DEVELOPMENT OF A PROGNOSIS TOOL TO PREDICT HEAT TREATMENT RESULTS FOR HETEROGENEOUS GAS QUENCHING OF STEELS

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Abstract

Heat treatment is usually preferred to achieve the pre-determined material properties of steel components thereby suited for several engineering applications. Gas quenching after austenitisation in vacuum is an established process for this purpose, as it is clean and environment friendly. The selection of quenching parameters depends on many factors such as sample geometry as well as material and the batches. The process parameters are adopted by many years of expert knowledge, complex calculations or from trial and error methods. This problem is addressed in this scientific study by developing a prognosis tool, which can predict the heat treatment results based on an artificial neural network (ANN). This is attained by training the ANN on the basis of experimental and numerical investigations. Therefore, the heat treatment experiments were carried out on specific components made from 42CrMo4 and 100Cr6 in a two chambered quenching setup, where N_2 gas act as quenching fluid. The cooling behaviour will be investigated under the variation of process parameters such as gas pressure, geometry and batches. The development of the microstructure and hardness as a function of the process parameters are analysed metallographically. For the detailed investigation as well as to improve the training quality of ANN, FEM simulations are developed and validated, which serves afterwards to research the influence of parameter variation numerically. Thereby, sufficient data are generated numerically and experimentally for the successful training of the ANN of the prognosis tool, which can finally predict the heat treatment results.

Keywords: Steel, material properties, heat treatment, FEM, ANN

1. INTRODUCTION

Heat treatment is a suitable method for achieving the desired properties of steels. In particular, gas quenching after austenitisation in vacuum is an economical, clean and environmentally friendly method for hardening of steels. The selection of the heat treatment parameters has to be accomplished by considering the steel grade, component geometry and batches as well as the furnace and quenching setup. Depending up on the type of steel the Time-Temperature-Transformation (TTT) behaviour and thereby the maximum achievable hardness and hardening depth varies based on the respective chemical composition. The quenching plant parameters such as ventilator velocity, gas pressure, gas type and quenching chamber size highly influence the flow traits and finally the thermal history of the component being quenched. The previous works [1-3] investigated the influence of flow velocity and gas pressure during gas quenching. This makes it obvious that, in addition to the purely metal-physical processes in the component, expertise on the thermofluid-dynamic processes is also required to estimate the appropriate boundary conditions and in particular the cooling conditions.The selection of heat treatment parameters requires a great deal of expertise, elaborate calculations or trial and error . In order to minimise the effort for the design of the heat treatment process, the development of a prediction tool based on artificial neural networks (ANN) is planned, which enables the prognosis of the heat treatment results. The scientific stages of development are presented in this paper.

2. EXPERIMENTAL SETUP AND NUMERICAL MODELING

To develop the prediction tool four stages are adopted. In the first stage the components are heat-treated with varying process parameters and the temperature history within the specimen is recorded. The flow inside the chamber and temperature characteristics are investigated experimentally and numerically. Validated CFD (Computational Fluid Dynamics) computations are adopted for obtaining the boundary conditions especially the local heat transfer coefficient (HTC) depending on the quenching parameters. Afterwards the heat-treated components are analysed in order to get an insight into the microstructure and hardness achieved. Furthermore, to generate sufficient data for the training of the ANN, FEM simulations are carried out considering variation of the HTC, which thereby guides to map the microstructure development and hardness. Based on the experimental and numerical results obtained, the ANN is trained. After succesful training of the ANN and its validation, this serves to predict the hardness values depending on the input process parameters, specimen geometry and batches. The experimental setup and procedures are described in the following sections.

2.1. Heat treatment setup

For this research a two chambered (IPSEN) quenching setup is selected where heating and quenching is accomplished in two separate chambers with quenching chamber dimension (L × B × H = 625 × 435 × 420 mm^3). The probe under investigation is a disc with diameter Ø = 125 mm and h = 25 mm (**Figure 1 (a)**) and from 42CrMo4. The oven temperature is set at 850 °C and the oven hold time (t_o) is 75 minutes in vacuum condition for proper austenitisation. Due to safety reasons higher t_o cannot be achieved. The quenching medium is N_2 gas with an average temperature of 70 °C. In this work the gas pressure is varied between 10 and 6 bar as well as a two layered batch with inline and staggered configuration is analysed (**Figure 1(b)**). Dummy probes from austenitic steel (1.4301) are adopted for constructing the charge in which the position of each probe is designated with convention: Layer-Row-Column (**Figure 1 (b)**).

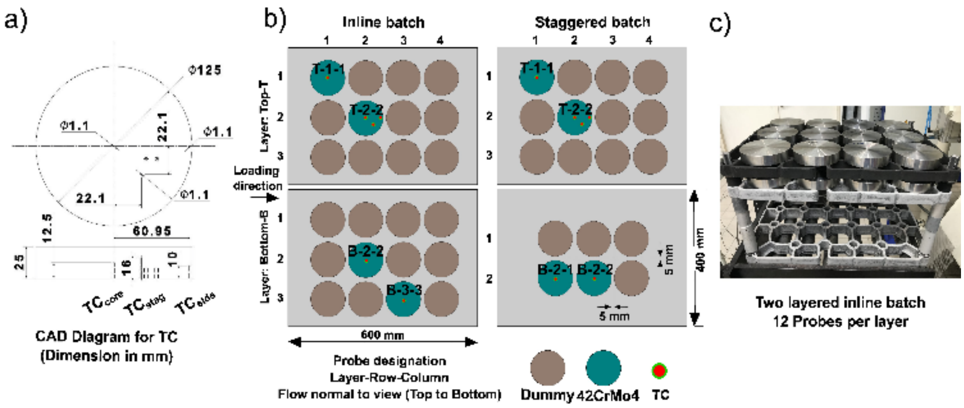

Figure 1 (a) CAD with TC positions, (b) Inline and staggered batch configuration with name convention, (c) Batch construction with dummy probes

Throughout the work the ventilator velocity is maintained constant at maximum (2970 1/min) which results an average velocity of 13.4 m/s at chamber inlet at atmospheric conditions [1]. K-Type thermocouple (TC) with a diameter of 1 mm is implemented for recording the cooling curve (DATAPAQ Tpaq21-3 Hz) for which holes of 1.1 mm are drillled within the probe for inserting the TC (**Figure 1 (a)**). Probe T-2-2 has 3 local measurements and other probes except dummys with one local measurement at the core. Space is also provided to pack the Datalogger with Isolation box below the batch (**Figure 1 (c)**).

2.2. Microstructure and mechanical properties

The heat-treated components are examined with regard to their hardness. Since the surfaces are not to be further influenced by further preparation, the Rockwell C method (HRC) is selected as the hardening method. This is characterized by the fact that in contrast to the Vickers or Brinell methods, no further surface treatment, such as grinding or polishing is required. The hardness evaluation pattern is shown in **Figure 2 (a)**. During the hardness measurement, the position of the specimens in the furnace is taken into account so that the specimens are always aligned in the same way. Furthermore, selected specimens are examined in detail metallographically. For this purpose transverse sections are prepared for microstructure analysis and hardness measurement according to Vickers (HV10). The preparation included cutting, grinding and polishing of the samples. The polished specimens were etched with Nital (2% HNO_3). In addition to the heat treatment of the discs, continuous (CCT) and isothermal (TTT) dilatometer tests using Dil 805 A/D (Bähr Thermoanalyse GmbH), are performed (**Figure 2(b)**).

The isothermal TTT served as input for the FEM simulations and the continuous cooling tests (CCT) for the further validation of the simulations. The data obtained in the experiments are used for validation of the FEM simulations and for training of the ANN.

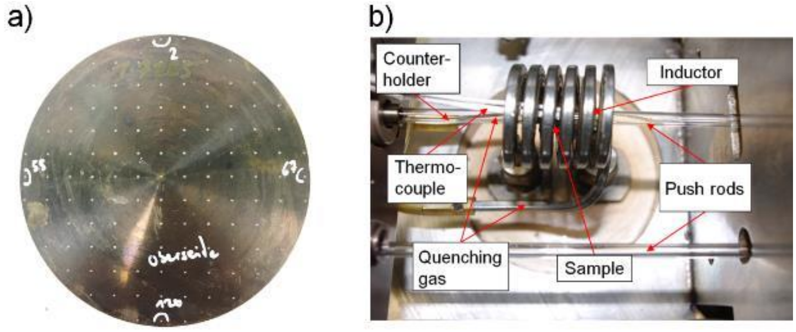

Figure 2 (a) Top side of the disc with pattern of indentations (HRC) (b) Dilatometer test setup

3. FEM MODELING

In order to generate further test data for training the ANN, various quenching processes are simulated for different HTC variations and the respective hardness values are calculated. The FEM simulation is performed by means of Deform™ HT using the JMAK model. Depending on the selected boundary conditions, i.e. the HTC, the FEM simulation calculates the temperature development in the component based on the heat conduction equation (**Equation 1**).

$$\rho c(\vartheta)\frac{\partial\vartheta}{\partial t} = div[\lambda(\vartheta)grad(\vartheta)] + \dot{W}(\vartheta, x, t) \qquad (1)$$

The approximate solution of the heat conduction equation requires the input of the heat capacity, density, thermal conductivity as well as the latent heat which occurs during the microstructure transformation. Furthermore, the calculation of the evolution of the microstructural constituents during quenching requires the input of isothermal TTT.The TTT is determined experimentally by using dilatometry. The other input data required for the simulation are calculated using JMatPro® V7.0 **(Figure 3)**. If the respective volume fractions *V* of the microstructure constituents (M: martensite, B: bainite, FP: ferrite/pearlite and RA: retainied austenite), are known, the hardness *H* can be calculated by applying the mixing rule (**Equation 2**).

$$H = \frac{H_M \cdot V_M + H_B \cdot V_B + H_{FP} \cdot V_{FP} + H_{RA} \cdot V_{RA}}{100\,\%} \quad with \quad V_M + V_B + V_{FP} + V_{RA} = 100\,\% \qquad (2)$$

Further information on heat treatment simulation using FEM can be found in [4-6]. Once the FEM simulations are validated, the boundary conditions (HTC) are varied from 100 to 2000 W/(m²K) to generate the training data for the ANN. A distinction is made between the HTC of the edge, the top side and the bottom side of the component.

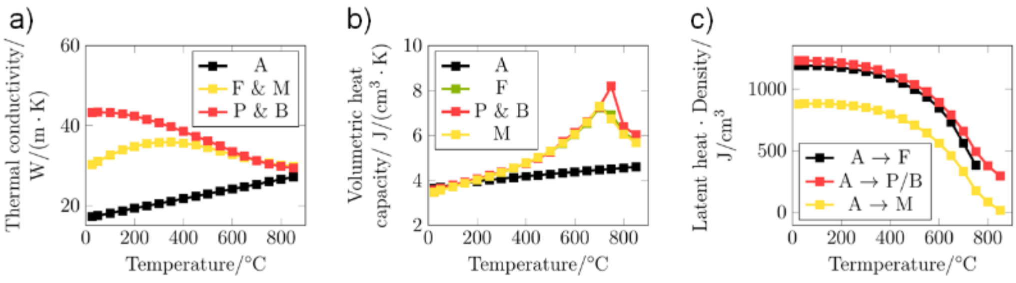

Figure 3 Material data of the microstructures of 42CrMo4 calculated using JMatPro®. a) Thermal conductivity, b) Volumetric heat capacity, c) Latent heat. The following abbreviations are used in the legends: A: austenite, FP: ferrite/pearlite, B: bainite. M: martensite.

4. MODELING ANN

Since the calculation of the HTC is still in progress, the results from the FEM simulations are first used to train the ANN. To train the network, the FEM simulation data and results are randomly assigned to a training data set (60 %), a validation set (20 %) and a test set (20 %). The input included the different HTC and the local coordinates of the sample (x,y). The output includes the hardness (HRC). This allows the calculation of the local hardness (HRC (x,y)) depending on the different HTC. By exploiting the symmetry constraints, a rotationally symmetric disc can be considered.The input and output data are normalized between zero and one. The test set is introduced to detect an overtrained mesh and calculate the prediction accuracy. The ANN's are systematically varied in terms of their architecture, i.e. the number of neurons in the hidden layer, as well as the features used (logsig, tansig, purelin) for each randomly grouped dataset. The number of neurons in the hidden layer is varied from 5 to 10. A total of 900 different ANN's are trained. The training of the ANN is performed using the Marquardt algorithm. In doing so, the algorithm minimised the mean square error (MSE) between the predicted and experimentally measured hardness by adjusting the biases "b" and weights "w" of all neurons. Training ends when the MSE of the training set is below a predefined threshold. The ANN with the lowest MSE was used for further calculations. For more information, please refer to [7-8].

5. RESULTS AND DISCUSSION

5.1. Influence of batch on heating trend and quenching

The case of 10 bar before quenching is analysed in detail in which the heating trend of probe positions are measured in oder to compute the effective hold time (t_e). The effective hold time is the time above which the specimen core is above 840 °C so that sufficient austenistisation occurs. The **Figure 4 (a)** shows the available t_e for the probes at measured positions. It clearly shows that for the disc from 42CrMo4 the t_e is not equal t_o and the $t_e < t_o$. From results it can be observed that top layer heats faster that bottom layer as well as the outer probes are faster than the inner probes which are marked in green, blue and red colors (**Figure 4 (b)**). This means based on the position of the probe within the batch it posses different t_e which may lead to non-uniform hardness values within the same batch. The probes in bottom layer and inner regions have poor t_e since the heat transfer is blocked by massive probes. The t_o must be considered higher so that all probes within the batch are sufficiently austenitised (from practice 30 min). However for the staggered configuration the t_e is improved for bottom layer since the path is less blocked. **Figure 5 (a)** depicts the quenching trend for 10 bar inline from the probe core for four probes within the batch from top and bottom layer. It shows that for the top layer the outer probes are cooled faster than inner but for bottom layer a mixed effect was observed (**Figure 5 (b)**) and asymmetrical. Comparing the two layers bottom is appeared to be faster than top, this may be due to the difference in t_e ($t_e < t_o$). This can lead to incomplete austenitisation as well as local flow traits are to be further investigated with CFD Simulations.

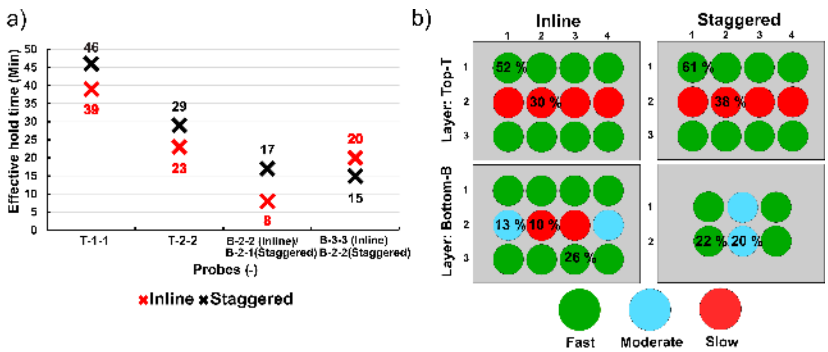

Figure 4 (a) Effective hold time for inline and staggered configuration (b)-Heating trend for inline and staggered configuration (% t_e from t_o)

It is interesting to observe the quenching trend within a probe (**Figure 5 (c)**), it shows the outer region is cooled faster and the core slower. This is also clear from the time for reaching the probe core from 800 to 500 °C ($t_{800/500}$) which can affect the microstructure development. The flow accelerates at the probe sides resulting in higher HTC and hence higher heat transfer. For staggered configuration a more uniform cooling is seen for the bottom layer (**Figure 5 (d)**) as the flow is directed to the probes from the top layer gap as well as the probes at bottom in staggered have almost similar t_e.

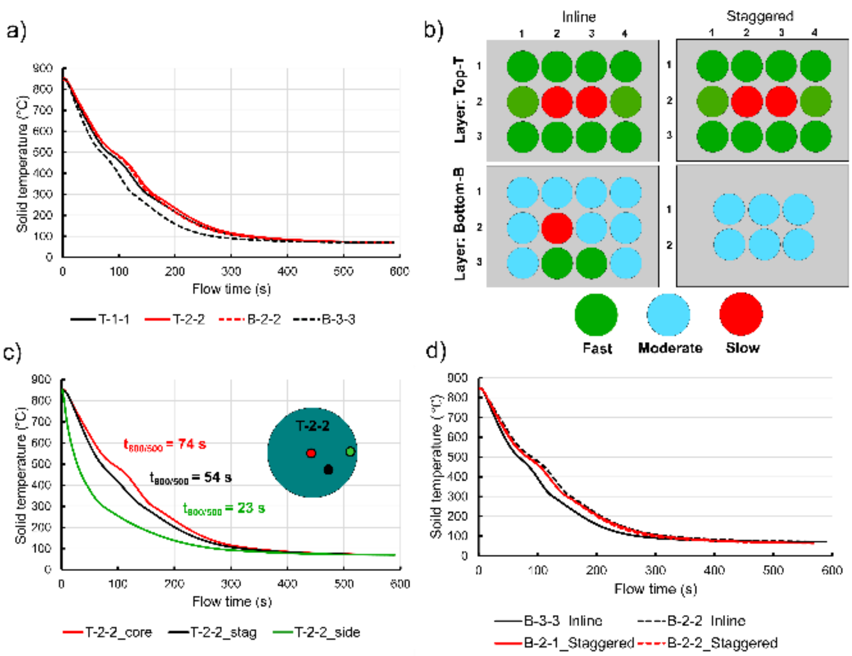

Figure 5 (a) Quenching curve from probe core for 10 bar, (b) Quenching trend for inline and staggered configuration, (c) Quenching trend within the probe T-2-2 for 10 bar quenching and (d) Quenching trend for inline and staggered configuration for 10 bar quenching

5.2. Influence of pressure on quenching

The influence of pressure is analyzed by varying it from 10 to 6 bar as seen in **Figure 6.** The increase of pressure can accelerate the rate of cooling in top and bottom layer. This is becasue the increase in pressure results in higher HTC [1]. HTC depends on Re (Flow Reynolds number) as well as Pr (Prandtl number) [9].

Based on the experimentally determined temperature curves, it can be seen that the process/furnace parameters, the geometry and the position of the specimens have a major influence on the cooling rates and thus on the resulting microstructure and hardness. By using FEM simulations and ANN, it will be possible to calculate the hardness as a function of the process/furnace parameters and the position of the specimens.

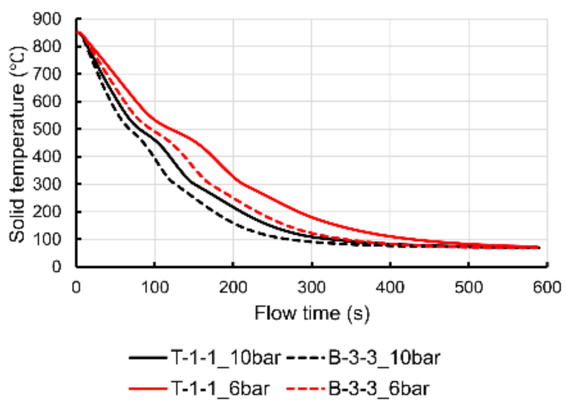

Figure 6 Influence of pressure on gas quenching (10 and 6 bar) for inline configuration

5.3. Results from FEM Simulation and ANN Modeling

The FEM results are first validated using continuous CCT. **Figure 7** shows good agreement between the hardness and the microstructure. It is found that isothermal TTT from the literature produce qualitatively reasonable but quantitatively deviating results with respect to the volume fractions of the individual microstructural constituents and thus the hardness. Based on the created material model, the further calculations for the variation of the HTC are carried out. **Figure 8** shows a typical example of the experimentally determined hardness of a heat-treated disc. It can be seen that there is higher hardness at the edge and lower hardness at the center. The maximum hardness is about 56 HRC and the minimum hardness approx. 30 HRC. It should be noted that the results of the hardness vary depending on the process and boundary conditions as well as the position of the sample in the batch, but qualitatively the results are comparable, i.e. higher hardness at the edge and minimum towards the core.

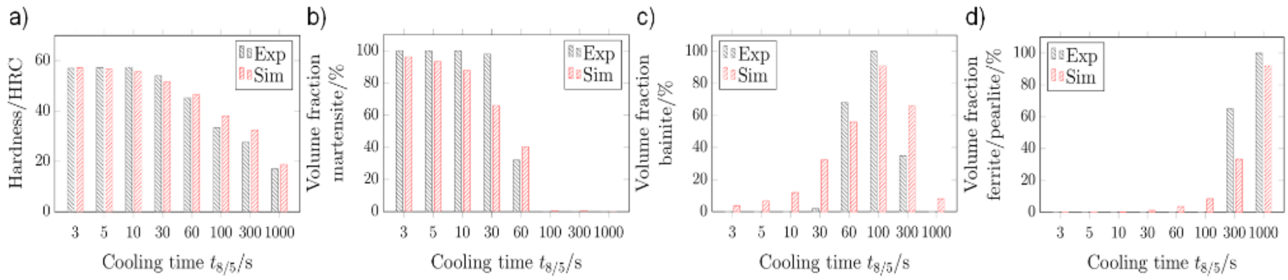

Figure 7 Comparison of experimental and simulated hardness as well as volume fractions of the different microstructures of the CCT samples of 42CrMo4 for different cooling rates. a) Hardness, b) Martensite, c) Bainite, d) Ferrite/Pearlite.

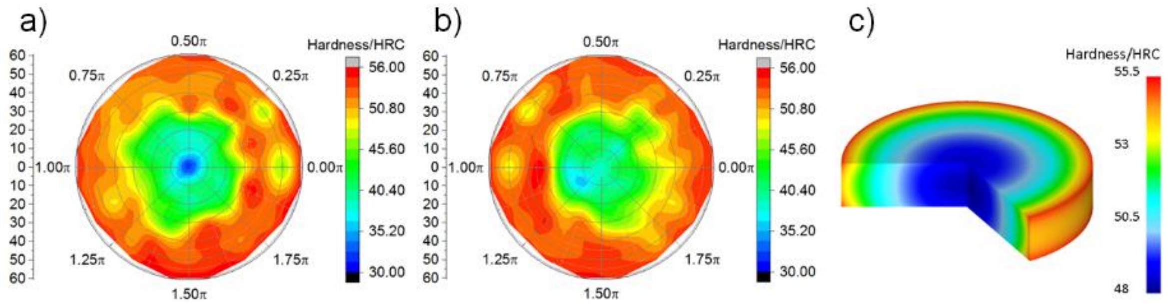

Figure 8 Example for the experimental hardness of 42CrMo4 (T-1-2, 10 bar, inline, ventilator velocity maximum) a) Top side, b) Bottom side and c) Example of simulated hardness by FEM (rotationally symmetric 2D)

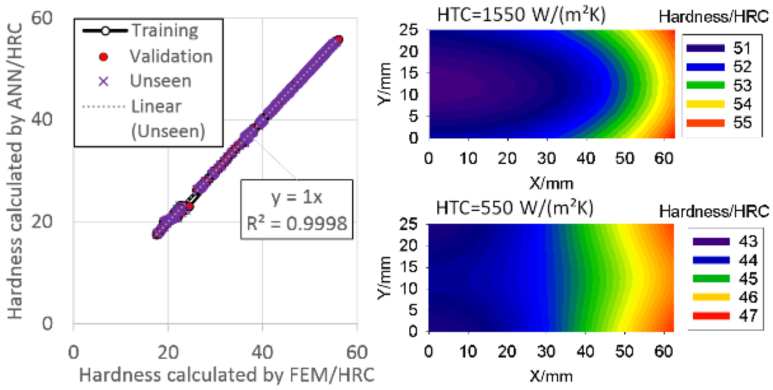

Figure 9 Comparison between the predicted hardness by FEM and ANN as well as hardness contour plots calculated by ANN

The results from the ANN are shown in **Figure 9**. The transfer of the FEM simulation results to the ANN worked very well. This is indicated by the linear regression of the unseen data and the coefficient of determination of almost 1. The results also shows examples of the hardnesses for HTC = 550 and 1550 W/(m²K). This illustrates the possibilities of the ANN training by means of the FEM simulations.

6. CONCLUSION AND OUTLOOK

Heat treatment experiments shows that the effective hold time is not equal to oven hold time and this depends on layer, batch and position of probe. The effective hold time is improved for bottom layer in staggered configuration. For inline and staggered configuration the outer probes in top layer are cooled faster than inner, also for the bottom layer in inline posses mixed quenching trend but for staggered with a uniform cooling trend. The rate of cooling within a probe is not uniform, where the edges are cooled faster than the core. The rate of cooling for top and bottom layers is increased with increase of gas pressure.

Heat treatment simulations using FEM requires the validation of the input data used and especially the TTT. Once the FEM model is validated, the results can be used for the extension of the experimental space as well as to train the ANN. With this method the ANN allows to calculate the hardness as a function of the HTC.

In further steps, depending on the selected furnace parameters such as pressure, ventilator velocity as well as the component geometry and the batch, the HTC are to be calculated by means of CFD and compared with the experiments presented. By coupling the furnace parameters with the HTC, it should be possible to predict the local hardness of the components as a function of the process parameters. Furthermore, based on optimization methods, it is feasible to define a required minimum hardness for a component and to predict the required furnace/process parameters by means of a prognosis tool based on ANN.

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