Semi-Automatic Optimization of Steel Heat Treatments for Achieving Desired Microstructure

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Abstract

The thermo-mechanical processing history together with the steel composition defines the final microstructure, which in turn produces the macroscopic mechanical properties of the final product. In many industrial processes it is therefore of paramount importance to find the optimal thermal path that produces the desired microstructure. In the current study an optimization method has been developed to calculate the optimal thermal path for producing desired amounts of microstructural constituents (ferrite, bainite, martensite) of a medium carbon, low-alloy steel, and a low carbon microalloyed steel. The optimization is performed for two separate industrial processes: induction hardening of a pipeline steel and a water cooling of hot rolled steel strip. The optimization workflow consists of first setting the desired amounts of microstructural constituents, and subsequent optimization of the thermal path, which produces these desired amounts. For the water cooling of a steel strip we additionally employed previously developed tool to calculate the cooling water fluxes that are needed to realize the optimized cooling path in water cooling line after hot rolling. To demonstrate the applicability of the method, we present results that were obtained for different case studies related to the industrial processes.

Keywords: constrained optimization, nonlinear optimization, steel, processing

1 Introduction

1.1 Background

The thermo-mechanical processing history together with the steel composition defines the final microstructure, which in turn produces the macroscopic mechanical properties of the final product. In many industrial processes, it is therefore of paramount importance to find the optimal thermal path that produces the desired microstructure.

In the case of pipe induction hardening, the gradient of material properties (microstructure, hardness and hardening depth) through the pipe body can be optimized by designing the thermal cycle i.e. rates of heating and cooling along with the peak temperature and soaking time. In the induction hardening processing, the thermal cycle is very easy and precise to apply and control. As regards, an optimization is required to reach the desired material properties through the final microstructure characteristics in an efficient way.

Higher heating rate is beneficial in many ways. However to some extent it can cause inhomogeneity and abnormal grain structure (Javaheri *et al.*, 2019a) in the steel. The heating rate can also change the critical phase transformation temperature, which cause difficulties for selecting the austenitization temperature. The minimum possible peak temperature can result in the finest prior austenite grain structure, which leads to formation of very fine final microstructure and consequently will improve the strength and toughness at the same time. Increasing the cooling rate in the industrial scale may affect the production cost. However producing hard and strong microstructure such as martensite or lower bainite would not be possible if the cooling rate is smaller than a certain level. All in all, an optimization should be performed to find the best and most efficient combination of above mentioned parameters.

In industrial practice of hot rolling of steel, steel manufacturers are forced to employ the most advanced processing routes in their production lines. The control of reheating, rolling and accelerated cooling forms the basis of producing new types of high-performance steels. The capability to accurately predict and control plate or strip temperature behavior and microstructure evolution during thermomechanical processing is of fundamental importance in commercial production. In the water cooling line, it is possible, within certain limits, control the resulting microstructure for a given steel composition. Since the line layout and other processing parameters limit the available cooling paths, the optimization script needs to take these effects in to account conveniently.

Optimization of thermal processing is a common task arising in metal processing (Jung *et al.*, 2018; Tavakoli, 2018). In current study we employ the optimization tools in Matlab programming language.

1.2 Aims

In the current study an optimization tool has been developed to calculate the optimal thermal path for producing desired amounts of microstructural constituents (e.g. ferrite, bainite, martensite). Since in the current implementation, the minimization algorithm applies an initial guess, we call this implementation as "semi-automatic", although for the water cooling of steel strip the choice of the initial guess was performed by automatically testing different cooling paths, as explained later.

The optimization is performed for two separate industrial processes: induction hardening of a medium carbon, low-alloy pipe steel (Javaheri *et al.*, 2019b) and a water cooling of a hot rolled low carbon steel strip (Pohjonen *et al.*, 2018a). The optimization workflow consists of first setting the desired amounts of microstructural constituents, and subsequent optimization of the thermal path, which produces these desired amounts applying the phase transformation model described in (Pohjonen *et al.*, 2018a; Pohjonen *et al.*, 2018b; Javaheri *et al.*, 2019b). For the water cooling of a steel strip, we additionally employed previously developed tool (Paananen, 2015; Pohjonen *et al.*, 2016) to calculate the cooling water fluxes that are needed to realize the optimized cooling path in water cooling line after hot rolling.

To optimize the induction hardening process for achieving desired gradient of microstructure and mechanical properties, initially, the heating cycle (austenitization) has been optimized regarding the rate of heating and peak temperature assuming a dwell time of 2.5 s aiming for the finest prior austenite structure. Then, three different scenarios for the cooling path have been considered to achieve three thoroughly different microstructures of i) fully martensitic structure (100%), ii) fully bainitic microstructure, equal amount of upper and lower bainite (50% each) and iii) mixture of martensite and bainite (30% martensite, 40% upper bainite, and 30% lower bainite).

To test the optimization tool in the context of water cooling of hot rolled steel strip, we set the desired fractions of bainite and martensite, and perform optimization to achieve these fractions within the water cooling line. In the case of water cooling, the line layout and rolling process set some limits for the possible cooling rates. Maximum overall cooling rate at the strip centerline ranges typically from 150 °C/s to 30 °C/s while minimum cooling rate due to radiation and convection ranges from 10 °C/s to 2 °C/s for the thin and thick plates, respectively.

2 Calculations

In the current study, an optimized piecewise linear cooling path was sought. The optimization of the path was realized with the Matlab Optimization Toolbox (Mathworks, 2020) using the fmincon function. The interior point minimization algorithm with nonlinear constraints (Byrd *et al.*, 2000) was chosen for the optimization. Since the heating and cooling rates are limited in practice, the constraints for these rates are defined for the optimization. Also, the maximum temperature changes and time intervals of the path can be limited to desired values. By setting the exact time intervals for the path, the optimization tool can be adjusted to given water cooling line layout, when the speed of the strip is known.

The workflow for the cooling path optimization is depicted in Fig. 1. The applied optimization method requires an initial guess for the optimized parameters, which is used as a starting point for the optimization. Here we use the starting temperature T_0, the temperature changes ΔT_i and time intervals Δt_i for each segment i of the piecewise linear temperature path as the optimization parameters, so that the parameters describe the thermal path. The thermal path optimizer applies the fmincon function, which runs a script that calculates the phase fractions that result from the thermal path. After the calculation, the optimizer script receives the final phase fractions, and calculates the difference to the desired phase fractions, $_i \chi_{i,des} - \chi_i$. Based on the optimization algorithm (Byrd et al., 2000; Mathworks, 2020) the thermal path is changed and the optimization proceeds to minimize the difference to the desired phase fractions.

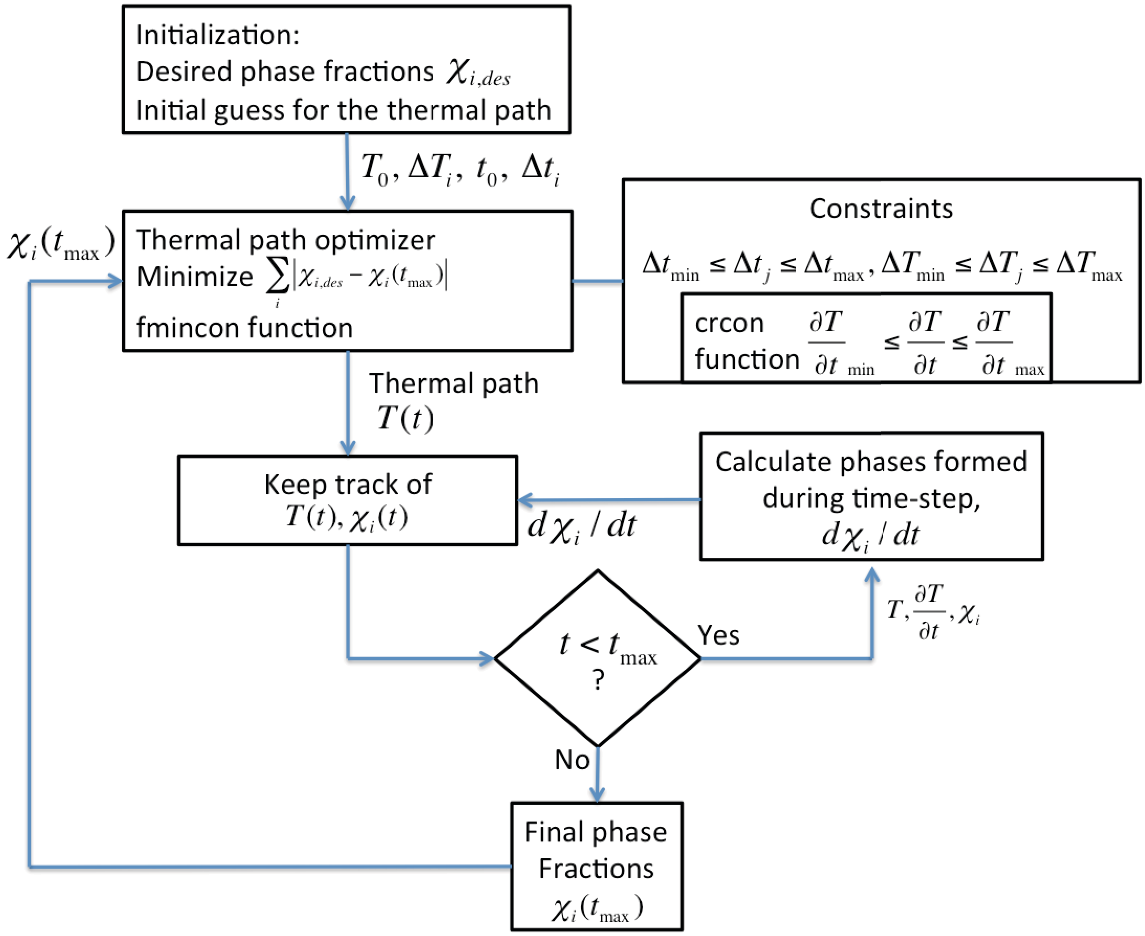

Figure 1. Optimization flowchart

Upper and lower bounds were set within the fmincon function call. From the application point of view, it is important to define the minimum and maximum cooling and heating rates, since even without additional cooling, the object cools by itself due to radiation and convection. Also, depending on the size and geometry and the applied forced cooling, there is maximum cooling rate that can be achieved. Too high or low heating rates can adversely affect the resulting microstructure. For this reason, the non-linear constraints for heating and cooling rates $\partial T/\partial t$ were set using crcon function (Mathworks, 2020) related to the fmincon minimization algorithm, to control the maximum cooling rate for each segment in the piecewise linear cooling path: $\frac{\Delta T}{\Delta t}_{\min} \le \frac{\Delta T_i}{\Delta t_i} \le \frac{\Delta T}{\Delta}_{\max}$. The phase transformation module has been described in detail generally in (Pohjonen *et al.*, 2018b), in context of induction hardening of medium carbon steel (Javaheri *et al.*, 2019b) and in the context of water cooling of hot rolled low carbon steel in (Pohjonen *et al.*, 2018a), where (Javaheri *et al.*, 2019b) and (Pohjonen *et al.*, 2018a) also include the transformation model parameters fitted for the steels that were used in these examples.

Since the minimization script finds a local minimum near to the initial guess, it is required to choose suitable initial guess, so that the algorithm can find a good minimum. For the test cases related to optimization of the cooling path of water cooled steel strips, we applied a script to automatically test nine different initial guesses for the cooling paths and then select the one that produced the best solution. The cooling paths described by the initial guesses are shown in Fig. 2.

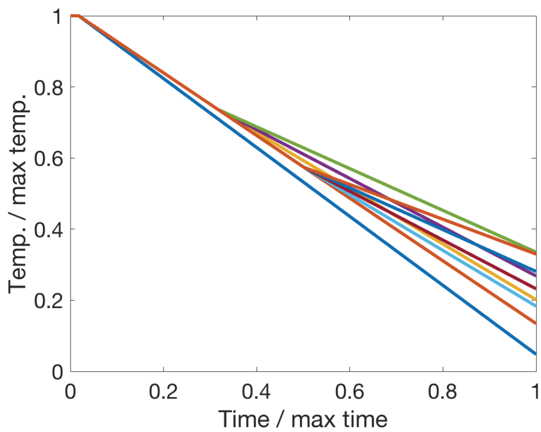

Figure 2. Thermal paths used as initial guesses for the optimization of the temperature path for water cooling of hot rolled steel strip.

After the thermal path to produce desired microstructure in the strip cooling line is optimized, another optimization script is used for calculating the required water fluxes. The water flux calculation is done by an approximate model presented elsewhere (Paananen, 2015; Pohjonen *et al.*, 2016). This model calculates the average temperature at the mid-depth of the steel strip. Approximate model was fitted using a more detailed but computationally heavier model (Pyykkönen *et al.*, 2012) so that the effect of strip temperature and water flux was studied with wide variety of parameters in detailed model. These results were used to form tables for mean cooling rate, k, under one cooling unit as a function of temperature and water flux. Later, the mean cooling rate for arbitrary temperature or water flux is calculated by using these tables and linear interpolation.

$$T_{i+1} = T_i + \frac{\Delta z\, l}{t_{strip} v_{strip}} k(T,\theta) \qquad (1)$$

where T is temperature, Δz is thickness, l is the length between two modelling points, v is velocity, k is average cooling rate and θ is the water flux. Subscript i denotes a modelling point.

For the induction hardening cases, the optimization time interval was longer, hence it was more suitable to find the initial cooling path by testing few different paths that already produce some amount of the desired phase fractions, so that the optimization script then is capable of finding how the changes of the path affect the resulting phase fractions. While the optimization for the steel strip was fully automated, the semi-automatic optimization was chosen for the induction hardening cases.

3 Results and discussion

3.1 Water cooling of hot rolled steel strip

In the case of steel strip cooling, the chemical composition and rolling procedure limit the possible phase fractions that can be obtained during water cooling. However, in some cases, even small changes to the final phase fractions may lead to desired change in the final properties of steel. Two different cases are presented where the fractions of bainite and martensite are 20 % bainite - 80% martensite for case i) and 40 % bainite - 60 % martensite for case ii). In these cases, five (time, temperature) points were chosen, at which the temperature is optimized. In reality, there could be even more fitting points, but this would make it more difficult to know what the constraints for different zones would be.

First, optimal cooling path to produce desired amounts of bainite and martensite is found through optimization presented in this work, then the water fluxes that produce this cooling path in the cooling line are calculated with an approximate model (Paananen, 2015). Finally, the cooling path that can be achieved in the cooling line (continuous line in Figures 4 and 6) was used as an input to phase transformation model, to check that even though there are some small differences in the thermal path of Figs 3 and 4, the desired phase fractions are still obtained.

3.1.1 Water cooling of steel strip case i), 20 % bainite, 80 % martensite

The optimized thermal path and phase fractions for water cooled steel strip test case i) are shown in Fig. 3. The path started from fully austenitic structure. The path was optimized to produce 20 % bainite and 80 % martensite. The optimized normalized water fluxes are shown in Fig. 4.

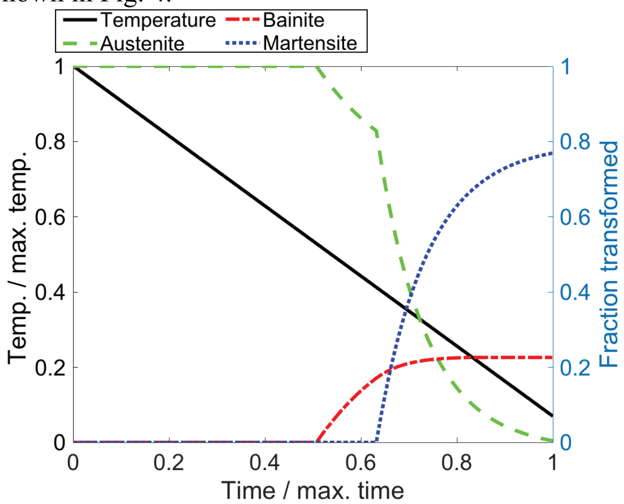

Figure 3. The optimized thermal path for strip cooling process test case i) (20 % bainite, 80 % martensite) and the fraction of phases formed as function of time.

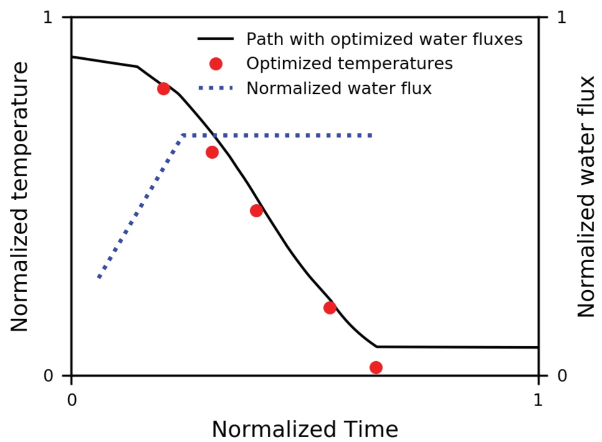

Figure 4. The optimized normalized water fluxes.

Target temperatures refer to temperatures that would be optimal to obtain the desired phase fractions the black line shows the thermal path estimated as result from these water fluxes.

3.1.2 Water cooling of steel strip case ii), 40 % bainite, 60 % martensite

The optimized thermal path and phase fractions for water cooled steel strip test case ii) are shown in Fig. 5. The path started from fully austenitic structure and it was optimized to produce 40% bainite and 60 % martensite. The optimized normalized water fluxes are shown in Fig. 6.

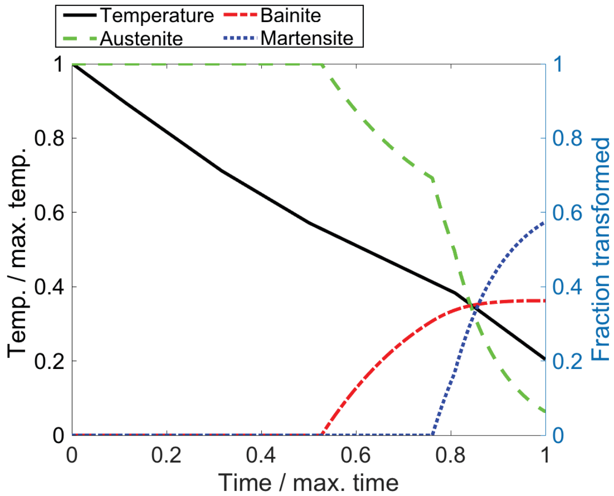

Figure 5. The optimized thermal path for strip cooling process test case ii) (40 % bainite, 60 % martensite) and the fraction of phases formed as function of time.

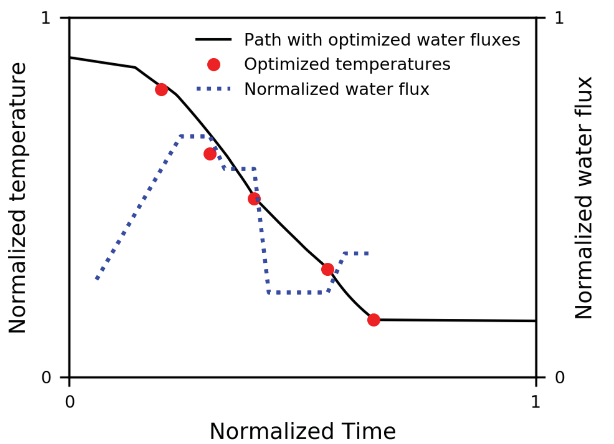

Figure 6. The optimized normalized water fluxes. Target temperatures refer to temperatures that would be optimal to obtain the desired phase fractions the black line shows the thermal path estimated as result from the optimized water fluxes.

3.2 Induction hardening

Typically, in the induction hardening process, in order to avoid a significant grain growth, the time when the material stays in highest temperature (the *peak temperature*) is few seconds. This time is called *dwell time*. In this study, a dwell time of 2.5 s was considered for all the calculations. Moreover, to achieve the finest possible grain structure, it is desirable to maintain the peak temperature as low as possible, while still achieving full austenitization.

For the optimization of the austenitization, we defined the objective function f_{obj}, which is minimized. The function $f_{obj} = |\chi_\gamma - \chi_{\gamma,des}| + T_p/a$, where $\chi_{\gamma,des} = 1.0$ is the desired austenite fraction (full austenitization). T_p is the peak temperature and a is a penalty parameter which affects how much the peak temperature contributes to the objective function. The parameter a was optimized so that the final value was the minimum that produced more than 99.5 % austenite during the heating and holding in the peak temperature. The physical austenitization parameters were the peak temperature and the heating rate, which was constrained between 50 °C/s and 100° C/s.

The minimum peak temperature satisfying this condition was found to be 795 °C with the minimum heating rate 50 °C/s. The found peak temperature, heating rate, and the chosen 2.5 s dwell time were used in the austenitization schedules for all of the induction hardening cases examined in this study.

3.2.1 Induction hardening case i), fully martensitic structure

The optimized thermal path for the induction hardening test case ii) is shown in Fig. 7. The path was optimized for full austenization at minimum temperature, 2.5 s dwell time, with 50-100 °C/s heating rate. Upon cooling the path was optimized to produce fully martensitic structure. For further experimental and applied studies, as well as serving as a suitable initial guess for other desired phase amounts close to this result, the actual values and cooling rates are presented in Table 1.

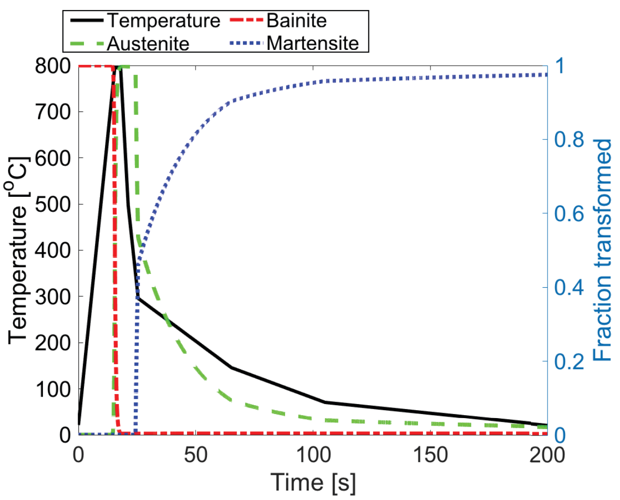

Figure 7. The optimized thermal path for induction hardening process test case i) (fully martensitic structure) and the fraction of phases calculated to form as function of time.

Table 1. The values of the time-temperature path of induction hardening test case i) shown in Fig. 7, as well as the corresponding heating (HR,+) and cooling rates (CR,-).

Time (s)	Temperature [°C]	HR+/CR- [°C/s]
0,0	21,0	50,0
15,5	795,2	0,0
18,0	795,2	-92,2
21,2	497,6	-47,3
25,5	295,9	-3,8
65,3	145,8	-1,9
105,1	70,8	-0,5
200,0	21,0	-

3.2.2 Induction hardening case ii), equal amount of upper and lower bainite (50% each)

The optimized thermal path for the induction hardening test case ii) is shown in Fig. 8. The path was optimized for full austenization at minimum temperature, 2.5 s dwell time, with 50-100 °C/s heating rate. Upon cooling the path was optimized to produce 50% upper bainite (which forms above 550 °C), 50 % lower bainite (which forms below 550 °C). For further experimental and applied studies, as well as serving as a suitable initial guess for other desired phase amounts close to this result, the actual values and cooling rates are presented in Table 2. Despite the minimization procedure, abount 10 % of the austenite transformed to martensite during cooling. A longer total time would be required to produce the desired fully bainitic microstructure.

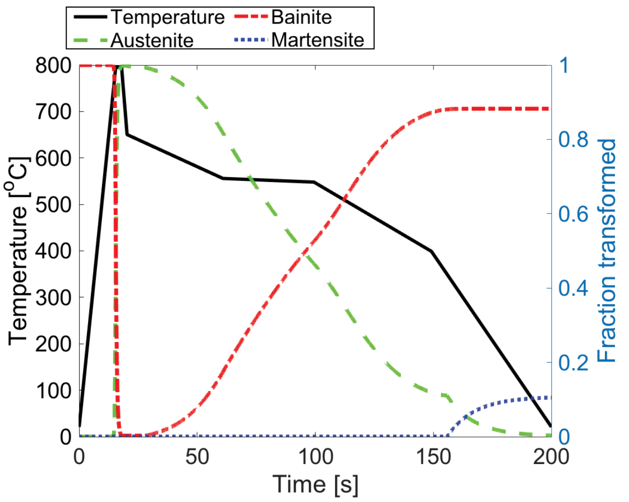

Figure 8. The optimized thermal path for induction hardening process test case ii) (50 % upper and 50 % lower bainite) and the fraction of phases calculated to form as function of time.

Table 2. The values of the time-temperature path of induction hardening test case ii) shown in Fig. 8, as well as the corresponding heating (HR,+) and cooling rates (CR,-).

Time [s]	Temperature [°C]	HR+/CR- [°C/s]
0,0	21,0	50,0
15,5	795,2	0,0
18,0	795,2	-62,5
20,3	650,3	-2,3
60,9	555,9	-0,2
99,4	548,0	-3,0
149,2	399,0	-7,4
200,0	21,0	-

3.2.3 Induction hardening case iii), 30% martensite, 40% upper bainite, and 30% lower bainite

The optimized thermal path for the induction hardening test case iii) is shown in Fig. 9. The path was optimized for full austenization at minimum temperature, 2.5 s dwell time, with 50-100 °C/s heating rate. Upon cooling the path was optimized to produce 40% upper bainite (which forms above 550 °C), 30 % lower bainite (which forms below 550 °C) and 30 % martensite. For further experimental and applied studies, as well as serving as a suitable initial guess for other desired phase amounts close to this result, the actual values and cooling rates are presented in Table 3.

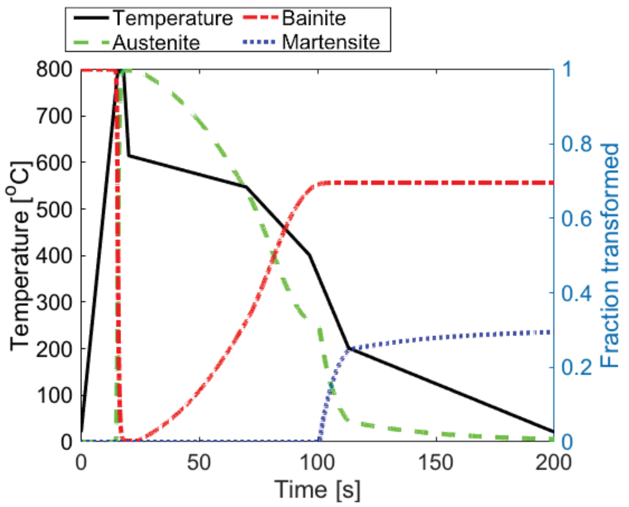

Figure 9. The optimized thermal path for induction hardening process test case iii) (30 % martensite, 40 % upper bainite, 30 % lower bainite) and the fraction of phases formed as function of time.

Table 3. The values of the time-temperature path of induction hardening test case iii) shown in Fig. 9, as well as the corresponding heating (HR,+) and cooling rates (CR,-).

Time [s]	Temperature [°C]	HR+/CR- [°C/s]
0,0	21,0	50,0
15,5	795,2	0,0
18,0	795,2	-84,4
20,1	614,5	-1,4
69,8	547,2	-5,5
96,5	401,1	-12,1
113,1	201,4	-2,1
200,0	21,0	-

4 Conclusions

Using the Matlab programming language (Mathworks, 2020), based on the algorithm described in (Byrd et al., 2000) an optimization script was created for finding the cooling path that produces the desired microstructural constituents (ferrite, upper and lower bainite, martensite) as well as finding suitable heating path for desired austenitization. The script was succesfully applied for several test cases related to water cooling of hot rolled steel strip and induction hardening. For the water cooling case, the script was fully automated by running a series of initial guesses for the thermal path and choosing the best result, while for the induction hardening cases, a user defined initial guess was used. For water cooling we additionally optimized the required cooling water fluxes needed to realize the optimized cooling path based on the earlier work (Paananen, 2015; Pohjonen *et al.*, 2016). Although the results of the presented test cases are not directly applied in the industrial practice as such, they are reasonably close to the actual production to demonstrate the practical applicability of the method.

5 Author contributions

Aarne Pohjonen: implementation of the thermal path optimization script, thermal path optimization simulations, writing of the article.
Vahid Javaheri: original idea of thermal path optimization on induction hardening process, induction hardening process related information, writing, editing.
Joni Paananen: implementation of the water flux optimization tool, water flux optimization, strip cooling related information, writing, editing
Juha Pyykkönen: strip cooling related information, writing, editing.

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References

R. H. Byrd, J. C. Gilbert, and J. Nocedal. A trust region method based on interior point techniques for nonlinear programming. *Mathematical Programming, Series B*, 89:149-185, 2000. doi: 10.1007/PL00011391.

V. Javaheri, S. Kolli, B. Grande, and D. Porter. Insight into the induction hardening behavior of a new 0.40% C microalloyed steel: Effects of initial microstructure and thermal cycles. *Materials Characterization*, 149:165–183, 2019a. doi: 10.1016/j.matchar.2019.01.029.

V. Javaheri, A. Pohjonen, J. I. Asperheim, D. Ivanov, and D. Porter. Physically based modeling, characterization and design of an induction hardening process for a new slurry pipeline steel. *Materials & Design*, 182:108047, 2019b. doi: 10.1016/j.matdes.2019.108047.

M. Jung, S-J. Lee, W-B. Lee, and K.I. Moon. Finite Element Simulation and Optimization of Gas-Quenching Process for Tool Steels. *Journal of Materials Engineering and Performance*, 27(8):4355–4363, 2018. doi: 10.1007/s11665-018-3492-6.

Mathworks. Matlab documentation, 2020. *https://www.mathworks.com/help/matlab/*.

J. Paananen, *Laskennallinen työkalu kuumavalssatun teräsnauhan jäähdyttämisen suunnitteluun*. University of Oulu, BSc thesis. 2015.

A. Pohjonen, M. Somani, J. Pyykkönen, J. Paananen, D. Porter. The onset of the austenite to bainite phase transformation for different cooling paths and steel compositions. *Key Engineering Materials*, 716:368-375, 2016. doi: 10.4028/www.scientific.net/KEM.716.368.

A. Pohjonen, A. Kaijalainen, J. Mourujärvi, and J. Larkiola. Computer simulations of austenite decomposition of hot formed steels during cooling. *Procedia Manufacturing*, 15:1864–1871, 2018a. doi: 10.1016/j.promfg.2018.07.203.

A. Pohjonen, M. Somani, and D. Porter, Modelling of austenite transformation along arbitrary cooling paths. *Computational Materials Science*, 150:244-251, 2018b. doi: 10.1016/j.commatsci.2018.03.052.

J. Pyykkönen, M. Somani, D. Porter, M. Holappa, T. Tarkka. Modelling of Thermal History and Microstructural Evolution on the Run-out Table of a Hot Strip Mill. In *Proceedings from the 6th International Quenching and Control of Distortion Conference*, 9-13 September, 2012 Chicago, IL, USA, pages 817–828, 2012.

R. Tavakoli, Thermal optimization of the continuous casting process using distributed parameter identification approach—controlling the curvature of solid-liquid interface. *The International Journal of Advanced Manufacturing Technology*, 94(1):1101–1118, 2018. doi: 10.1007/s00170-017-0978-6.