HEAT TREATMENT OF STEELS – VIRTUAL OPTIMIZATION OF MICROSTRUCTURES, MECHANICAL PROPERTIES, STRESSES AND DISTORTIONS

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ABSTRACT

Cast steels are characterized by a large variety of mechanical properties and microstructures after the heat treatment process in dependence on their final application. Process variations like differences in austenitization time and temperature, cooling conditions and chemical compositions play the significant role for high quality cast products. Process simulation with MAGMASOFT® is able to predict phase contents as well as mechanical properties including theses process variations in heat treatment and supports therefore a robust industrial heat treatment process design. Industrial examples for microstructure optimization of cast steels for a chain link will be given within the paper.

Furthermore residual stresses in the cast part based on the temperature history are calculated over the entire casting and heat treatment process. In the high temperature range like in the austenitization process for steels the material behavior is dominated by creep effects. The application of a unified creep model allows the quantitative prediction of stress reduction from the casting process linked to inelastic deformation during heat treatment.

In fast water or oil quenching processes stresses are built up again because of high thermal gradients in the steel casting, in addition the volume increase due to the diffusion-less martensitic phase transformation increases stresses tremendously. Quench cracks because of high levels of tensile stresses as well as large amounts of distortion are results of these phenomena. Thus a compromise between desired material properties, namely high strength martensitic microstructures and acceptable stress levels to minimize distortion and avoid crack risks, has to be found in order to deliver desired properties of the steel casting. As industrial examples, the results of the virtual experimentation for a chain link and a brake disc will be discussed.

KEYWORDS

cast steel, distortion, mechanical properties, microstructure, virtual optimization, residual stresses, simulation

INTRODUCTION

Microstructures as well as mechanical properties of steels are highly dependent on the exact heating and cooling conditions of the steel heat treatment process. Main process parameters are the cooling effect of the quench media as well as the chemical composition of the cast material. Within one casting, variations in quench hardness of a few hundred HV can easily occur due to local differences in cooling rates in correspondence with microstructure variations.

Usually a compromise between high strength and a reasonable ductility has to be found for the final application of the casting. Therefore fast quenching processes are often followed by a tempering step in order to transform high strength brittle martensitic microstructures in more ductile annealed

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microstructures which are closer to the thermodynamic equilibrium and reduce at the same time the amount of residual stresses, but keep also a reasonable strength level.

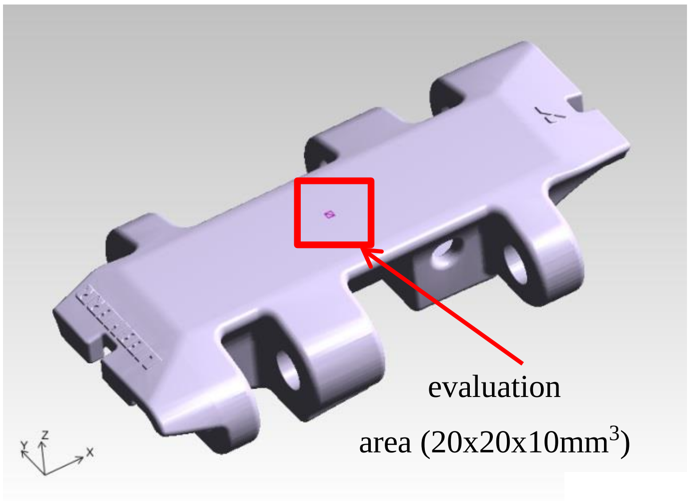
Within this paper different industrial examples for steel castings are given. For the optimization of microstructures as well as mechanical properties and stress calculations over the entire casting and heat treatment process a chain link was chosen. The consequence of different quenching conditions on the amount and direction of distortion for a steel brake disc is discussed as another relevant application for process optimization in stress calculations.

1. HEAT TREATMENT SIMULATION

The heat treatment module in MAGMASOFT® for steel alloys couples local heating and cooling rates in the casting known from a temperature field calculation with the alloy composition through regression analysis to predict microstructures and mechanical properties throughout the casting. The calculated temperature profiles during the heat treatment are the basis for the steel property and microstructure prediction, which are state of the art for steel heat treatment process simulation. Within the heat treatment process, the steel casting is exposed to a certain temperature regime to get the required transformations:

- Austenitisation above Ac3 temperature in order to form 100% austenite with a homogeneous distribution of the alloying elements over the entire casting
- Fast quenching in a quench medium like water or oil in order to get martensite and/or bainite with a high strength and hardness level
- Tempering step at moderate temperatures (~400-600°C) for the increase of the ductility and elongation values and reduction of residual stresses inside the casting.

Goal of the heat treatment process is to obtain required material properties by a specific microstructure change which depends on the chemical composition as well as on the temperature profile. As an example for a typical heat treatment process the results for a low alloyed carbon steel (GS34CrMo4) chain link are presented. In Fig. 1 the geometry of the chain link is shown.



evaluation

area (20x20x10mm^3)

Fig. 1: Geometry of the chain link and size of the evaluation area (investigated area for microstructure and mechanical property characterization in optimization); the length of the chain link is ~1.6m

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In Fig. 2 the calculated temperature curves of the maximum, minimum and average temperature during one typical heat treatment process consisting of austenitization, quenching and tempering can be seen.

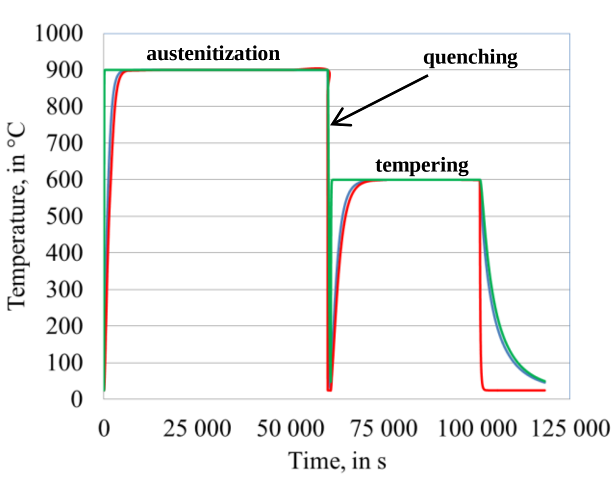

Fig. 2: Calculated temperature curves during one typical heat treatment process of the steel casting (process steps are: austenitization, quenching and tempering)

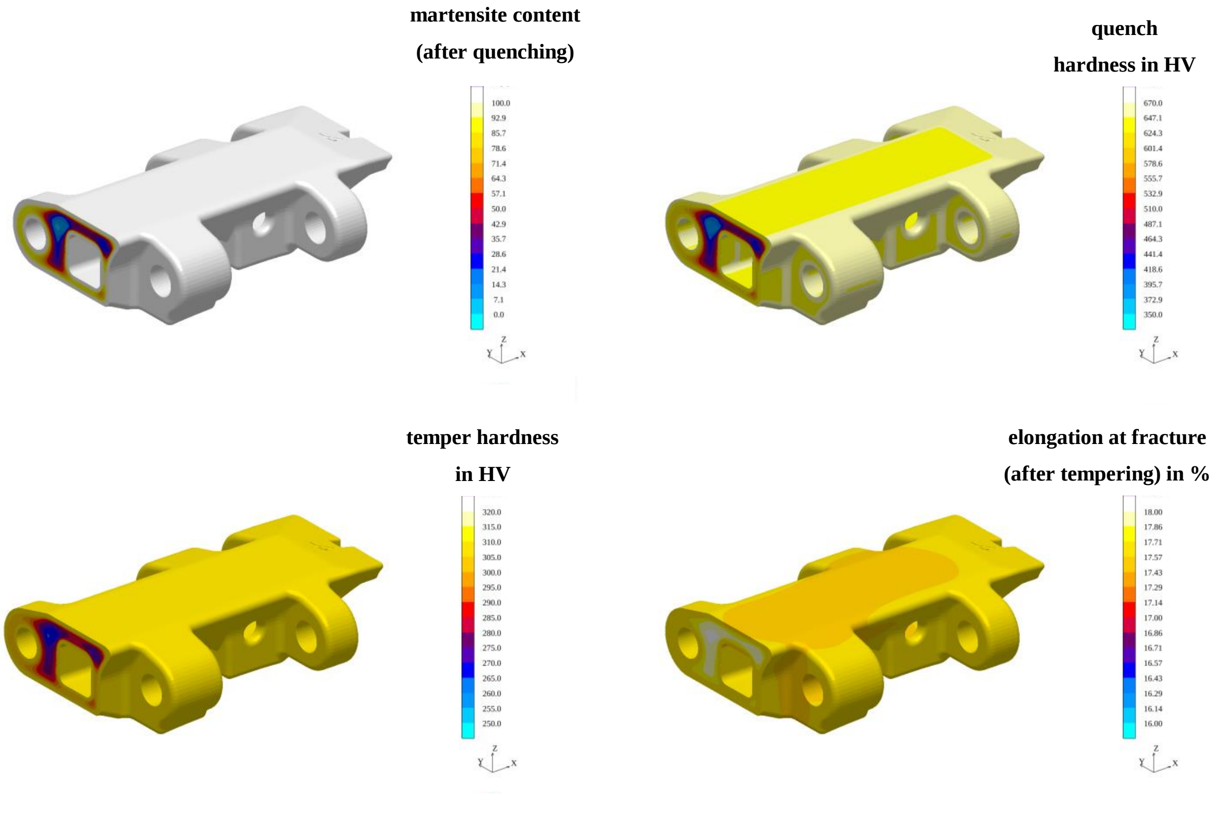

Fig. 3: Typical results of the heat treatment simulation for the chain link (cross section): Martensite content after quenching, quench and temper hardness as well as elongation after tempering for a low alloyed steel with a carbon content of 0.4% (water quenching, austenitization time 1000min at 900°C, tempering time 667min at 600°C)

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For this one typical heat treatment process various microstructure results as well as mechanical properties are visualized in Fig. 3 for a chosen cross section of the chain link. Martensite contents after quenching, hardness in quenched and tempered condition and elongation at fracture values for the entire steel casting are presented (other phases like bainite and pearlite are calculated as well; they are not presented in the paper). As expected martensite content and quench hardness on the surface are higher compared to the inside of the casting because of higher cooling rates during quenching. Because of the higher quench hardness of the original microstructure after quenching also the temper hardness is higher on the surface of the casting meanwhile elongation values after tempering are a bit lower in the same area.

2. VIRTUAL PROCESS OPTIMISATION OF HEAT TREATMENT

One single calculation like shown in the previous section cannot give any information about the robustness of the heat treatment process and the optimal heat treatment conditions for a particular part and steel grade. Therefore the different influencing parameters have to be investigated systematically to obtain the process optimum. In order to minimize the experimental work and to plan the heat treatment process efficiently recently developed statistical methods can be used applied with process simulation [1- 3].

Thanks to advances in both software and hardware, the time required to carry out a single simulation continues to decrease. This means that an optimization program can run a sequence of simulations “in the loop” and can be used to carry out a large number of virtual experiments in a comparably short time. The relevant quality criteria can be automatically assessed by the software after each virtual casting trial. After having run the virtual experiments, all results are available to the engineer for statistical assessment (guided by the software), supported by a 3D visualization of the process. The investigations described in this paper have been carried out using the software MAGMA[5] using its fully integrated capabilities for virtual optimization.

In setting up an automatic optimization, the heat treatment process parameters which are to be varied and their respective variation ranges need to be identified (e.g. chemistry, quench medium or austenitization time). Then, a sequence of virtual experiments is set up similar to a “Design of Experiments (DoE)” for real plant trials. The software uses statistical methods to aid the engineer when setting up the sequence, so that the fewest experiments necessary are required to gain as much information as possible from the results. Evaluating a sequence of virtual experiments helps to understand how strongly the effect of each parameter on the quality criteria is. In many cases, this gives valuable information to the engineer to significantly improve the production process in terms of quality or production costs [1-4].

On top of this, a true automatic optimization can be carried out to propose an optimal heat treatment process/process operating point. An automatic optimization is driven by the analysis and evaluation of the relevant quality criteria. Objectives can, for example, be “maximize the temper hardness” or “maximize tensile strength after heat treatment”. Virtual automatic optimization is focused on fulfilling several objectives, which may be in competition with each other, at the same time so the best compromise needs to be found [1-4].

The following process parameters are varied in the virtual experiments of the heat treatment process for the chain link:

- Carbon content (0.3 – 0.4%; step 0.025)
- Austenitization temperature (900°C and 940°C)

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- Quench media (representative heat transfer coefficients for water, oil and air quenching)
- Austenitization time (667min – 1000min; step 167min)
- Tempering time (333min – 667min; step 167min)

This leads to a total calculation of 270 different virtual heat treatment experiments in MAGMA[5] by application of automatic optimization. Not only the calculations but also the investigation of results is done automatically. Therefore an area of interest (a so called evaluation area, shown in Fig. 1) was chosen for the investigations because different positions of the casting show quite a large variety in microstructures as well as in mechanical properties (as it can be seen in Fig. 3 for one single simulation of the heat treatment process).

The two main objectives for the optimization are:
- Hardness after tempering
- Elongation after tempering

In order to show also the influence of the process variations on the microstructure and properties after quenching, the following objectives are added:

- Martensite content after quenching
- Hardness after quenching

In Fig. 4 the resulting correlation between objectives and process parameters is presented. Red color corresponds to a positive correlation of the process parameter with the objective, blue color to a negative one.

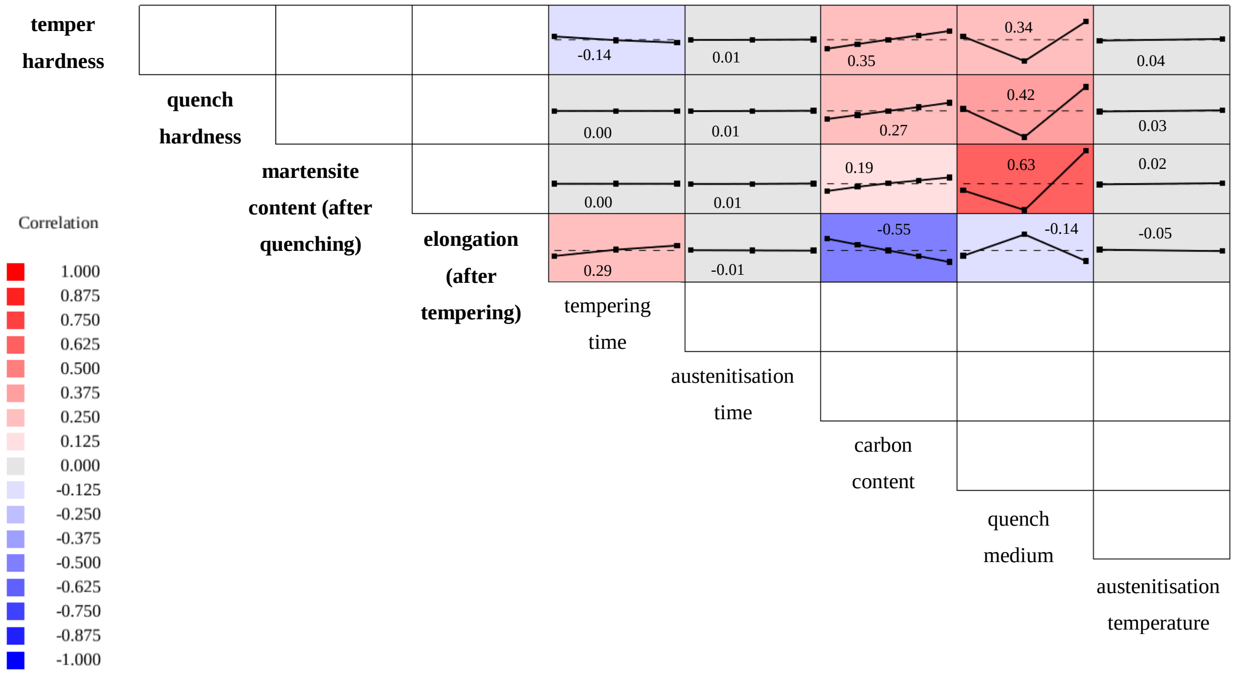

Fig. 4: Correlation matrix between process parameters and objectives

The following conclusions can be made by these virtual experiments:

- Quench hardness, martensite content and temper hardness are mainly dependent on the quench medium and carbon content

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- Elongation and hardness after tempering is also influenced by the tempering time
- Elongation after tempering is influenced by the quench medium
- Austenitization time and temperature have only a very small influence on the microstructure and mechanical properties (note: complete austenitization was always assumed)

In Fig. 5 and Fig. 6 the main influencing parameters quench medium and carbon content on the temper hardness and elongation after tempering are shown (results for different austenitization times, austenitization temperatures and tempering times). Each dot reflects the outcome of a single virtual experiment in the evaluation area of the part.

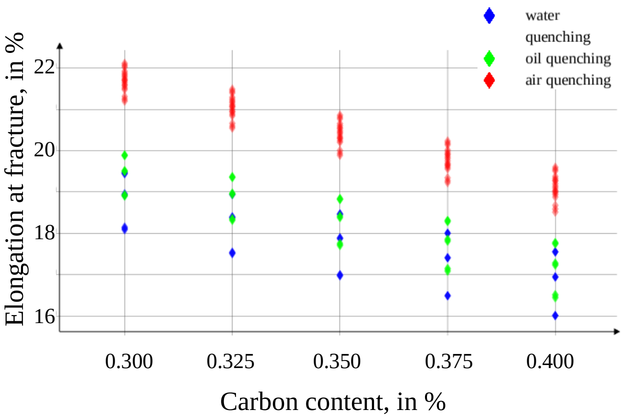

Fig. 5: Overview for all results, influence of carbon content and quench medium on the average elongation values after tempering in the evaluation area

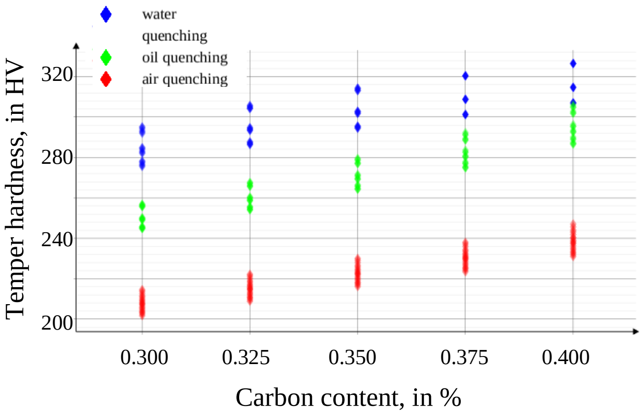

Fig. 6: Overview for all results, influence of carbon content and quench medium on the average temper hardness in the evaluation area

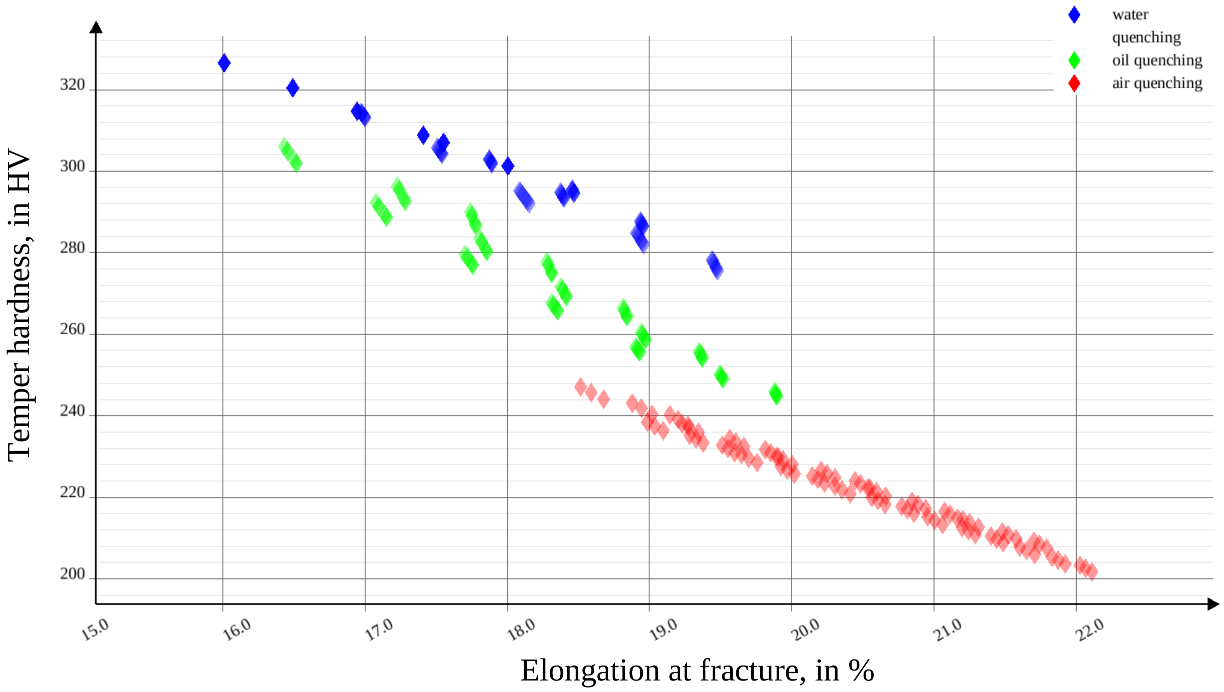

Fig. 7: Possible combinations of average temper hardness and elongation values in the evaluation area after tempering for the investigated process variations of the heat treatment process

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In Fig. 7 the possible combinations of temper hardness and elongation are presented. As expected the two main objectives are contradictory and show a negative correlation. So a compromise has to be found in order to satisfy both requirements. In dependence on the exact requirements for hardness and elongation after tempering a suitable design can be chosen in Fig. 7.

Moreover with focus on heat treatment process robustness, differences and variations in results can easily be reported by the application of automatic virtual experimentation. As it can be seen in Fig. 8 especially for the oil quenching process the expected variety inside the small evaluation area of 20x20x10mm^3 can be relatively large. This fact has to be considered especially in terms of comparison with experimental results where locations for samples have to be defined with accuracy.

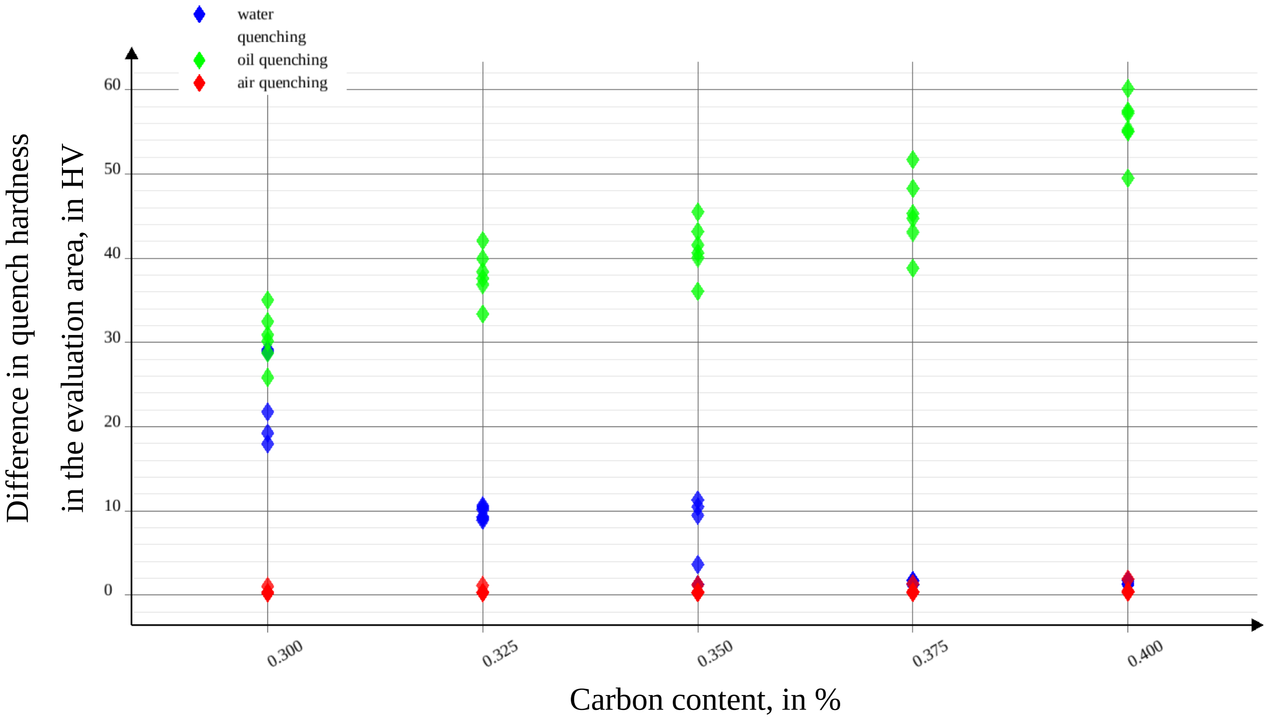

Fig. 8: Maximum difference in quench hardness in dependency on cooling medium and carbon content inside the evaluation area

3. STRESS PREDICTIONS OF THE ENTIRE CASTING AND HEAT TREATMENT PROCESS

During the casting and heat treatment process inhomogeneous temperature fields arise. These temperature fields cause not only differences in microstructure but also shrinkage of the casting as well as residual stresses and distortions. The stress distribution as well as related strains and displacements during the solidification and further cooling of the castings over the entire casting process are calculated with a time independent elasto-plastic model. The interface between cast material and surrounding core and mold material is enforced by a contact algorithm. Thus shrinkage constraints due to sand forms or cores are considered in the simulation of residual stresses. Temperature dependent nonlinear material behavior of mechanical as well as thermophysical material parameters is taken into account.

Moreover calculation of stresses and deformations during heat treatment based on thermal calculations of the heat treatment process are performed considering the stress state at the end of the casting process. In order to simulate the heat treatment processes of steel cast parts, a time

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dependent constitutive creep model is implemented for heating processes where residual stresses from the casting process are released to deformation due to creep effects [5].

The time dependency in the mechanical response of the material is described in different ways depending on what type of phenomena are considered. Hence, different models and approaches have been proposed in literature to include time effects. The approach is based on a classical creep formulation where time effects are taken into account via Norton's power law, to mainly describe the nonlinear behaviour of stress relaxation at high temperature. Nevertheless, the implementation is unified in the sense that the model is generalized to include nonlinear conditions which are also taking place at lower temperatures. This is mainly achieved by selecting an appropriate hardening law, which can be adapted to different conditions at different temperature levels and by augmenting the Norton's power law, with a temperature sensitive part in it [5].

Moreover the volume increase as well as increase in strength level due to martensite formation is considered by application of material data of the thermodynamic software JMatPro version 8.0 (General Steel module) during the fast quenching process which follows the austenitization step. Stresses are built up and increase tremendously due to the volume change as a result of martensite formation.

For the evaluation of stresses in the casting as well as in the heat treatment process one typical heat treatment cycle from the previous chapter with a good compromise for strength and ductility level for the chain link was chosen:

- Austenitization at 900°C for 833min
- Oil quenching
- Tempering at 600°C for 500min

In Fig. 9 the complete production cycle of the casting is presented. Interesting points in time in terms of residual stresses are marked from A to D.

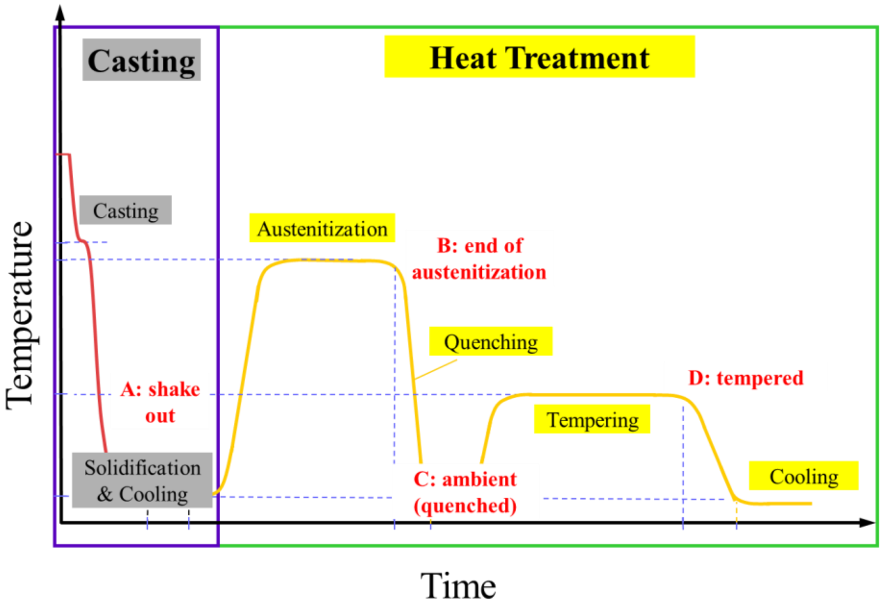

Fig. 9: The complete production cycle: Casting and heat treatment process

Usually stresses are built up during solidification and cooling until shake out of the sand form. The maximum principal stress (criterion for the maximum tensile stresses) and minimum principal

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stresses before shake out are presented in Fig. 10. Some areas for higher tensile loads can be observed. Nevertheless the general stress level is quite low and even reduced at room temperature in ambient condition after the external constraint of the sand form is removed. No critical values above the strength level of the material are exceeded during solidification and cooling and therefore no cracks are expected due to high tensile stresses inside the chain link.

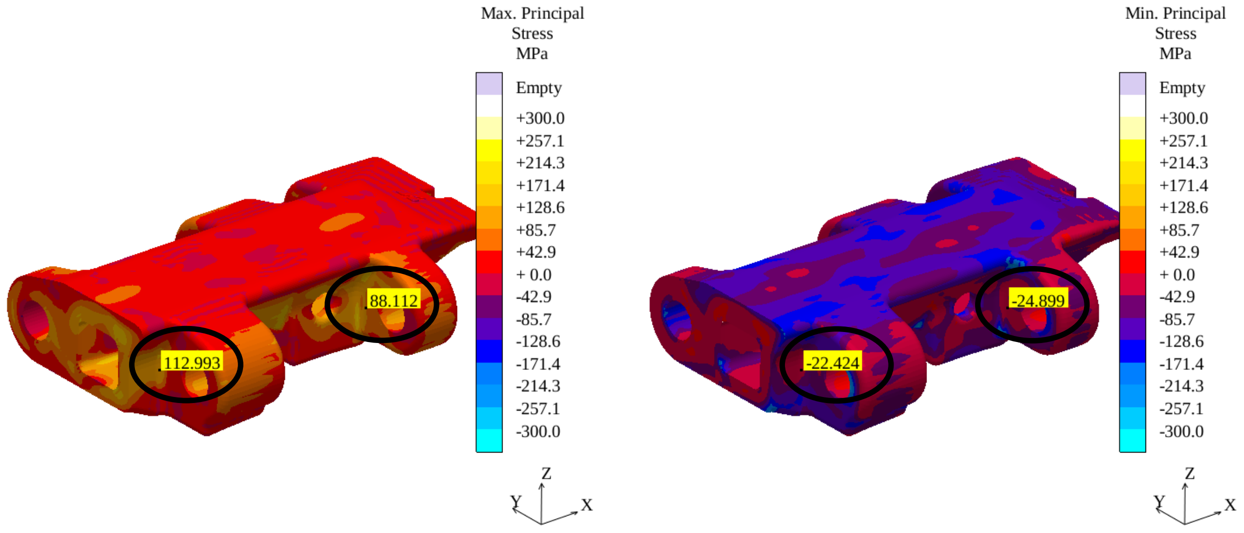

Fig. 10: Maximum and minimum principal stresses before shake out of the sand form (step A)

In the next step of the production process, stress relief due to creep processes during austenitization takes place, so that nearly no stresses are left at the end of austenitization (Fig. 11). The casting is almost stress free at the end of austenitization.

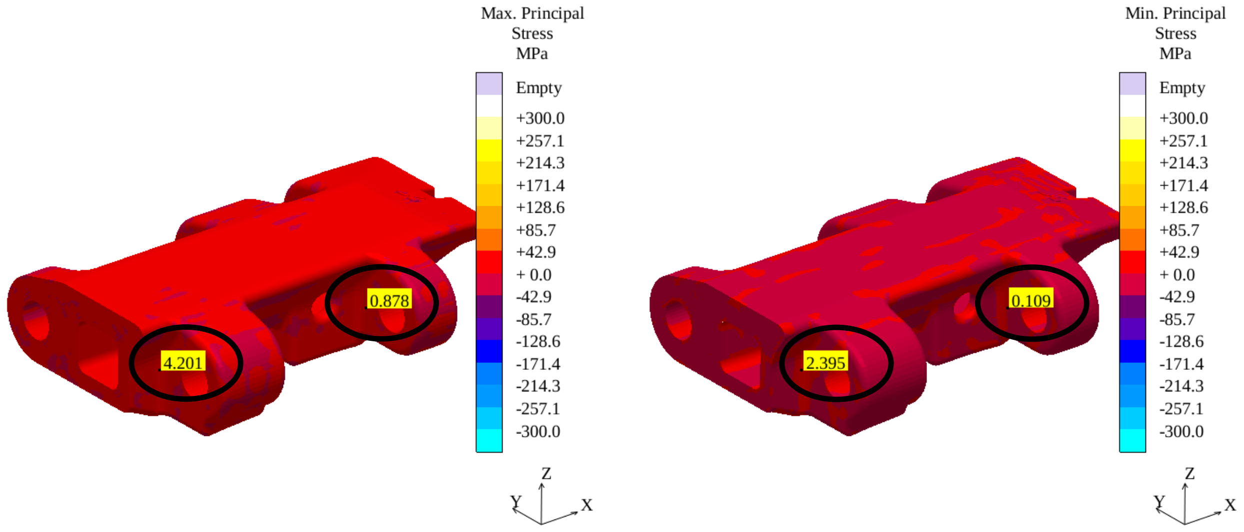

Fig. 11: Maximum and minimum principal stresses at the end of austenitization (step B), the casting is nearly stress free

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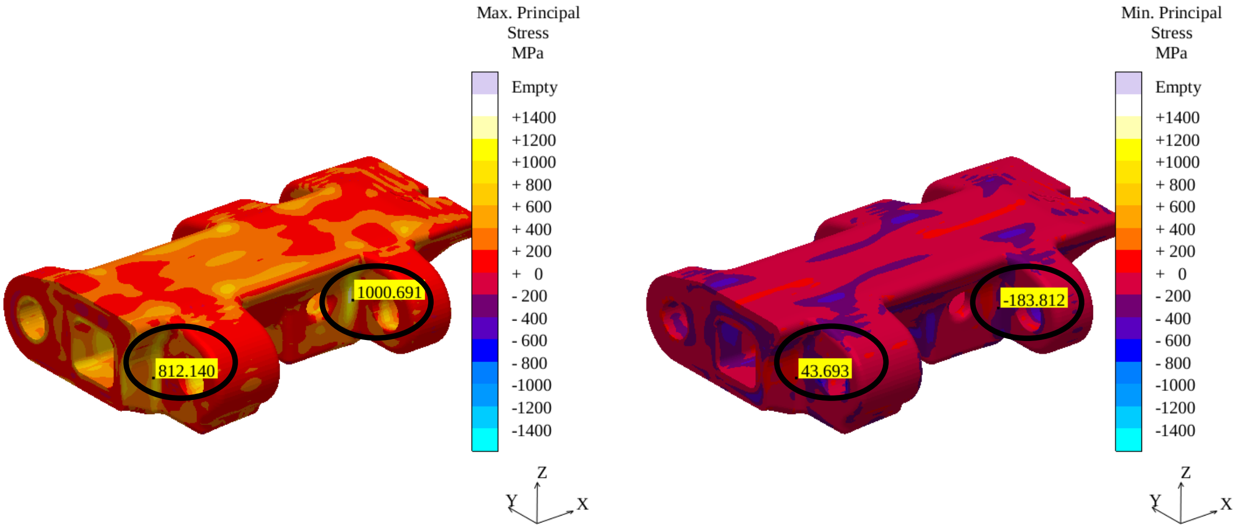

Fig. 12: Maximum and minimum principal stresses at ambient temperature (quenched state), high tensile stress due to martensite formation are found (step C)

In consequence of the austenite to martensite transformation and the corresponding volume change large stresses are built up during the oil quenching process of the casting as it can be seen in Fig. 12. These tensile stresses might be critical in terms of crack formation in some areas of the casting. The subsequent tempering leads again to a stress reduction due to creep processes in the high temperature range (Fig. 13).

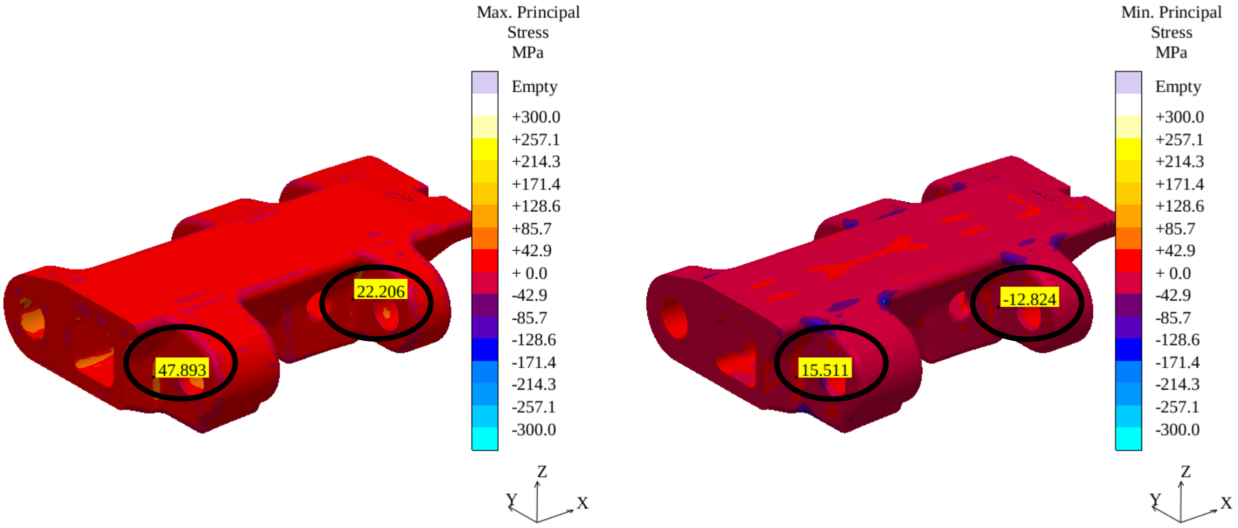

Fig. 13: Maximum and minimum principal stresses at the end of tempering (step D)

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4. OPTIMIZATION OF QUENCH CONDITIONS

Although the focus of the stress calculation for the chain link are tensile stresses and quench cracks, distortion plays the significant role during quenching of steel brake discs. Therefore exact quenching conditions need to be known in order to fulfill the optimization objective to minimize the distortion at the end of the quenching process. As influencing parameter, variations in quenching conditions are applied.

It is usually a big challenge to minimize distortion since a few of these brake discs are quenched on top of each other together. This quenching procedure will lead to slower cooling of some inner zones which are not so severely cooled in the quench medium like outer areas. The geometry of the brake disc is presented in
Fig. 14. The calculations are done for a low alloyed carbon steel with 0.25% carbon (GS25Mn5). The material data are calculated with the thermodynamic software JMatPro version 8.0 (General Steel module). A stress-free non-distorted geometry was always assumed at the end of the austenitization process so that only the quenching process from 900°C to room temperature was calculated thermally with the heat treatment module in MAGMA[5]. Based on the temperature field, residual stresses and distortions are predicted as well.

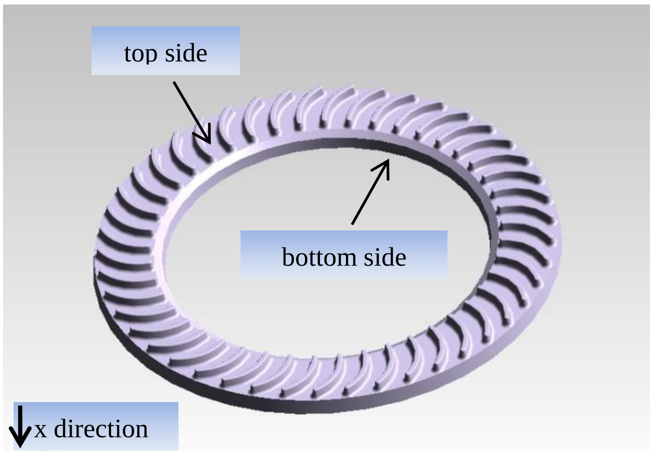

Fig. 14: Geometry of the brake disc (inner diameter ~800mm)

Displacement results for the brake disk are presented in Fig. 15 for different water quenching conditions. Besides homogeneous quenching in water (considered by application of a representative heat transfer coefficient for the quench media) inhomogeneous quenching conditions, where a faster quenching of the top side or the bottom side was assumed, are investigated as well.

The results are presented in Fig. 15. As it can be seen, especially inhomogeneous water quenching leads to substantial levels of distortion of the brake disk of a few millimeters. In dependence if it was faster quenched from the top or bottom side also the direction of deformation changes. Especially when the bottom side of the brake disc is more rapidly in water quenched large distortions are observed. The oil quenched brake discs show generally less amount of distortion. Faster oil quenching from the top side delivers the best results in terms of distortion in the oil quenching process. During quenching the brake disc is first bent in one direction and later in the other direction. Therefore a more or less flat profile of the brake disc is observed at the end of the quenching process. Also for oil quenching, faster quenching of the bottom side leads to larger amounts of distortion compared to homogeneous quenching conditions.

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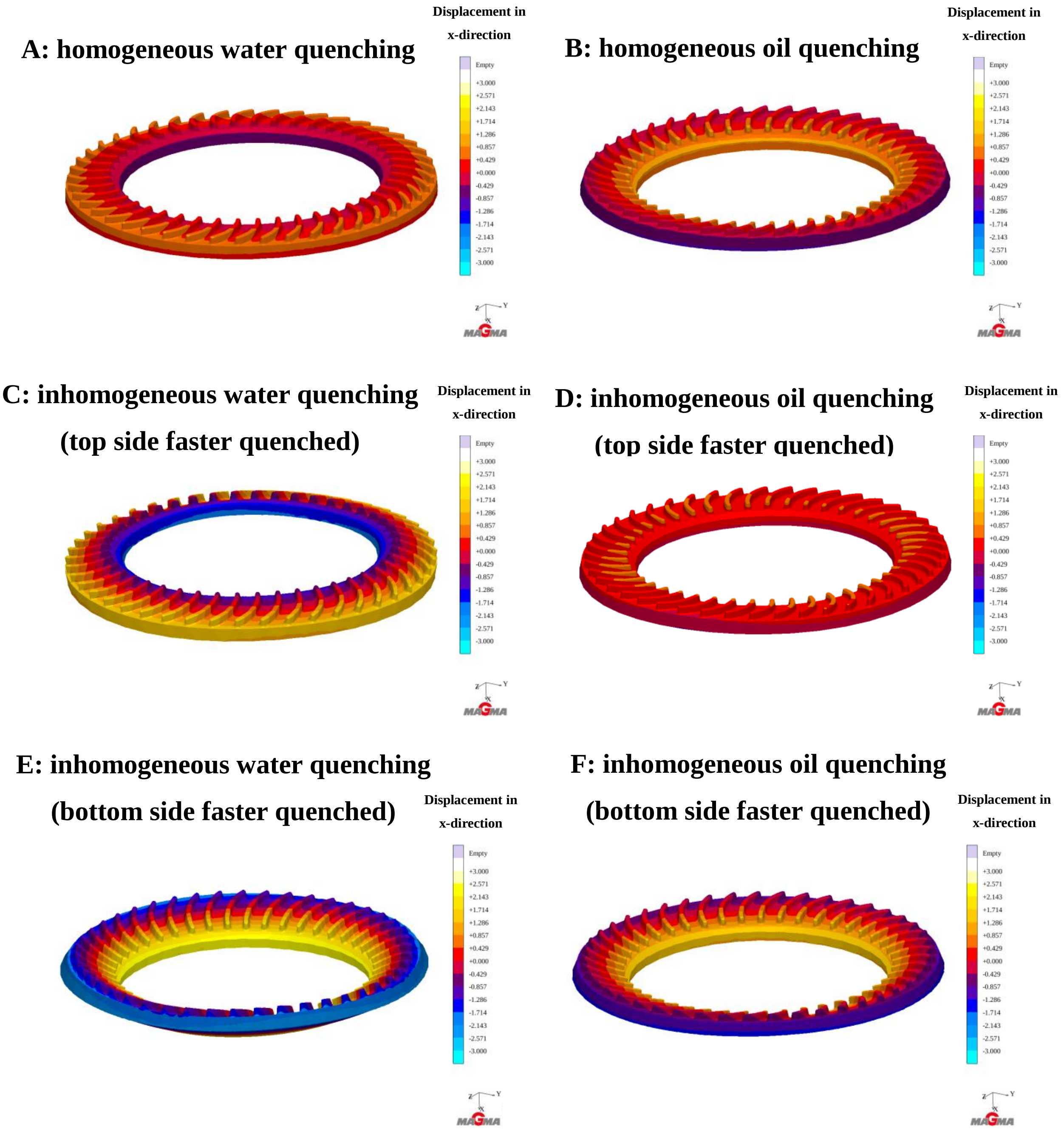

Fig. 15: Displacement in x-direction for a brake disk presented with a distortion factor of 15 (quenching from 900°C to room temperature was considered for different quenching conditions A-F)

In Table 1 the maximum difference in the displacement results is summarized in dependence on the quenching conditions and cooling rate. The level and direction of distortions as well as the residual stress level is always dependent on the exact geometry of the casting and the exact quenching conditions. Optimization can successfully be used to minimize the amount of distortion and improve the quality of the casting.

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Table 1: Maximum difference in displacement for different cooling conditions of the brake disk obtained by virtual optimization

Rank	**Quenching condition**	**Average cooling rate on the top surface of the casting between 900°C and 100°C in K/s**	**Maximum difference in displacements in x-direction in mm**
1	inhomogeneous oil quenching (top side faster quenched)	2.0	1.0
2	homogeneous water quenching	14.8	1.7
3	homogeneous oil quenching	2.7	2.0
4	inhomogeneous oil quenching (bottom side faster quenched)	2.1	3.0
5	inhomogeneous water quenching (top side faster quenched)	8.0	3.8
6	inhomogeneous water quenching (bottom side faster quenched)	11.1	5.1

SUMMARY

Within the paper an overview was given how process variations in a steel heat treatment process influence microstructure as well as material properties of steel castings. Virtual optimization was applied in order to investigate the influence of different process parameters on microstructure and properties of cast steels and to find a good compromise between strength and ductility of the material. Moreover stresses inside the casting at different points in time over the entire casting and heat treatment process are calculated. Especially high stresses during the quenching process in connection with martensite formation are built up. Finally the consequence of cooling conditions on the distortion of a steel casting brake disc is presented within the paper, where optimization is applied succesfully in order to minimize the distortion.

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