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# Thermo-metallurgical modelling of steel cooling behaviour during quenching or welding

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## ABSTRACT

This paper deals with including the metallurgical behaviour of steels into thermo-mechanical studies. For this purpose, a new model of anisothermal cooling phase transformations is proposed and applied to the thermo-metallurgical simulation of quenching. Developed in the thermodynamics framework of simple materials with memory variables, the originality of this model lies in the choice of the temperature time derivative $\dot{T}$ as an independent variable and in its easiness and rapidity of identification. The first validation presented deals with dilatometric tests and show the ability of the model to simulate all CCT deductible tests even for some tests not used for the identification. Finally, a second stage of validation of the model in a more complex situation that dilatometric tests is presented. It concerns with the simulation of a steel cylinder quench which show quite good accuracy of the numerical results and confirm the validity of the model.

## 1. INTRODUCTION

Many studies of nuclear components, involving for instance dissimilar joints or underclad defects, require the numerical simulation of thermo-metallurgical phenomena caused by heat treatment or welding in order to determine the residual stress field. The aim of this work is then to include the metallurgical behaviour of steels (and specifically their phase transformations) into thermo-mechanical studies. For this, a new model of anisothermal phase transformations has been proposed and developed in the EDF finite elements code. Developed in the thermodynamics framework of simple materials with memory variables, its originality lies in the choice of the temperature time derivative $\dot{T}$ as an independent variable and in its easiness and rapidity of identification.

The derivation of the model has been presented in detail in a previous work [7] and it is quickly reminded in a first part. Then, the identification of the model and a first stage of validation against dilatometric tests is presented and shows the ability of the model to simulate all CCT diagrams (Continuous Cooling Transformations) deductible tests even for some tests not used for the identification. A much important validation against dilatometric tests and with the model available in the Sysweld software [5] have also been carried out in a previous work [7] and have shown quite good results even for some dilatometric records not included into the CCT diagrams and have exhibit the easiness and rapidity of identification the proposed model. Finally, a second stage of validation of the model in a more complex situation that dilatometric tests is presented with the simulation of a steel cylinder quench which shows quite good accuracy of the numerical results and confirm the validity of the model.

## 2. DESCRIPTION OF THE MODEL

### *2.1. Evidencing structural transformations*

A dilatometric test (see Figure 2.1) evidences the different structural transformations (or solid state phase changes) occurring in ferritic steel subjected to welding or quenching operations. First, during heating a transformation from ferrite + pearlite (F+P) to austenite ($\gamma$) takes place. This transformation involves volumetric contraction and modification of some thermo-mechanical characteristics (especially thermal expansion coefficient and yield stress). Then, during cooling, depending on the rate, the following transformations can appear :

from austenite to ferrite + pearlite (1)

from austenite to bainite (2)

from austenite to martensite (3)

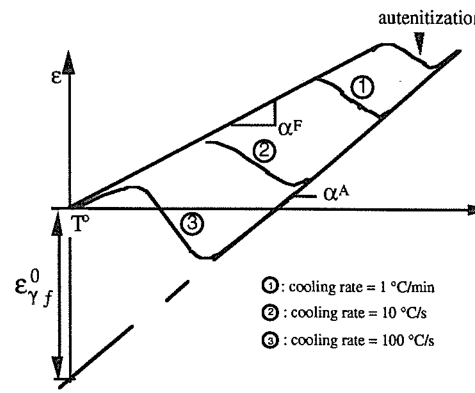


Figure 2.1 : Schematic dilatometric curves

These different transformations may be total, partial or consecutive. They involve volumetric expansion and give rise to metallurgical constituents having mainly fairly different plastic properties. That's why mechanical computations of residual stresses require, first, the simulation of the thermo-metallurgical behaviour of steel exhibiting such phase transformations.

### *2.2. State variables of the model*

As suggested by the dilatometric tests and in accordance with common approach, we choose to describe the metallurgical structure at a given material point by the quantity $\mathbf{Z} = (Z_1,Z_2,Z_3,Z_4)$, which components are the respective proportions of ferrite, pearlite, bainite and martensite. Then, to include a memory effect of time-temperature history on metallurgical evolutions we choose to develop the proposed model in the framework of thermodynamics of simple materials with memory variables. More precisely, the temperature was chosen as the pilot variable and to take into account a cooling rate effect on the structural evolutions we also include, *a priori*, the temperature time derivative $\dot{T}$ as an independent variable. Lastly, due to the austenite stabilisation phenomenon, the martensite starting temperature Ms, present in the Koïstinen-Marbürger law is also introduced as a internal variable.

### *2.3. Cooling stage model*

We suppose that the evolution of phases is ruled out by a differential equation of the first order (1), except for the martensitic one which is described by the Koistinen-Marburger law (2) in which Ms is assumed to be constant and equal to $Ms_0$ as long as the proportion of transformed austenite remains below a threshold Zs. Thus, with the hypothesis and variables adopted, we obtain :

$$\dot{z}(t) = f(T, \dot{T}, z, Ms) = f(T, \dot{T}, z)\,\frac{[T - Ms]^+}{T - Ms} \qquad \text{with } z = \{Z_1, Z_2, Z_3\} \qquad [1]$$

$$Z_4(T, z, Ms) = [1 - \sum_{i=1}^{i=3} Z_i]\,\{1 - \exp(\beta.[Ms - T]^+)\} \qquad [2]$$

where $\beta$ ($°C^{-1}$) is a material parameter and $[X]^+$ is the positive part of X.

$$\text{and } Ms(\mathbf{z}) = Ms_0 + A.[\sum_{i=1}^{i=3} Z_i - Z^S]^+ \qquad [3]$$

## 2.4. *Determination of the metallurgical evolutions*

As it seemed difficult to propose a simple form of model dependence on $\dot{T}$ based on physical mechanism or thermodynamics formalism, it was decided to impose no specific form for the metallurgical internal variable evolution equations and to use, for the determination of the metallurgical evolution rates, the known values of the evolution function derived from the CCT diagrams. Indeed, this diagrams constitute a set of time-temperature histories for which the metallurgical evolutions $\mathbf{Z}(T(t))$ are known and are each one a particular solution of evolution equations. Then, the time differentiation of these experimental $\mathbf{Z}(T(t))$ evolutions gives rise to the knowledge of a set *E* of the values of the *f* function for every state $\{T, \dot{T}, \mathbf{z}\}$ found in CCT diagrams. This identification can be carried out very easily and quickly by a computer program of discretization of the CCT diagrams.

Thus, for any thermal loading, the time integration algorithm of the constitutive law (1) use some special interpolation technique in the set *E* (where the states are now independent) to evaluate the rate of transformations for a given state $\{T, \dot{T}, \mathbf{z}\}$, without imposing any restrictions on the form of the *f* function [7-8].

Finally, the options selected have the advantage of enabling simple and fast (less that half a day) identification of the model and data preparation requiring only CCT diagrams. Furthermore, this option to impose no specific form for the metallurgical variable evolution equations allows to add any experimental result in the identification data of the model without any difficulties.

## 2.5. *Heating stage model*

During heating the only transformation able to occur is the transformation into austenite which not strongly depends to the heating rate. Then, we choose to describe this kind of transformation the same model as those proposed by Leblond [5] and for which :

$$\dot{z}_\gamma(T, z_\gamma) = \frac{Z_{eq}(T) - z_\gamma}{\tau(T)} \qquad [4]$$

where $z_\gamma$ denotes the austenite proportion and $Z_{eq}$ and $\tau$ are two temperature depending functions.

But, in order to keep an easy and quick model identification, we propose to simplify the form of the $\tau(T)$ function and perform this identification with the only $Ac_1$ and $Ac_3$ data (quasi-static temperatures of start and end of the austenitic transformation). More precisely, the $Z_{eq}$ and $\tau$ functions are defined as follow [9] :

$$Z_{eq}(T) = \begin{cases} 0 & \text{if } T \leq Ac_1 \\ \dfrac{T - Ac1}{Ac_3 - Ac_1} & \text{if } Ac_1 \leq T \leq Ac_3 \\ 1 & \text{if } T \geq Ac_3 \end{cases} \quad [5]$$

and $$\tau(T) = \begin{cases} \tau_1 & \text{if } T \leq Ac_1 \\ \tau_1 + \dfrac{T - Ac_1}{Ac_3 - Ac_1}(\tau_3 - \tau_1) & \text{if } Ac_1 \leq T \leq Ac_3 \\ \tau_3 & \text{if } T \geq Ac_3 \end{cases} \quad [6]$$

with $\tau_1$ et $\tau_3$ positive constants.

## 3. VALIDATION AGAINST DILATOMETRIC TESTS

In order to validate the presented model, two kinds of tests were performed. The first concern was to ensure that the model enables correct simulation of all the tests used for its identification i.e. twenty-nine tests defining the CCT diagram of the French 16MND5 (SA 508) steel selected to identify the model [3-4-7]. Then, using the same CCT diagram, we defined twenty-eight other thermo-metallurgical histories where the cooling rates differed from those of the records selected to identify the model. The purpose of this second series of tests is to check the model's capacity to correctly simulate these tests, which are compatible with the identification data but not integrated in them.

For all the twenty-nine tests defining the CCT diagram and the twenty-eight deduced from the CCT diagram, the imposed thermal load and resulting metallurgical response are known. So this first validation consists in numerical simulation of these tests and comparison of computed starting and finishing temperatures for each transformation and the final proportions of the constituents formed with the experimental one (cf. figures 3.1 and 3.2 where the experimental and computed CCT diagrams are superimposed in a [Temperature - Cooling rate at 700°C] reference frame).

Finally, to simplify quantification of the experimental versus computed result deviations, we define, for a given test n, the overall discrepancy on the transformation starting and finishing temperatures and on the final composition by (cf. tables 3.1 and 3.2 which show the comparison between experiments and simulation in terms of overall discrepancies) :

$$\Delta Tdn = \Sigma_i (Td_i^n - T'd_i^n).Z'f_i^n \quad ; \quad \Delta Tfn = \Sigma_i (Tf_i^n - T'f_i^n).Z'f_i^n \text{ and } \Delta Zfn = \Sigma_i (Zf_i^n - Z'f_i^n).Z'f_i^n$$

where $Td_i^n$, $Tf_i^n$ and $Zf_i^n$ (i = 1 to 4) are the transformation starting and finishing temperatures and the final composition corresponding to a given numerical test n and $T'd_i^n$, $T'f_i^n$ and $Z'f_i^n$ are the same variables corresponding to a given experimental test n.

| ΔTD (°C) | ΔTF (°C) | ΔZF (% absolute) |
|---|---|---|
| 0,97 | 2,63 | 0,57 |

Table 3.1 : Mean overall errors on simulation of the twenty-nine tests used for model identification .

| ΔTD (°C) | ΔTF (°C) | ΔZF (% absolute) |
|---|---|---|
| 1,47 | 2,28 | 0,69 |

Table 3.2 : Mean overall errors or simulation of the twenty-eight tests not used for model identification.

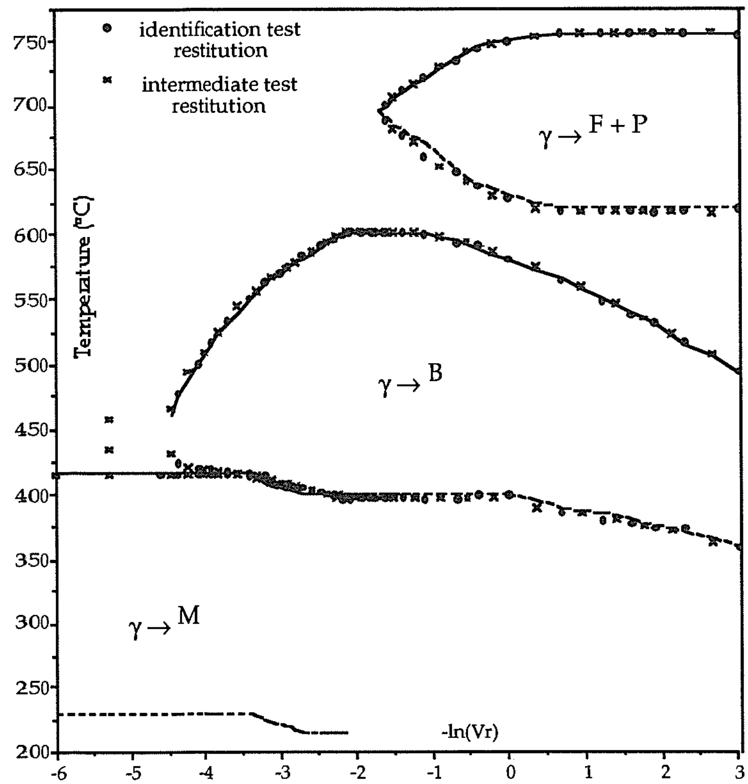


Figure 3.1 : Comparison for the proposed model between experimental and simulated transformation starting and finishing temperatures for twenty-nine identification tests and twenty-eight intermediate tests.

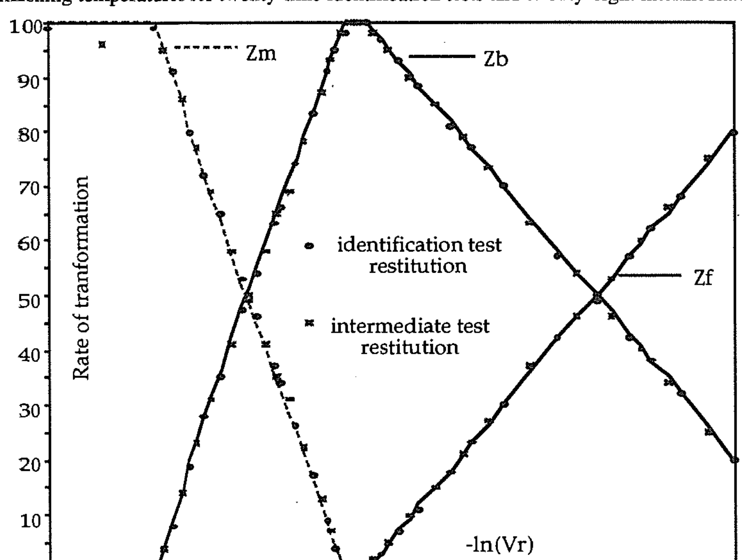


Figure 3.2 : Comparison for the proposed model between experimental and simulated final proportions of phases formed for twenty-nine identification tests and twenty-eight intermediate tests.

The conclusion on this first series of tests is that the model simulates perfectly all CCT diagram deductible tests used or not for its identification. Indeed, the discrepancies observed between experimental and computed results are of the same order of magnitude as the accuracy (and significance) of the experimental data, in a context where cooling rates range from -0.05°C/s to -400°C/s. A more complex validation through dilatometric tests fairly different that those used for CCT diagrams building can also be found in [7].

## 4. VALIDATION AGAINST STEEL QUENCHING

### *4.1. Description of the experimental process*

In order to validate the proposed model in a more complex situation that dilatometric tests, we have realised a quenching operation for a French 16MND5 steel. The chosen piece is a cylinder of 150 mm length and 100 mm diameter and the quench is a water quench at 25 °C after austenitization of one hour at the same austenitization temperature (900°C) that the CCT diagram used for the model identification. In order to allow a good thermal simulation, thermal records have been realised during all the process for different points located inside the cylinder and at its surface. Finally, after the quench, the cylinder has been cut and hardness measurements (under 5 kg) and metallurgical examinations have been carried out in order to characterise the metallurgical components formed during the quench. All these experiments was made in the Material Department of the EDF Research Division and with the collaboration of the Ensam Paris for the thermal recording [3].

### *4.2. Thermal simulation*

The exploitation of the experimental temperature evolution have allowed to determine the different stage of cooling : film boiling, nucleate boiling and natural convection and then an estimation of the thermal flux for each of these stages of cooling. Then, this first estimation of thermal flux has been modified to adjust as well as possible the numerical result with the thermal recording.

The figure 4.1 shows for different points the comparison between experimental and numerical evolution of temperature (which has been determined with taking into account the thermal dependence of the thermal properties and flux). For all the measurement points, the agreement between simulation and experiment seems quite good.

### *4.3. Metallurgical simulation and comparison with experimental measurements*

Then, the thermal evolution computed previously was used to determine the metallurgical evolution due to the quench with the proposed model identified with the CCT diagram show figures 3.1 and 3.2.

Finally, to compare the computed phase proportions with the experimental measurements, we have determined the numerical hardness from the numerical phase proportions with a linear law of mixture ; the hardness of each phase being determined by measurements.

The figure 4.2 show the comparison between numerical and experimental hardness evolutions along radius at 10, 38 and 75 mm from the upper surface (respectively denoted by H10, H38 and H75 in the figure). As for the temperature, the hardness numerical results seem quite satisfactory with a mean error between simulation and measurements of the same order that the experimental uncertainty (less than 10 Hv5).

## 6. CONCLUSION

We have proposed a metallurgical behaviour model for steel cooling which originalities are to include T among its variables, to not suppose any particular form of the metallurgical evolution function and to require only primary data such as the CCT diagrams for its identification.

The first validation elements presented, corresponding to dilatometric tests, show that, since the model is identified with CCT diagram data, it is able to well simulate all thermo-metallurgical histories derivable from this diagram, even those not used for its identification. Furthermore, identification of the model would appear to be simple and fast, and compatible with the subsequent inclusion of any tests in addition to the conventional CCT diagram identification data.

Since the model was deemed satisfactory, it has been introduced in the EDF thermo-mechanics finite element code (*Code Aster®*), together with various models described in the relevant literature for simulation of the mechanical effects of metallurgical phenomena [1-2-8]. It thus enables full simulation (thermal, metallurgical and mechanical) of operations such as welding or quenching with recording of the residual stresses induced [1-8-10] and the quench simulation here presented confirm its capability to well describe the metallurgical evolutions caused by welding or quenching cooling down.

## 7. REFERENCES


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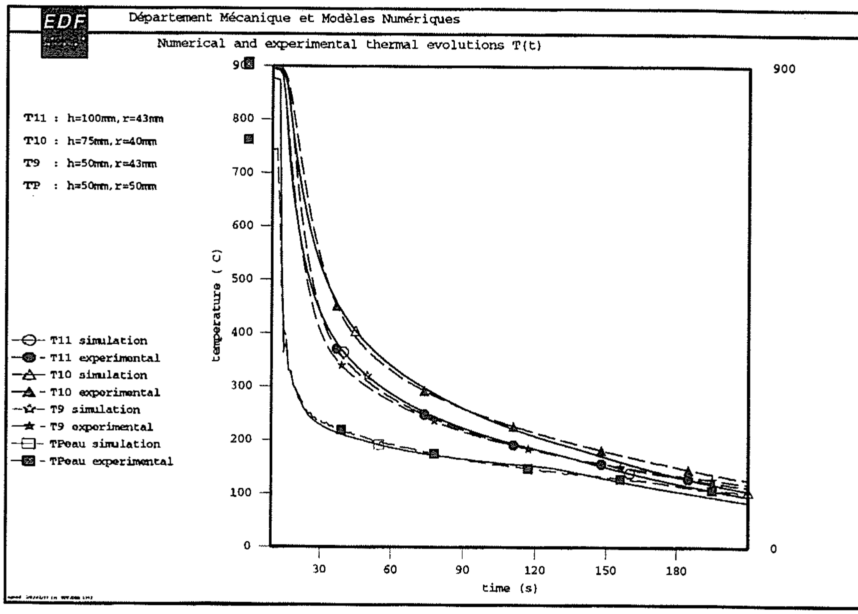


Figure 4.1 : Numerical and experimental thermal evolutions during the quench cooling down.

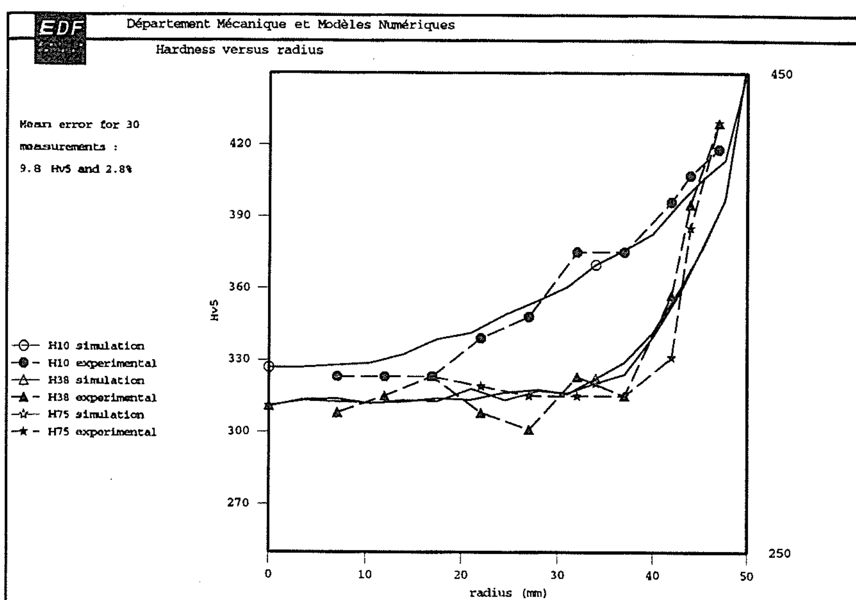


Figure 4.2 Numerical and exprimental hardness versus radius at 10, 38 and 75 mm from the upper surface.