Universitat Politècnica de Catalunya

Master in Numerical Methods in Engineering

Industrial Training

Final report

Topic: Modelling of microstructural phase change and prediction of mechanical properties of steels during quenching stage in hot forming processes.

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Date: 28/02/2017

The company and the problem

Starting on November 24, and under the supervision of Dr. Fernando Rastellini, the industrial training has been being carried out in the company called Quantech ATZ. This company devotes to software development for the simulation of industrial processes, like thick sheet forming, progressive die or stretch forming among others.

The work carried on has been around a particular process called hot stamping, in which a sheet of metal is heated above austenitizing temperature, and then is press-shaped and cooled down by refrigerating the dies.

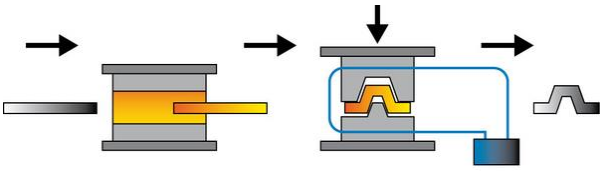


Fig 1. Hot stamping process. Extracted from:
http://automotive.arcelormittal.com/europe/products/UHSS/Usibor/EN

Currently the software the company has developed (Stampack) offers solutions using only thermal and mechanical problems. However is an industry need being able to predict the final material properties of a piece, and to do so it is necessary to know which is the final microstructural composition of the material. By simulating these kind of processes, industrial companies are able to save time and money as they can avoid having to carry out stamping tests with consequent destructive inspections.

Further, being able to couple the microstructural changes with the thermal and mechanical fields can increase the quality of the overall solution.

Phase formation in steels

Steel can be found to exist in different solid forms depending on how the atoms of iron, carbon and other alloyants arrange themselves on the atomic level. Each of the possible atomic arrangement receives the name of phase; the most common ones are:

- Austenite: Has a structure of FCC (Face Centered cubic) and is the parent phase of all possible transformations.
- Ferrite: Has a structure of BCC (Body Centered Cubic) and is formed of only iron atoms.
- Cementite: Is a carbide with an orthorhombic structure of Fe_3C.
- Perlite: Is a combination of ferrite (88 %w) and Cementite (12 %w).
- Bainite: Is a planar structure of cementite with ferrite on the dislocations.
- Martensite: Has a BCC structure and is supersaturated with carbon.

The phase transformation mechanism mainly involves the atoms of iron and carbon; more precisely on how the atoms of carbon diffuse among the iron. In order to induce any kind of phase transformation, the first requirement is the presence of free austenite and therefore the material has to be heated above the so-called austenitizing temperature. Once this temperature is reached the piece can be cooled down and depending on the cooling path the final composition of phases may vary.

For instance if the material is submitted to a slow cooling, the carbon has enough time to diffuse and ferrite is obtained; on the other hand for fast cooling rates, the carbon has no time at all to diffuse and remains trapped inside the iron forming the Martensite phase.

Also important to say, is that for transformations to take place, first a nuclei must form; this is called the incubation time.

General description of the approach

The problem that arises when trying to determine how microstructure evolves is that the available data (in form of TTT/CCT diagrams) is useful only for coolings at a constant rate or sudden cooling followed by an isothermal transformation, but in neither case for an arbitrary cooling curve.

A possible way to solve this engineering problem is by solving problems involving differential equations describing the physics of the problem, however those methods are not much studied; and also require to work at the mesoscale, which makes its computational cost prohibitive.

The approach used consists in discretizing the arbitrary cooling curve into a set of steps, and then for each one compute them as isothermal transformations [and using information from TTT diagrams].

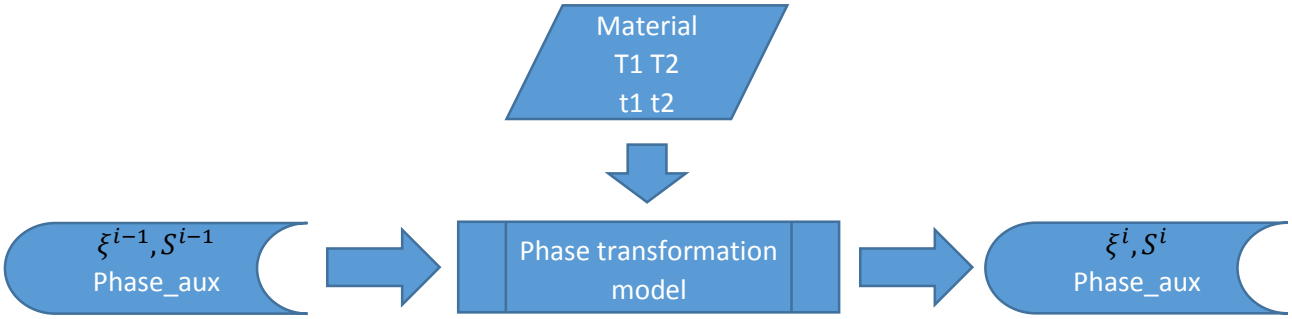
The final implementation is based on Scheil additivity rule, which states that under certain conditions an anisothermal process can be understood as the sum of consecutive isothermals ones; and the JMAK model, which describes the exponential growth of steel phases.

Implementation

Once the mathematical model was determined through looking at various scientific papers, it was coded inside Matlab environment; and once the implementation had been validated, the code was translated into Fortran.

That code in Fortran is intended to be used as a subroutine, that later can be integrated inside the company commercial code.

In the framework of hot stamping, the calculation of microstructural evolution is computed after every step of the thermal problem. Being that it may be that the timestep size required for the microstructure problem is considerably smaller than the thermal one, a substeping is done inside the subroutine. This substeping is driven by an iterative process, such that the solution the subroutine gives is guaranteed to be inside certain tolerance.



The subroutine has as input the type of material being simulated, and the time-temperature range of a step. Then using the internal variables coming from the previous time step, it computes the volume fraction ξ, the incubated fraction S, and other auxiliary variables.

Results

One of the first results obtained was regarding a method that supposedly improved the calculation of the incubation time by making use of CCT diagrams.

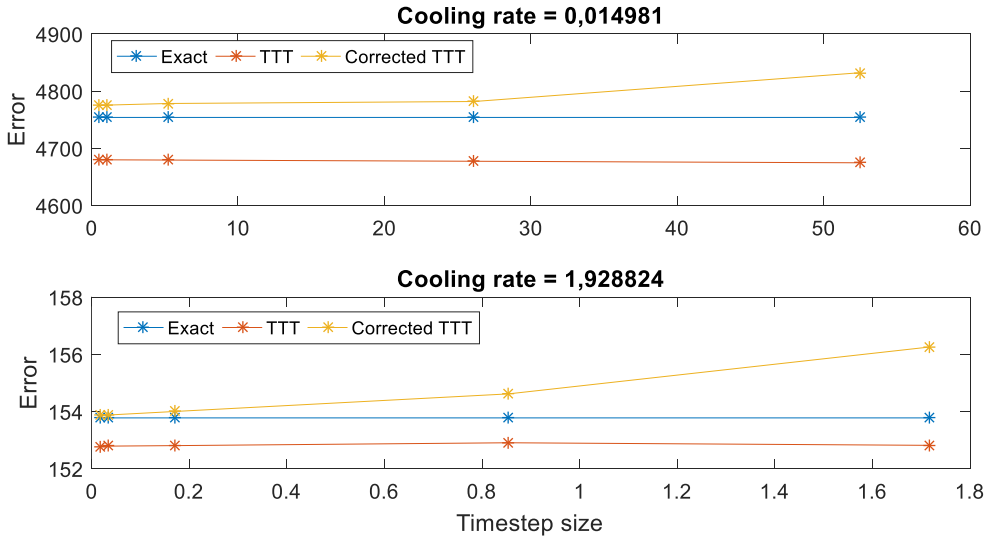


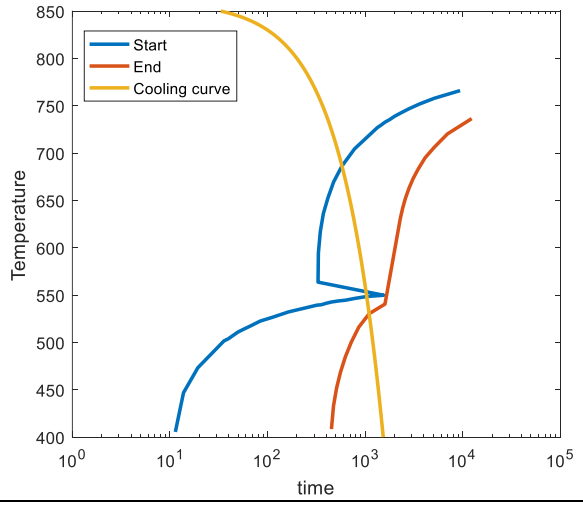
Figure 2. Convergence comparison

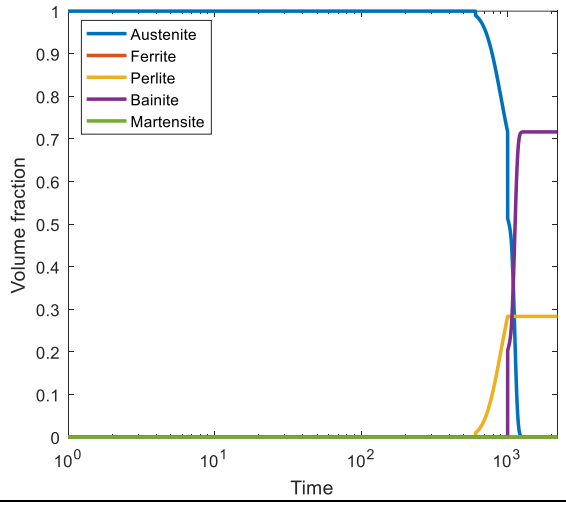
After coding both methods, it was seen (Fig 2) that the correction yielded to a faster convergence towards the exact incubation time, however the correction was extremely expensive, and it was decided to not apply it and let the iterative scheme use the proper number of time steps.

Regarding the validation of the overall implementation, the tests carried out consisted in simulating the phase transformations of cooling curves of constant cooling rate such that the solution could be compared with available data.

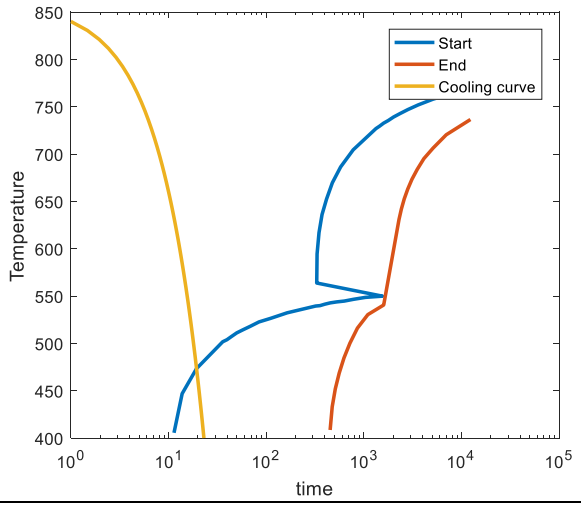
The next two sets of results show the solution of a eutectoid steel cooled down at 0.3 K/s and 20K/s.

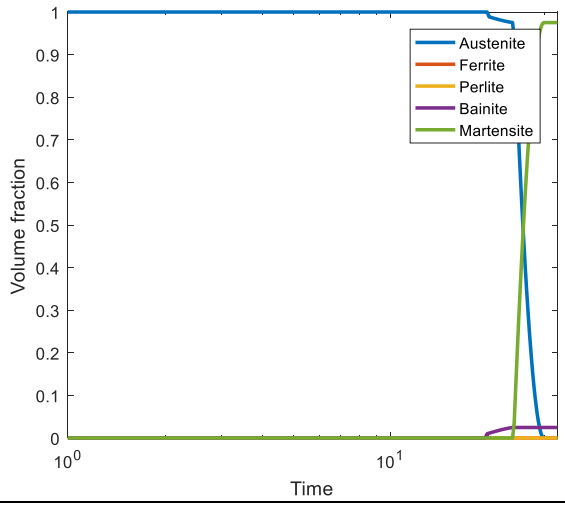
	Cooling Rate (K/s)	Ferrite fraction	Pearlite fraction	Bainite fraction	Martensite fraction	Austenite fraction	Incubation time
Data	0.3	0.0003	0.3142	0.6853	0.0000	0.0000	575.40
Simulation		0.0000	0.2834	0.7165	0.000	0.0000	603.93





	Cooling Rate (K/s)	Ferrite fraction	Pearlite fraction	Bainite fraction	Martensite fraction	Austenite fraction	Incubation time
Data	20	0.0000	0.0000	0.0699	0.9293	0.0007	19.31
Simulation		0.0000	0.000	0.02469	0.9752	0.0000	20.15





Work done (weekly summary)

- Week 1 (start 24/10/2016)

  Bibliographic research about the phase change phenomena (mostly books) and how to model it (scientific papers). Several models were found, based in its practicability the models based on JMAK equation are set to be the main interest, as other models are not well studied or are too computationally expensive.

- Week 2 (start 30/10/2016)

  Programing in Matlab environment the part of the code that computes the incubation time. The model using only TTT information and the one using an additional CTT correction were tested. Also the code for the phase transformation was started but presented wrong behaviour and results.

- Week 3 (start 07/11/2016)

  Programing in Matlab environment the part of the code that computes the time evolution of the steel phases (both diffusive and displacive transformations). Correction of a problem related with initial conditions. Model seems to work although further tests are required.

- Week 4 (start 14/11/2016)

  The model fails to compute a proper evolution for transformation involving consecutive diffusive ones (Perlite and Bainite). This problem is solved using a fix inspired in one of the papers. Using logarithmically spaced substeps is tried, it results not worth it.

- Weeks 5 and 6 (start 21/11/2016)

  Research and implementation of models applicable to hypo and hypereutectoid steels. Research of models to determine the material properties using the cooling history and steel phase fractions.

- Week 7 (start 05/12/2016)

  The Matlab code is moved to Fortran. Additional functions and subroutines had to be coded in order to serve as a substitute of built-in Matlab functions. First tests in Fortran.

- Week 8 (Start 12/12/2016)

  Finished implementation in Fortran of the code working in Matlab. Addition of substepping process for the substepping in order to guarantee the results to be inside certain tolerance.

- Week 9 (start 02/01/2017)

  Writing of the internal report describing the available models to solve the problem, detailing the models decided to use and its implementation, and showing the results of the validation tests carried out. Optimization of the code in order to reduce computation time.

- Weeks 10 and 11 (start 09/01/2017)

  Continuation of the writing of the internal report. New structure of the code is tried in order to improve performance. Testing empirical equations useful to substitute the need of data in the form of TTT diagrams.

- Week 12 (start 23/01/2017)

    Incorporation to the internal report of a performance comparison between the two coded subroutines. Finishing the internal report.

Conclusions

This internship, has supposed to me, the great opportunity of working in a company in the field I like, and furthermore doing a work which will have direct application to a commercial code.

One of my first tasks was getting familiar with phase transformation modelling, at this stage I had to cope with carrying out a research stage from scratch, learning how to filter scientific papers that were not useful to my purposes. From this work a numerical model able to predict time evolution of steel phase transformations was obtained.

After that, I had to code the implementation of that model and verify it properly worked. This stage helped improving my programing skills, especially when it comes down to optimization, as for a commercial code, performance is also crucial aspect.

Regarding the results that the implementation is able to provide, although at first it may seem that a 5% error is considerably high, it is important to also consider that the implemented method is based in empirical formulations; and also that there are several possible sources of error as for instance ‘bad resolution’ in the TTT diagrams.