Description of consecutive diffusive transformations in proutectoid steel using JMAK equation

Albert Capalvo[a,1,]

[a] *Universitat Politcnica de Catalunya*

Abstract

The use of the JMAK equation for describing the evolution of micro structures in steel during quenching has been extensively used since the models of exponential grow were stated decades ago.

The main interest in these thermal processes resides in high cooling rates, fact that yielded to a lack of advances in the formulation such that it could describe the behaviour of a treated material under moderately slower ones.

In this paper modifications on the JMAK equation in order to consider two consecutive diffusive transformations (such Bainite and Perlite) have been done by means of correcting the so-called fictitious time and adjusting the phase fraction of previous steps. Also formulation in order to decompose the Ferrite+Perlite fraction is introduced.

Additionally, an improvement on the calculation of incubation time is tested. This correction comes from making use of data coming from CCT diagrams, instead of just using isothermal transformation information.

Keywords: phase transformation, diffusive, JMAK, quenching, proeutectoid steel

1. Introduction

In simulations of heat treatment of steels, knowing the evolution of the material microstructure is crucial in order to determine the thermal and mechanical properties of the studied piece. By having precise results coming out of these simulations, industry can shrink the prototyping step, saving both time and money. One of those processes is the so called hot stamping, in which the material is heated above austenitization temperature, and then shaped and quenched at the same time.

Since many decades ago, coming from the work of Davenport and Baine, the behavior of steel under cooling conditions has been registered in the form of TTT and CCT diagrams, however those only covered particular case scenarios, which made its use very theoretical and as a guide. This changed when Scheil additivity rule was postulated, and therefore mathematical models could be introduced in order to describe the exponential grow of steel phases. The most important family of these models is the JMAK ecuation [1–5] to describe diffusive transformations and the Koistinen-Marburger [6], describing displacive ones.

The first notorious work implementing those ecuations in order to simulate phase evolution during continuous cooling can be found in [7, 8], and its use has been extended in time suffering minor modifications [9–15].

Microstructure change does not only have influence over the thermal and mechanical problems by means of the material properties dependence, but also trhough more implicit couplings. One of those is the latent

Email address: albert.capalvo@estudiant.upc.edu (Albert Capalvo)

heat, which is the heat generated due to changes in microstructure. In [11, 16, 17] expressions determining this latent heat can be found.

To asses final properties, the most common method is using the rule of mixtures, which simply states that a final property is the sum of the phase properties weighted with the phase fraction. This information is often extracted from experimental charts, however the reader is addressed to [18, 19] in which some expressions are presented, especially regarding to hardenability, which is one of the parameters of most interest.

Although, the JMAK model has been extensively used, there is a void under certain cooling conditions, or material types, which does not allow the model to describe the full range of possible transformations. Those are transformations with proeutectoid phases and cooling rates low enough to involve multiple diffusive transformations. The lack of study in those fields can be possibly explain by the fact that in the framework of heat processing cooling rates are kept extremely high, so that those transformations do not often take place.

However, it is believed that a proper implementation should consider them as the can affect the computation of incubations times (and therefore overall precision), or that certain material can be presented isothermal transformation curves shifted enough so that multiple diffusive transformations can take place even at high cooling rates.

2. Mathematical model

All procedure stated in this section, has been done accepting the validity of the Scheil additivity principle. The cooling law to which the piece is subjected has been discretized as a set of isothermal transformations, and therefore information regarding material parameters can be extracted from TTT diagrams.

Index 'i' represents the timestep, 'k' the phase numbering, symbol ξ to volume fraction. Additionally index 'k' can sometimes take value other than numerical in order to refer to specific phases such as austenite γ, ferrite f, perlite p, bainite b or martensite m.

2.1. Incubation time

Previous to the transformation of unstable austenite to any of the stable phases, a nuclei must be formed so that the transformation can begin. The incubation time describes the moment in which those nuclei have grown enough and is determined by sum of the partial fraction incubated in each timestep. The incubation period can be considered concluded when:

$$\int_{t=0}^{t=t} \frac{dt}{t_s(T)} = 1 \xrightarrow{\text{discretize}} \sum_{i=1}^{n} \frac{\delta t_i}{t_s(T_i)} \geq 1$$

However, as pointed in [20], this approach is not completely accurate and propose correcting the incubated fraction using additional material data coming from the CCT diagrams. The modified criteria for incubation time is now

$$\sum_{i=1}^{n} \frac{\delta t_i}{t_s(T_i)} \cdot \frac{1}{\phi_o} \geq 1$$

Where the correction factor ϕ_i is computed as

$$\phi_i = \int_{t=0}^{t=t_{s,i}^{CCT}} \frac{dt}{t_s^{TTT}}$$

2.2. Phase transformation

The JMAK ecuation is obtained integrating the differential ecuation describing the rate of of growth of a given phase [21], while considering linear growth ($r = 1$)

$$\dot{\xi} = (1-\xi)^r \frac{n}{\tau}\left(\frac{t}{\tau}\right)^{n-1}$$

Yields to the most common expression

$$\xi_k^i = 1 - exp(b_k(T_i)t^{n_k(T_i)})$$

This last equation can be modified such that it can consider transformations which saturate at $\xi_k^{end} = \xi_k^{max}$. Additionally the time t is substituted by a fictitious time $(\tau_k^i + \delta t)$, allowing for a certain independence from the incubation time, and further aiding the computation of the evolution of consecutive diffusive transformations together with the term $(\xi_\gamma^{i-1} + \xi_k^{i-1})$; which usually does not affect the result, as for single transformations $\sum \xi_k = 1$. The final expression becomes:

$$\xi_k^i = \xi_k^{max}\left(\xi_\gamma^{i-1} + \xi_k^{i-1}\right)\left(1 - exp(b_k(T_i)(\tau_k^i + \delta t)^{n_k(T_i)})\right)$$

Under normal circumstances the fictitious time is calculated as

$$\tau_k^i = \left(\frac{-ln(1-\xi_k^{i-1})}{b_k(T_i)}\right)^{\frac{1}{n_k(T_i)}}$$

However given the case of a second diffusive transformation, the volume fraction of the transforming phase at the previous timestep is adjusted using the amount of free austenite.

$$\xi_k^{i-1} \rightarrow \frac{\xi_k^{i-1}}{\xi_k^{i-1} + \xi_\gamma^{i-1}}$$

Where the material parameters $n_k(T_i)$ and $b_k(T_i)$ can be extracted from the TTT diagram as

$$n_k(T_i) = \frac{ln(\frac{ln(1-\xi_{s,k}^i)}{ln(1-\xi_{f,k}^i)})}{ln(\frac{t_{s,k}^i}{t_{f,k}^i})} \qquad b_k(T_i) = \frac{-ln(1-\xi_{s,k}^i)}{(t_{s,k}^i)^{n_k(T_i)}}$$

An important consideration made by Carlone et al.[13] is that the JMAK model is only valid when the parent phase (austenite) transforms into another single phase (eutectoid steels). This problem arises for hypo and hypereutectoid steels for temperatures below Ae1.

It can be seen in a Fe-C diagram that below Ae1 temperature austenite decomposes [simultaneously] into ferrite and perlite . However as transformation evolves, ferrite is limited by the perlite, so using two independent avrami equations (as [8] proposes)may not describe accurately the transformation.

Alternatively, it is possible to compute the ferrite-perlite phase using one single Avrami equation, and split the fraction into its components using the lever rule and the equilibrium fraction.

$$\xi_F^i = \begin{cases} \xi_{FP}^i & \xi_{FP}^i < \xi_F^{max,i} \\ \xi_F^{max,i} & \xi_{FP}^i \geq \xi_F^{max,i} \end{cases} \qquad \xi_P^i = \begin{cases} 0 & \xi_{FP}^i < \xi_F^{max,i} \\ \xi_{PF}^i - \xi_F^{max,i} & \xi_{FP}^i \geq \xi_F^{max,i} \end{cases}$$

where the maximum ferrite can be obtained using the lever rule $\xi_F^{max,i} = \frac{C_P - C_0}{C_P - C_\alpha}$,being for a pure iron-carbon steel

$$C_\alpha = -1.189 \cdot 10^{-4} T + 0.1085$$

$$C_P = 0.3429 \cdot 10^{-3} T - 1.793$$

always considering that the effect of other alloyants can be computed making use of the concept of equivalent carbon content.

Regarding the displacive transformation, despite the most used model is a modified Koistinen-Marburger equation [6], the last does not describe a complete austenite to martensite description once M_f is reached. Finally the Yu model is used [11, 13].

$$\xi_m^i = \begin{cases} \xi_\gamma \left(1 - \left(\frac{T_i - T_{M_f}}{T_{M_s} - T_{M_f}}\right)^2\right) & \xi_m^i \geq \xi_m^{i-1} \\ \xi_m^{i-1} & \xi_m^i < \xi_m^{i-1} \end{cases}$$

3. Numerical implementation

The previous mathematical model has been implemented in Fortran 90 and compiled using gcc. The code works as a subroutine which can be implemented inside any other code, requiring as input the time-temperature range of a step coming from a thermal problem.

The subroutine carries out a substepping process using a iterative scheme, so that the results can be guaranteed to be inside a given tolerance. Due to its reversible nature, the proeutectoid ferrite is only taken into consideration in the incubation time, as JMAK model is not valid for the austenite to proeutectoid ferrite transformation.

4. Results of the incubation calculation

Before showing the validation of the phase transformation, it is presented the results of the two methods for computing the incubation time. In this case the timestep size has been set to be fix (the iterative process is not carried out) in order to isolate the effects of the correction.

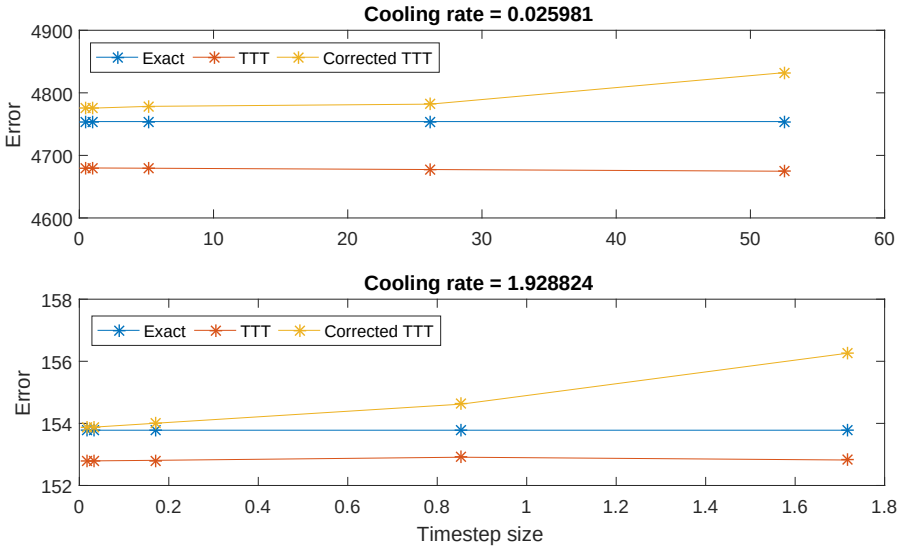

Figure 1: Convergence plot of TTT vs corrected TTT

It can be seen in figure 1 that as the timestep is refined the corrected TTT method converges towards the exact solution, while pure TTT does not visually present any convergence. Also note that the absolute error is much higher for slower cooling rates.

However the corrected TTT comes with an extremely higher computation cost, due to the addition of inner loops for the computation of the correction factor and the calculation of the integral limit $t_{s,i}^{CCT}$. Is for this reason that is preferable to use no correction and let the iterative scheme refine the time discretization where needed.

5. Validation of phase transformation

The first validation has been using an eutectoid steel and setting a constant cooling rate of 0.3 Ks^{-1} such that two diffusive transformations take place.

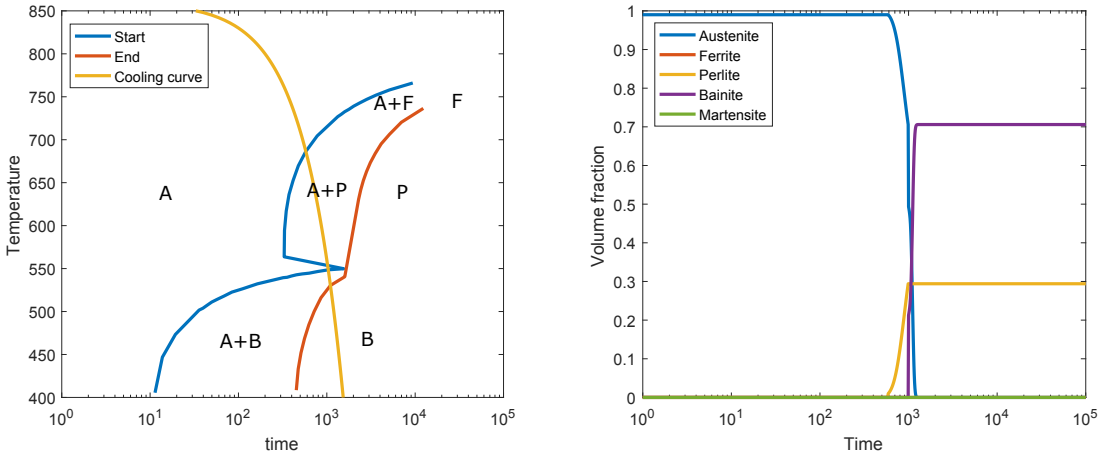

Figure 2: Time evolution of eutectoid steel cooled at 0.3 Ks^{-1} .Left: Cooling curve over CCT diagram. Right: Evolution of steel phases

Table 1: Final volume fractions for the eutectoid steel cooled at 0.3 Ks^{-1}

	Ferrite	Pertile	Bainite	Martensite	Austenite
Data	0.00	0.31	0.69	0.00	0.00
Computed	0.00	0.29	0.71	0.00	0.00

It can be seen in figure 2 that the initial and final time of transformations does match, further taking a look at the table 1 the final volume fractions are inside a 2% error compared to the exact solution.

Performing the same cooling rate to a proeutectoid steel, results are presented in figure 3 and table 2. For this type of material the start and end time does also match, but the error in the volume fraction increases to a 5%. Additionally the ferrite+perlite phase decomposition seems to yield to a misrepresentation of the perlite fraction.

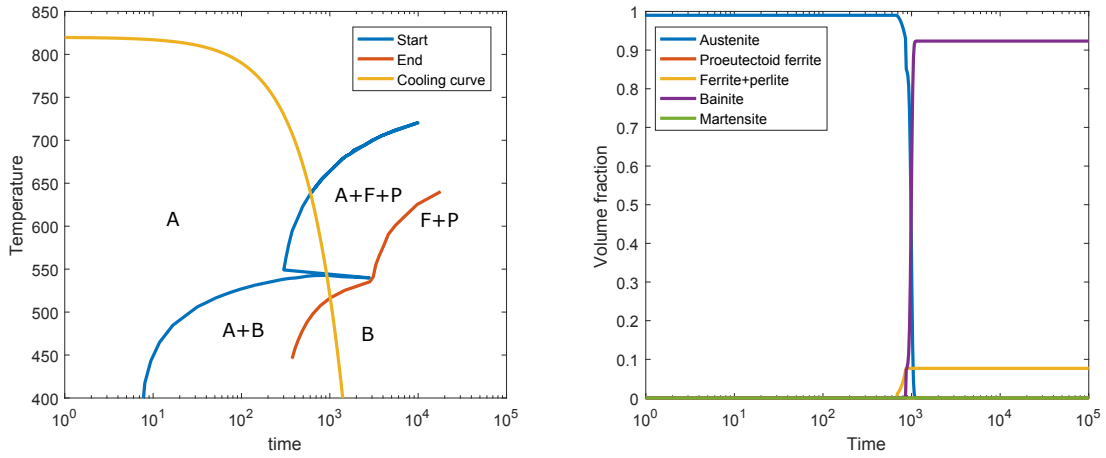

Figure 3: Time evolution of proeutectoid steel cooled at 0.3 Ks^{-1} .Left: Cooling curve over CCT diagram. Right: Evolution of steel phases

Table 2: Final volume fractions for the proeutectoid steel cooled at 0.3 Ks^{-1}

	Ferrite	Pertile	Bainite	Martensite	Austenite
Data	0.10	0.02	0.88	0.00	0.00
Computed	0.08	0.00	0.92	0.00	0.00

6. Conclusions

In this paper two aspects of the usage of JMAK equation and Scheil Additivity rule have been studied; first comparing the incubation time between using only TTT data and correcting it with CCT data, and secondly improving JMAK equation such that it could take into account consecutive diffusive transformations and transformation in proutectoid steels.

Regarding the method for computing the incubation time, it came out that while the CCT correction provides more accurate results, its computational cost is very high, being that the use of an iterative scheme is the best way to proceed.

About the modifications introduced, it has been shown to work both for eutectoid and proeutectoid steels. In the first case the error is in the order of 2% while in the second case a 5%. Also came out that the Ferrite+Perlite decomposition yields to an excess in the ferrite fraction.

Overall it has been seen that even though its simplicity, the JMAK model can describe phase transformations within an acceptable error at a low computational cost.

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