VMS), proposed by [27, 28], suggest a general framework that has new variant of mixed variational form [29–33]. This stabilization is also used for the elasto-plastic solver presented in the previous section. A brief recall of the steps is presented here.

We first decompose the velocity and the pressure fields into resolvable coarsescale and unresolved fine-scale:

$$v = v_h + \tilde{v}, \tag{4.53}$$

$$p = p_h + \tilde{p}, \tag{4.54}$$

This decomposition is also made on the weighting functions. The fine-scales are mainly calculated using the residual based terms derived consistently. The finescale are then embedded in the large-scale problem as additional terms, and they are tuned by stabilization parameters. This approach gives a better stability and accuracy of the standard Galerkin formulation.

Second, the fine-scale problem is modeled, which is defined on the sum of element interiors and expressed with respect to the time-dependent large-scale parameters. It is then substituted in the coarse-scale problem, and the approximation of the fine-scale solution within each element is given by:

$$\tilde{v} = \sum_{\mathcal{T}_h} \tau_v \tilde{P}_u(R_u), \qquad (4.55)$$

$$\tilde{p} = \sum_{\mathcal{T}_c} \tau_c \tilde{P}_c(R_c), \qquad (4.56)$$

where  $R_u$  and  $R_c$  are the finite element residuals.  $\tilde{P}_v$  and  $\tilde{P}_p$  are projection operators.  $\tau_v$  and  $\tau_c$  are stabilization parameters used for tuning. Hence, the finescale explicit appearance is eliminated while still taking their effects into account. More details can be found in [2, 34].

For a simpler notation,  $f_m$  and  $f_c$  are used as the source terms in equations (4.51) and (4.52), with the addition of the explicit terms of equation (4.50) into  $f_m$ . By inserting the subscales expression, we can finally write the stabilized finite element problem. The coarse-scale variational formulation is now written as:

$$\begin{cases}
(\rho\partial_t(v_h+\tilde{v}), w_h) + (\rho(v_h+\tilde{v}) \cdot \nabla(v_h+\tilde{v}), w_h) - (p_h+\tilde{p}, \nabla \cdot w_h) \\
+ (2\mu\varepsilon(v_h):\varepsilon(w_h)) + (\gamma\delta\Delta t\nabla(v_h+\tilde{v}):\nabla w_h) = (f_m, w_h) \quad \forall w_h \in W_{h,0}, \\
(\nabla \cdot (v_h+\tilde{v}), q_h) = (f_c, q_h) \quad \forall q_h \in Q_h,
\end{cases}$$
(4.57)

and the fine scale one:

<

$$\begin{cases}
(\rho\partial_t(v_h+\tilde{v}),\tilde{w}) + (\rho(v_h+\tilde{v})\cdot\nabla(v_h+\tilde{v}),\tilde{w}) - (p_h+\tilde{p},\nabla\cdot\tilde{w}) \\
+ (2\mu\varepsilon(\tilde{v}):\varepsilon(\tilde{w})) + (\gamma\delta\Delta t\nabla(v_h+\tilde{v}):\nabla\tilde{w}) = (f_m,\tilde{w}) \quad \forall\tilde{w}\in\tilde{W}, \quad (4.58) \\
(\nabla\cdot(v_h+\tilde{v}),\tilde{q}) = (f_c,\tilde{q}) \quad \forall\tilde{q}\in\tilde{Q}.
\end{cases}$$

At this stage, one can make two assumptions for the sake of simplifying the resolution of the fine-scale equation. First we consider the subscales as quasi-static and second we approximate the convection by  $(v_h + \tilde{v}) \cdot \nabla(v_h + \tilde{v}) \approx v_h^c \cdot \nabla(v_h + \tilde{v})$ . Then, we formulate the expression of  $\tilde{v}$  and  $\tilde{p}$  by replacing them into the coarse-scales equation, and we apply the integration by parts, finally the system of equations to solve becomes:

$$\begin{cases}
\left(\rho\partial_{t}v_{h}, w_{h}\right) + \left(\rho v_{h}^{c} \cdot \nabla v_{h}, w_{h}\right) - \left(p_{h}, \nabla \cdot w_{h}\right) + \left(2\mu\varepsilon(v_{h}) : \varepsilon(w_{h})\right) + \left(\gamma\delta\Delta t\nabla v_{h} : \nabla w_{h}\right) \\
-\sum_{K\in\mathcal{T}_{h}}\left(\tau_{v}R_{v}, \rho v_{h}^{c} \cdot \nabla w_{h}\right) - \sum_{K\in\mathcal{T}_{h}}\left(\tau_{c}R_{c}, \nabla \cdot w_{h}\right) = \left(f_{m}, w_{h}\right) \quad \forall w_{h} \in W_{h,0}, \\
\left(\nabla \cdot v_{h}, q_{h}\right) - \sum_{K\in\mathcal{T}_{h}}\left(\tau_{v}R_{v}, \nabla q_{h}\right) = \left(f_{c}, q_{h}\right) \quad \forall q_{h} \in Q_{h}, \\
(4.59)
\end{cases}$$

where  $R_u$  and  $R_c$  are the finite element residuals defined by

$$R_v = f_m - \rho \partial_t v_h - \rho v_h^c \cdot \nabla v_h - \nabla p_h, R_c = f_c - \nabla \cdot v_h.$$
(4.60)

In the strongly anisotropic meshes case with widely stretched elements, the stabilization parameters definition remains an open problem and has an important role in the stabilization coefficients design. In this work, a particular choice of the stabilization parameters proposed in [2] will be adopted.

If we compare the previously described stabilization with the standard Galerkin method, additional terms evaluated on the elements are involved. These terms, obtained by the substitution of  $\tilde{u}$  and  $\tilde{p}$  into the large-scale equation, represent the sub-grid scales effects and importantly they account for the reshaped surface tension terms. They consistent way to introduce them to the Galerkin formulation in order to overcome the instabilities of the standard formulation specifically in convection dominated flows and to deal with spurious oscillations in the pressure field.[35].

#### 4.5 Fluid-structure interaction framework

It exists in the literature different types of fluid-solid coupling. Some of the works consists of solving the fluid physics alone and then transferring the data to another domain to solve the solid physics in a different software. In the previous sections, the boiling and evaporation model consists of having one domain with immersion to solve all the physics in one meshed domain. In this work, a novel fluid-solid coupling will be presented and called adaptive immersion method. As we can see in figure (4.6), this method consists on working in two different domains simultaneously, with only one software.

Figure (4.6) represents a one time-step procedure. First, the Navier-Stokes equation are solved with the convection diffusion reaction (CDR) equation to simulate the boiling and evaporation with the heat transfer between the solid and the fluid. This part was explained in this chapter (chapter 4). This is done in a fluid-solid domain where the solid is immersed in the fluid domain using the level function described above. Afterwards, the temperature distribution is transferred to a solid mesh alone to prevent solving the solid physics in the fluid domain which is a unnecessary computational cost. In the solid domain alone, the phase transformation calculations are done as described in chapter (2). Subsequently, the mechanical response in solved as described in chapter (3) and the shape of the solid in updated using the moving mesh method (MMM) presented previously. Finally, the solid is re-immersed in the fluid-solid domain by the techniques presented in this chapter, to proceed to the next time-step.

By doing so, the computational cost is reduced since the solid solvers are only solving on a solid mesh. In addition, this procedure makes the user to have more control on the solution, since one can choose different meshes for the solid an the fluid, different time-steps, and be more accurate in each domain.



Figure 4.6: Fluid-solid coupling representation

#### 4.6 Thermo-hydrodynamic framework

Another framework was proposed in [36] for very large test cases. Generally the industrial test cases of the quenching process can consist of large and complex solid parts which takes sometimes 30 hours of quenching. For that reason to reduce the computation cost, a new framework is proposed that divides the direct simulation into two parts: the Thermo-hydrodynamic part to compute the properties of the boiling part, and the thermal part of the solid. This method works as follows:

#### • The thermo-hydrodynamic part:

This part is the boiling and evaportation with a contant temperature on the solid for few seconds of the quenching. After a steady state is achieved, the heat flux is averaged locally (on each node) over this time. This process is applied using the same equations described in this chapter (chapter 4). Once the the heat transfer coefficient (HTC) is calculated, it is transferred to the solid mesh alone.

#### • Thermal Simulation:

This part consists of simulating the solid alone with the HTC transferred from the whole domain. Navier-stokes equations are not solved in this part, which makes the simulation faster specifically for large industrial applications. The work presented in chapter (2) and (3) will be applied in this part of the simulation.

For more information about this model refer to the thesis of in [36].

#### 4.7 Numerical validation

In this section, 2D and 3D simulations will be performed showing all the physical phenomena happening in the quenching process, with the presented fluid-solid coupling.

#### 4.7.1 Quenching of a 2D rectangular bar

The rectangular piece with  $8x2cm^2$  dimensions, was initially at  $780^{\circ}C$ , and the surrounding is at  $20^{\circ}C$ . The fluid-solid domain has approximately 21000 elements and 10000 nodes while the solid domain has 4000 elements and 2000 nodes. The material and thermal properties are all temperature and phase dependent. The calculations start with a Navier-Stokes study and CDR coupling for the fluid and solid together. And then at the time step, as seen in figure (4.6), the temperature is transferred to a solid domain alone to do a phase transformation and mechanical analysis. Finally the latent heat calculated will be transferred to the fluid-solid domain with the immersion of the new solid shape to proceed with the next timestep.

As results, figure (4.8) shows the anisotropic mesh adaptation described in the chapter, where the mesh is adapted to the fluid-solid interface, to the vapor bubbles. In addition, figure (4.7) represents the solution in both domains at the same timestep. We can notice the shape change in the solid domain is transferred to the fluid-solid domain. In figure (4.9) we can see the deformation of the piece during the cooling process. It is important to note that this deformation is magnified in order to visualize the shape change, but in general the deformation is small.

Figure (4.10) represents the core temperature history throughout the quenching process with and without the phase transformation effect. It is clear the phase transformation affects the cooling process at some point in the quenching. Because of the latent heat generated, we can see the decrease in the cooling speed around 50 seconds. Finally, concerning the fraction distribution, figures (4.14) describe the martensite and the pearlite fraction distribution. The difference between the fraction distribution seen here and in simulations with a heat transfer coefficient (HTC) assumption, is that the distribution is not uniform. This is an important point to stop on, since with the HTC the boundary conditions are uniform on all the piece, while here it depends on the boiling structure. For example, in figure (4.8)it is clear that the vapor bubbles are not uniform all along the piece. This explains

#### 4.7. NUMERICAL VALIDATION

why in figure 4.11 the martensite does not exist on all the boundary line. Same for figure 4.12, the pearlite transformation is faster from the top than the bottom. This also explains the importance of the piece orientation during quenching, which gives different microstructure distribution.



Figure 4.7: The rectangular piece at the final stages of quenching in both domains



Figure 4.8: Mesh adaptation on the solid and vapor bubbles



Figure 4.9: The deformation in the Y direction of the steel piece



Figure 4.10: Temperature history in the piece, with and without phase transformation



Figure 4.11: Martensite Fraction Distribution at the end of the quenching.



Figure 4.12: Pearlite Fraction Distribution half way of the quenching.



Figure 4.13: Pearlite Fraction Distribution at the end of the quenching.

Figure 4.14: Phases distribution

# 4.7.2 Quenching of a 3D cylinder

A 1080 steel cylinder with 380 mm diameter and 750 mm height is simulated based on the test case found in [37]. The mesh have approximately 3,000,000 elements and 500,000 nodes for the fluid-solid domain, and 700,000 elements and 120,000 nodes for the solid domain. The initial temperature of the cylinder is  $850^{\circ}C$  and  $20^{\circ}C$  for the surrounding.

Figure (4.15) represents the cylinder during quenching with the vapor bubbles. As mentioned before, the heat transfer while considering boiling and evaporation, will not be uniform at the piece interface. The piece orientation can play a major role in the cooling process since the gravity is taken into account. Some of the vapor bubbles can be stuck and work as thermal insulators. Before any comparison one must note that the sensor here is in the core but shifted downward in the z direction. This is because of aforementioned uneven cooling, and this could be clearly seen in figure (4.17) where the phase fractions are clearly not uniform. The effect of the latent heat on the cooling is clear even in this test case. Nevertheless, the temperature difference seen in this test case in comparison with the others is because of first the difference in the sensor place, and second the different heat transfer procedure while it includes boiling and evaporation. Finally, figure (4.18) shows the shape change of the cylinder during cooling including the elasticity, plasticity, thermal, and phase transformation stresses and deformations.



Figure 4.15: Cylinder quenching.



Figure 4.16: Temperature history in the cylinder.



Figure 4.17: Phases fraction distribution in the cross section of the cylinder (at 30s of quenching).


Figure 4.18: Cylinder deformation at 0, 10, 20, and 30s (magnification by 10).

## 4.8 Conclusion

The boiling and evaporation model was presented in this chapter. This model was already developed and used as a tool for this thesis for the completeness of the process. In addition, a new fluid-structure framework was presented that allows the coupling of this model with the solid modeling presented in the previous sections.

To conclude, at this stage the process could be fully simulated. What was presented in this chapter is responsible for the heat transfer and the behaviour happening in the water. This model was not enough to cover all the process, for that reason a framework was presented that couples the work of this chapter with the ones presented in chapter (2) and (3). This framework allows a full simulation taking into account all the physics happening in the quenching process while using only one software.

This model was tested on 2D and 3D simulation and validated. However, the presented test cases were simple geometries. In the following section, the whole framework will be applied on industrial examples with complex geometries.

### 4.9 Résumé en français

Le chapitre 4 présente la stratégie générale, en terme de modélisation et de mise en œuvre numérique, permettant de simuler une trempe avec transformations de phases dans le solide. Plus précisément, deux maillages distincts sont utilisés: l'un dans lequel le solide est immergé dans le fluide à l'aide d'une méthodologie levelset combinée à de l'adaptation anisotrope de maillage, l'autre représentant le solide seul, permettant d'effectuer les calcul de transformations de phase et de mécanique du solide décrits dans les deux chapitres précédents. Sur le premier maillage, les équations de Navier-Stokes puis l'équation de conservation de l'énergie sont résolues par une méthode éléments finis, stabilisée, pour Navier-Stokes, par une technique VMS similaire à celle présentée pour la mécanique du solide. Cependant, l'originalité de cette partie réside dans la prise en compte d'un changement de phase liquide – vapeur à l'interface solide – fluide. Ce changement, décrit rigoureusement dans le cadre level-set, se modélise par deux termes sources, l'un dans l'équation de transport de la fonction level-set, l'autre dans l'équation de la chaleur. Ces termes dépendent d'un taux de transfert surfacique de masse dont une expression est dérivée, ne faisant donc pas apparaître de coefficients de transferts issus de résultats expérimentaux. Navier-Stokes et la thermique résolues, le champ de température est projeté sur la maillage solide, lequel est réactualisé une fois les transformations de phases et le déplacement calculés. Le solide est alors réimmergé dans le milieu fluide, et la chaleur latente transférée à son tour du maillage solide au maillage global. Ce chapitre se termine par deux simulations de trempe, l'une en 2D l'autre en 3D, mettant en avant la prise en compte de la chaleur latente, et donnant une comparaison avec la littérature.

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# Chapter 5

# Industrial application

## Contents

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### 5.1 Introduction

All the numerical tools developed and describe in previous chapters will applied on an industrial scale in this chapter. In other terms, this chapter aims to test the potential of the full eularian framework for fluid and thermo-elasto-plastic treatment on complex 3D geometries. As a reminder, the industrial application we are simulating is the quenching process. This work is part of the INFINITY ANR chair with several industrial partners that provides experimental data on the quenching process.

As mentioned previously, the aim of this thesis is to achieve a full model to simulate the fluid and the solid part at the same time. It is important to recall that prior to this work, stabilized finite elements solvers were developed in the CFL team that simulates multi-phase flows, and the elasticity. However, the metallurgic and mechanical parts were still missing, specifically the plastic deformation of the solid. So the first objective in this work was to add the phase transformation happening in the steel during the quenching. This is an important physical phenomena as described before, since the purpose of quenching is controlling the microstructure and also it affects the cooling process. In addition, steel is the most used metal in most of the industrial application, with the most complicated microstructure evolution. The second objective was to simulate the geometrical change in the part. The non-homogeneous cooling with the metallurgical phases variation at different points in the solid during quenching, lead to thermal and plastic stresses that could affect the shape of the solid at the end of the process. In the industrial context, this is an important part to prevent events as cracking and significant deformation in the end product. The full model is a coupling between all the physical phenomena described in the previous chapters. It consists of solving the heat exchange between the fluid and the solid with the boiling and evaporation effect, and the metallurgical and mechanical physics in the solid simultaneously.

The importance of this model comes in the control of the process. An accurate model helps the industrial partner to simulate the process without doing experimental tests that are costly. Moreover, it is easy to add more details to the model that helps the quenching process: agitators, stirring devices, etc. Also it give a flexibility to choose different types of fluids and solids, tanks size, position and orientation of the solid.

In the next sections, two industrial test cases given from FAURECIA will be presented. All the setup and the process will be described in the industrial and numerical contexts. Results will be compared to the experimental results provided by the industrial partner.

## 5.2 Provided data from the industrial

For every simulation, the setting of the problem is given with the needed data:

- 1. The solid geometry, mainly an .STL file that gives the surface mesh.
- 2. The size of the tank, and the position of the solid in the tank.
- 3. The initial solid and fluid conditions (Temperature, stresses, metallurgical phases)
- 4. The material properties (density, heat capacity, thermal conductivity, young's modulus ...)
- 5. The Temperature Time Transformation (TTT) diagrams for the phase fractions calculations.
- 6. Experimental results that serves as a comparison at the end of the simulation.

These data are enough to set the simulation and to validate the model by comparing the numerical results to the experimental ones.

#### 5.2.1 Thermal and mechanical properties

For each material used, the thermal and the mechanical properties given are temperature dependant. Since the properties change with temperature, it is important to update them at each time-step. In addition, since we are taking the phase transformation into consideration, the properties are given for each phase at different temperature. Using the JMAT PRO software, all the mechanical and thermal materials can be retrieved by giving the chemical composition of the material used. Table (5.1) is an example of some of the given material properties for two different phases (noting that not all the material details can be given for confidentiality reasons).

Given the temperature distribution of the solid, the properties of each phase can be retrieved at each point of the solid. As a recall, a linear mixture rule is used to define the properties at each point with respect to phase fractions and temperature:

$$P(T,\xi_i) = \sum_{1}^{N} P_i F_i \tag{5.1}$$

where P is the total thermal or mechanical property,  $P_i$  is the thermal or the mechanical property of the  $i^{th}$  phase at the given temperature, and  $F_i$  is the volume fraction of the  $i^{th}$  phase.

Austenite			Pearlite				
$T(^{o}C)$	$ ho \left( kg/m^3  ight)$	$C_p\left(J/kg/C\right)$	E(GPa)	$T(^{o}C)$	$ ho \left( kg/m^3  ight)$	$C_p\left(J/kg/C\right)$	$E\left(GPa\right)$
25	8112.46	452.26	198.93	25	7844.77	450.18	210.45
50	8097.18	460.44	196.72	50	7837.49	460.77	209.39
100	8066.79	474.24	192.27	100	7822.66	480.42	207.11
150	8036.62	485.85	187.79	150	7807.46	499.51	204.44
1000	7553.22	624.63	106.38	1000	7479.80	714.46	95.90

Table 5.1: Some of the tabulated materials for two different phases.

## 5.2.2 Metallurgical data

As described in chapter 2, we are using the temperature time transformation (TTT) diagrams to calculate the phase fractions during the quenching process. Using the same software (JMAT PRO) the TTT diagrams can be given in a tabulated form for each percentage of each phase. In general we only need two states of each phase, the starting state (0.1%) and the ending state (99.9%). The table below is an example of different phases diagrams.

The "-1" in the table designate the range where the phase could not transform, it can be seen in figure (5.1).  $T_{ps}$ ,  $T_{pf}$ ,  $T_{bs}$ , and  $T_{bf}$  are the starting and the final temperatures for the pearlite and bainite phases respectively. At each time-step, we can find the starting and ending time of each phase at a given temperature, which is enough information to calculate the phase fractions. In addition to the table given, the martensite starting  $(M_s)$  and ending  $(M_f)$  temperatures are given.



Figure 5.1: TTT diagrams for the given data in table (5.2).



Figure 5.2: Solid geometry and mesh.

Pearline				Bainite			
0.1 %		99.9 %		0.1 %		99.9~%	
$T(^{o}C)$	t(s)	$T(^{o}C)$	t(s)	$T(^{o}C)$	t(s)	$T(^{o}C)$	t(s)
450.0	8.471	450.0	0.241	450.0	105.511	450.0	8.427
460.0	7.118	460.0	0.207	460.0	88.656	460.0	7.240
470.0	6.065	470.0	0.180	470.0	75.536	470.0	6.303
480.0	5.239	480.0	0.159	480.0	65.251	480.0	5.564
490.0	4.588	490.0	0.142	490.0	57.146	490.0	4.984
500.0	4.074	500.0	0.129	500.0	50.744	500.0	4.533
700.0	175.021	700.0	-1	700.0	2179.74	700.0	-1
710.0	2145.85	710.0	-1	710.0	26724.9	710.0	-1
720.0	-1	720.0	-1	720.0	-1	720.0	-1

Table 5.2: TTT diagrams in a tabulated form.

#### 5.3 Quenching of a steel part: Test case 1

The first test case is a steel part that has a denture section as seen in the CAD representation in figure (5.2).

The part passes through different stages, first the area of the denture is heated, then it passes through a forging process to get the denture. The piece is then quenched directly after the forging process. Therefore, the initial conditions of the quenching process are not evident, the temperature distribution on the piece is not homogeneous, and the phase fractions as pearlite and martensite are not zero. For that reason, a forging simulation is done on  $\text{FORGE}^{(\mathbb{R})}$  where one can retrieve the temperature and the phase fractions distribution after the denture is made. In addition, the final mesh could be also retrieved as seen in figure (5.2). The solid mesh is then immersed in whole domain which is the quenching tank. The solid is



Figure 5.3: Initial temperature distribution of the solid

approximately 15 cm long with thickness of 5 mm, and the whole domain has a size of  $0.6 \times 0.6 \times 0.3 m^3$ .

### 5.3.1 Simulation Set-up

The part is made of steel and all the properties are given in a tabulated form as described before. The initial temperature distribution of the solid is given in figure (5.3), while the water temperature is  $T_w = 22.5^{\circ}C$  with the physical parameters of the water and the vapor described in table (5.3). The quenching time is 4 seconds and is divided in an equal time interval of 0.01 seconds. An anisotropic mesh was made with approximately 6,000,000 elements and 1,000,000 nodes, while the solid mesh is approximately made of 1,000,000 elements and 200,000 nodes. For this simulation, the mesh adaptation was not used to reduce the computational cost. Instead, the mesh is done to have very fine elements near the interface with a gradually coarser mesh away from the interface as seen in figure (5.4).

In the whole domain, the Navier-Stokes equations coupled with the convection diffusion reaction equation are solved taking into account the boiling and evaporation as described in chapter 4. In the solid domain, both phase transformation equations and the elasto-plasticity one are solved to get the fraction distributions with the latent heat, and the geometrical change of the solid (chapter 2 and 3).



Figure 5.4: Immersed solid in the whole domain

	$\mu (Pa.s)$	$ ho \left( kg/m^{3} ight)$	$c_p\left(J/kg/C\right)$	$k\left(W/m/K\right)$
Water	$1.0.10^{-3}$	1000	4185	0.6
Vapor	$1.2.10^{-5}$	1.0	2010	0.025

Table 5.3: Physical parameters of the water and vapor.

### 5.3.2 Results and discussions

The liquid/vapor phase evolution can be found in figure (5.5). The temperature difference between the solid and the water is so high that the vaporization happens directly at the interface. That can be seen in the first picture of figure (5.5) at 0.5 seconds. When the simulation continues the bubble starts to form and solid surface.



Figure 5.5: Vapor/liquid phase evolution during the boiling at times t = 0.1, 0.5, 0.7, 1, 1.5 and 2 seconds

In addition figure (5.6) show the pearlite, ferrite, and martensite phase fraction distribution after 2 seconds of quenching.



Figure 5.6: Pearlite, ferrite, and martensite fractions distribution

This was the first version of this test case, the full piece was simulated with the mesh extracted from  $\text{FORGE}^{(\mathbb{R})}$ . In the next section, a newer version of the piece will be presented with a comparison with experimental results.

#### 5.4 Quenching of a steel part: Test case 1 prime

In this section, the same piece simulated previously will be presented. The same initial conditions and properties still applies for this test case. However, this time a different mesh will be used. Since retrieving the mesh directly from FORGE<sup>(R)</sup> causes some problems in the mesh (overlapping surfaces, not a smooth mesh on the sharp edged...) that leads to a high computational cost, a cleaner one will be used. Figure (5.7) shows the difference between the previous and the current mesh. In addition, to reduce more the computational cost, and by the help of the piece symmetry, half of the piece will be simulated. The mesh in figure (5.8) is done using the same procedure as before. The mesh consists of approximately 4,000,000 elements and 400,000 nodes for the fluid-solid domain, and 90,000 elements and 20,000 nodes.



Figure 5.7: Difference between the previous mesh and the clean mesh.



Figure 5.8: Solid geometry and mesh immersed in the whole domain.

#### 5.4.1 Results and discussions

Figure (5.9) shows the temperature evolution in the teeth of the part with and without phase transformation. It is clear that with phase transformation, the cooling rate changes at some point because of the latent heat. Moreover, the simulations seem different from the experimental that is because of the difference in the assumptions made. In fact, the reference is a reverse engineering process, where the heat transfer coefficient is retrieved from the experimental results and then used to simulate the cooling process. While the simulation done in this work is direct boiling simulation which gives different results in the cooling process, but the same steadystate temperature. In addition, the real application comes with agitating the piece during quenching, while the simulation is made with static state of the piece. Figure (5.10) shows the martensite fraction in one of the teeth. Most of the micostructure is composed of martensite, which give good hardness in the teeth. Figure (5.11) shows the boiling process in the thermo-hydrodynamic framework during the quenching process. Finally, figure (5.12) shows the deformation of the piece at the end of the process. The deformation is so small that it can not be seen, for that reason a magnification of 1000 to visualize the deformation.



Figure 5.9: Temperature vs time in the teeth of the part.



Figure 5.10: Martensite distribution in the teeth of the part.



Figure 5.11: Boiling in the thermo-hydrodynamics framework.



Figure 5.12: Deformation of the part after quenching. The right figure is a magnification of the deformation by 1000.

## 5.5 Conclusion

To conclude, the full framework of the quenching process was tested on more complicated cases at an industrial level. The simulations shows good results with big meshes and complex shapes. Although the results showed a little difference with the simulation, but this is only because some assumptions are still be made as the agitation of the piece which it has a major effect on the piece. However, we can say that at this stage the model is ready to be used on industrial cases to simulate real life applications.

## 5.6 Résumé en français

Le dernier chapitre de ce manuscrit présente une application industrielle fournie par la société Faurecia. La simulation de la trempe est précédée d'une simulation du forgeage de la pièce effectuée avec le logiciel Forge et permettant de fournir le champ de température et les fractions de phase (perlite et martensite) en fin de forgeage et donc en début de trempe. Cette simulation est présentée dans deux versions, l'une où le maillage découlant de l'étape de forgeage est utilisé tel quel, l'autre utilisant un maillage "lissé" et prenant en compte certaine symétries géométriques. Les résultats montrent l'évolution des phases liquide et vapeur, les distributions obtenues en perlite, ferrite et martensite, la pièce déformée, ou encore une comparaison avec l'expérience de l'évolution de température.

## Chapter 6

## **Conclusions and perspectives**

## Contents

<b>6.1</b>	<b>Conclusions</b>
<b>6.2</b>	Perspectives
6.3	Résumé en français

#### 6.1 Conclusions

In this thesis a complete framework for the quenching process was presented. All the physical phenomena happening in is process were presented throughout the chapters with numerical methods and physical modeling. The main focus in this work was on the physics happening in the solid and the coupling with the fluid behavior.

It was shown that in the literature many researcher has worked on this process. Their work was either on the fluid or on the solid alone, while some of the works included the coupling between the solid and the fluid but with some assumptions. In this work, we used finite elements models already developed in the research team with the addition of more models to have a complete framework. The focus of the team was on the fluid part of the process, for that reason this thesis was dedicated for the solid behavior.

We have seen that the physical phenomena happening in the solid affect each other, and they are affected by the fluid behavior. The boiling and evaporation define the cooling process of the solid, thus the metallurgical change in the solid is affected. Both the temperature and the metallurgical change in the solid affects the stresses and the deformation of the solid. Throughout the chapters, each physical phenomena is presented and modeled, with 2D and 3D test cases for validation.

In chapter 2, the phase transformation in steel is presented, with all its physical background. A finite element numerical model was developed in the software of this research team to simulate the creation of every phase during the quenching process. It was shows that this process affects the cooling rate of the solid and it is important to include it the framework. This model was tested and validated by test cases, and it was the first contribution of the thesis.

In chapter 3, the mechanical response of the solid was modeled. This process was shown to be affected by the temperature change and the phase transformation. The changes in the temperature leads to thermal expansion or shrinking, in addition to plastic deformation due to low plastic limits because of the high temperature. The phase transformation creates some discontinuity between two different phases which also leads to deformation and stresses. First we presented the elastic solver already developed in this team, where it model the basics of all deformations in the solid. The contribution of this thesis was to add the thermal, plastic, and phase transformation parts of the deformation. The plastic deformation includes highly non-linear resolution of equation that were presented in a return mapping algorithm. All these contribution were tested in benchmark test cases to validate the model. At this stage, all the physics happening in the solid were modeled and coupled as seen in figure (1.3). In chapter 4 the fluid part is presented with a phase change model. In the research team, a high fidelity phase change model was developed that simulated the boiling and evaporation process. This model has shown very good results in many applications. In addition, many other powerful tools exists in the software as the level-set approach, anisotropic mesh adaptation, and a VMS stabilized Navier-Stokes model that was used to have a rigorous model. In this thesis, all these models were used and coupled with the solid behavior with a new framework. This is the third thesis contribution, a novel hybrid fluid-structure interaction framework that works simultaneously on both the solid and the fluidsolid domains. This method shown faster resolution since all of the physics are solved in only one software. Furthermore, it helped manipulate each domain alone: different time-steps, different mesh ...

After each part was tested and validated, and the whole model was working on benchmark test cases, it was interesting to test this model on industrial applications. This project is in the scope of the INFINITY chair that groups many industrial partners. In chapter 5, several quenching process done in FAURECIA were tested with this model and has shown good results compared to the experimental ones provided by the industrial. It confirms the rigorousness of the model and its ability to tackle large scale problems with complex shapes.

#### 6.2 Perspectives

Although this model shown good results especially on industrial and complex applications, some of modifications and enhancement could be done to have a better model. The aim is to create an industrial software with a friendly user interface for an easier use of the model. Some challenges still exist to improve this work.

First, concerning the solid resolution, the phase transformation model is only limited to steel applications, it could be extended to deal with other types of alloys. Moreover, the plasticity added in this model is a first version and could be enhanced. For instance, the non-linearity existing in the plasticity resolution can be model differently to give better and faster results.

Second, some of the quenching setting were not taken into account, for example: agitation, solid motion, fluid alimentation. These features also help to be more close to the reality.

#### 6.2. PERSPECTIVES

Third, the computational time can still be large for very big test cases since some of the applications involves very complex shapes and long quenching time as 30 hours. The new thermo-hydrodynamic framework presented in chapter 4 was a major enhancement on the computational time, however a faster solver could still be done. One of the of the enhancement that could be done is to couple this model with the artificial intelligence (AI) technology. AI has been interfering with finite elements simulations lately to guide the model to have more precise solutions in faster calculation times.

Finally, also with the help of AI specifically deep reinforced learning, some of the process settings can be defined. For example the piece orientation, the initial temperatures, the agitation rates, etc. could be optimized using the deep reinforcement technique. This way we can have a better quality in the resulting quenched solid.

## 6.3 Résumé en français

Ce chapitre conclusive résume chaque chapitre seul avec les contrubutions ajoutées. Dans le premier chapitre, la physique de la transformation de phase dans les aciers est introduite, et implémenté numériquement avec des cas tests de validation. Le deuxième chapitre porte la physique de changement de forme de la pièce à cause des déformations elastique, plastique, thermique, et de transformation de phase. En fait la partie elastique existait dans l'équipe bien que les autre types de déformations ont été ajoutés et testés pas des cas tests 2D et 3D. Finalement les deux dernier chapitres decrivent le framework globale de la trempe industrielle numerique en prenant en compte toutes les physiques existant. Ce framework est appliqué sur des géométries simples et compliqué au niveau industriel. En addition, quelques perspectives ont été proposés pour avoir un modèle plus général et compatible avec des problèmes non linéaires. En plus, ce modèle peu être couplé avec l'intelligence artificielle pour avoir des solutions plus rapides et précises.

## 6.3. RÉSUMÉ EN FRANÇAIS

## RÉSUMÉ

La trempe est un processus de refroidissement très important adopté de nos jours par la plupart des industries, en particulier les industries automobile, aérospatiale et nucléaire. L'importance de ce procédé vient de sa capacité à contrôler la microstructure, à avoir de meilleures propriétés thermiques comme la dureté et la limite d'élasticité, et à relâcher les contraintes résiduelles. Néanmoins, il s'agit d'un processus très complexe puisqu'il comprend plusieurs phénomènes physiques à la fois sur le fluide et sur le solide. Au niveau du liquide, du fait du contact direct avec une surface chaude, le liquide va s'évaporer et atteindre le point d'ébullition. Au niveau du solide, il existe des contraintes, des déformations qui modifient la forme de la pièce et des transformations de phase qui génèrent de la chaleur latente. Un modèle d'ébullition d'évaporation est été utilisé pour simuler ce qui se passe dans l'environnement du solide. L'importance de ce modèle vient de sa capacité à donner une description réelle du transfert de chaleur qui se produit entre le solide et le fluide. Le changement de température dans le solide affectera à la fois la transformation de phase et la réponse mécanique de la pièce. Dans ce projet, un modèle hybride est développé pour résoudre à la fois l'ébullition et l'évaporation, les paramètres de transformation de phase et la réponse mécanique. Dans un domaine Fluide-Solide, Navier-Stokes couplé avec l'équation de la chaleur est résolu pour donner une distribution de température dans le solide. Dans un domaine Solide uniquement, les paramètres de transformation de phase ainsi que les contraintes et les déformations, à l'aide d'un solveur thermo-élasto-plastique, sont calculés en fonction de la distribution de température transportée depuis le domaine Fluide-Solide. La nouveauté de ce modèle est sa capacité à travailler sur deux domaines différents simultanément, et à donner une meilleure résolution sur chaque domaine, en plus de sa complétude pour simuler toute la physique se produisant dans le processus de trempe.

## MOTS CLÉS

Couplage fluide-structure, Ebullution et évaporation, Transformation de phase, Elasticité, Plasticité, Contraintes thermo-élasto-plastique.

### ABSTRACT

Quenching is a very important cooling process adopted nowadays by most of the industries, in particular automotive, aerospace and nuclear industries. The importance of this process comes from its ability to control the microstructure. to have better thermal properties as hardness and yield strength, and to release residual stresses. Nevertheless, it is a very complex process since it includes several physical phenomena on both the fluid (quenchant) and the solid. On the fluid level, because of the direct contact with a hot surface, the fluid will evaporate and reach the boiling point. On the solid level it exists stresses, deformations that changes the piece shape, and phase transformation which will generate latent heat. A boiling and evaporation was used to simulate what is happening in the surrounding of the solid. The importance of this model comes with its ability to give a real description of the heat transfer happening between the solid and the fluid. The temperature change in the solid will affect both the phase transformation and the mechanical response of the piece. In this project, a hybrid model is developed to solve the boiling and evaporation, at the same time phase transformation parameters and the mechanical response. In a Fluid-Solid domain, Navier-Stokes coupled with the heat equation is solved to give a temperature distribution in the solid. In a Solid domain only, the phase transformation parameters along with the stresses and deformations, using a thermo-elasto-plastic solver, are calculated based on the temperature distribution transported from the Fluid-Solid domain. The novelty of this model is its ability to work on two different domains simultaneously, and to give a better resolution on each domain, in addition to its completeness to simulate all the physics happening in the quenching process.

#### **KEYWORDS**

Fluid-structure interaction, Boiling and evaporation, Phase transformation, Elasticity, Plasticity, Thermoelasto-plastic stresses.