

Analysis of a Thermomechanically Coupled Forming Process Using Enhanced Design and Analysis of Computer Experiments

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Abstract

In this paper, a thermomechanically coupled forming process consisting of an inductive heating, an automated workpiece transfer and positioning, and a forging step with integrated cooling is analysed. To accomplish this, real-world experiments and a detailed thermomechanically coupled finite-element analysis (FEA) of the process are combined. Design and Analysis of Computer Experiments (DACE) is used to separately compute surrogate models for both elements as well as a two-stage metamodel of the process, which emerges by enhancing the DACE metamodel for the FEA with an empirical model of the systematic deviations of the FEA from the real-world experiments. In order to compute the DACE models, in all steps, a meaningful subset of the observations has to be identified, since DACE does not scale well with an increasing number of experiments due to the inversion of the correlation matrix. Furthermore, the assumption of deterministic output does not hold for all modelled responses, which is factored in by incorporating a nugget effect. The results on the practical application are presented and a statistical validation of the DACE models is performed.

Keywords

Metamodelling, Kriging, Design and Analysis of Computer Experiments (DACE), Nugget Effect, Sampling, Functionally Graded Material (FGM), Finite-Element Analysis (FEA)

1 Introduction

A differential thermal process control provides the possibility of establishing different functional zones within workpieces made of a single material. The localised induction of heat within the mechanical forming process, also denoted as thermomechanical coupling, allows reducing the number of additional process steps without losing flexibility in the design of the product [1]. In contrast to composite materials, the resulting functionally graded materials are economical and easy to recycle [2]. Thus, this technology offers a novel potential for an innovative production. Nevertheless, comprehensive knowledge about the process is necessary to control the phase transformations, which essentially determine the properties of the final workpiece [3].

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The combination of extensive experimental investigations and detailed computer simulations is the key to understanding complex engineering processes. The real-world experiment represents the original system, which can only be modelled by allowing restrictions and simplifications. However, measurements during or after the real process are usually expensive, time-consuming, and not accurately reproducible. For some properties, an in-process measurement is not even possible. In these cases, detailed computer simulations based on physical or phenomenological equations offer an alternative. Their output is usually deterministic, but systematic deviations from the real-world behaviour can occur due to simplifications and unknown coefficients in the internal equations. Thus, the output of a simulation should always be validated against real-world experiments.

The main idea of this work is the combination of the freedom from systematic modelling error provided by real-world experiments and the reproducibility and high resolution of the output of a computer simulation in order to compute a two-stage metamodel of a complex thermomechanically forming process using Design and Analysis of Computer Experiments (DACE) [4], [5], [6]. The lower-stage models are also based on DACE and describe the output of the computer simulation as well as the measurements obtained from the real process. Based on the empirical models of the process, the systematic deviations of the computer simulation from the real-world experiment are determined. The two-stage metamodel ultimately emerges by combining the DACE metamodel of the computer simulation and the model of the systematic deviations.

A steel shaft with different functional zones is used as an exemplary application for functionally graded materials. The corresponding forming process and the thermomechanically induced phase transformations are introduced in section 2. For this process, a finite-element analysis (FEA) has already been realised, which is briefly described in section 3. The computation of DACE models is presented in the three following sections. First, the measurements obtained from the real-world experiments are empirically modelled in section 4. To accomplish this, a white-noise process has to be integrated within the covariance function [7], [8]. The output of the FEA is modelled in section 5. The computer experiments based on the FEA are designed to analyse the whole parameter region and compensate inaccuracies of the empirical models due to a low sampling density. The systematic deviations of the FEA output from the results of the real-world experiments are identified and modelled in section 6. For each model, sampling techniques have to be used in order to identify a representative subset, where the requirements of each model are different, thus, leading to different methods. In section 7, the results of the case study are presented. Conclusions are drawn and an outlook on possible methodical improvements is provided in section 8.

2 Thermomechanically coupled forming process for functionally graded material

The thermomechanically coupled forming process, which is considered in this study, consists of an inductive heating, an automated workpiece transfer and positioning, the actual forging process, and the cooling within the forging dies (Figure 1). The workpiece, a shaft with a flange in its centre, is made of CrV-alloyed steel (51CrV4). The process-integrated introduction of different functional zones is caused by phase

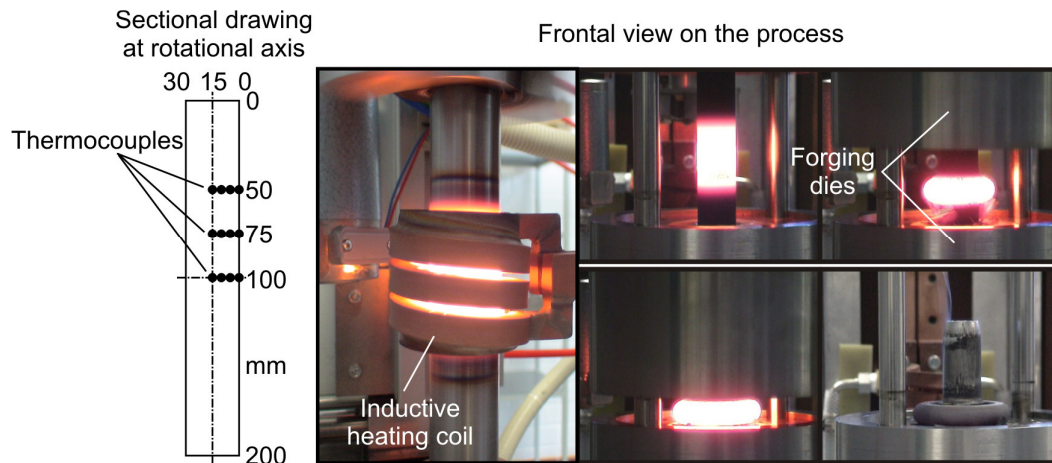


Figure 1: Process sequence, dimensions of the workpiece, and measurement positions

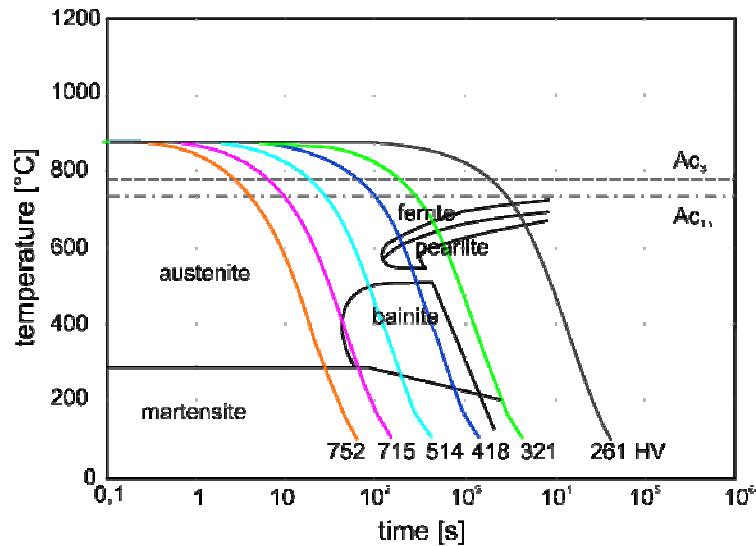


Figure 2: Time-temperature-transformation diagram for the continuous cooling of 51CrV4 [9] with exemplary temperature trajectories

transformations induced by different local temperature levels and cooling rates, which determine important workpiece properties, such as hardness, damping, and mechanical strength [1], [3].

The interdependence of the cooling rates and the phase transformations is shown in Figure 2. For local temperatures above AC_1 , the austenitisation of the material is initiated, which is completed when AC_3 is reached. The cooling of the workpiece begins directly after the heating. Depending on the cooling rates, a local martensitic phase transformation, which leads to a high hardness, can take place in the flange of the workpiece. At lower cooling rates, bainitic phase transitions occur or even a microstructure similar to the initial state can be the result. If the local temperature trajectories in the workpiece during the cooling phase are known, an estimation of the phase transformations is possible by means of the time-temperature-transformation diagram (Figure 2).

Within the actual forming process, there are no control variables which can influence the cooling of the material since the forging parameters are fixed at maximum pressure and speed in order to obtain high deformation degrees [1]. Thus, the cooling mainly depends on the temperature gradients within the workpiece after the heating, and, therefore, the focus of this study is on the analysis of the temperature evolution before the forming step, which can be controlled by varying the power of the inductive heating P and the heating time t .

3 Finite-element analysis of the forming process

The process is simulated completely in a single thermomechanically coupled analysis, which comprises the process steps electromagnetic heating with a simple heat-source model, free and tool-shape-determined forging, and cooling of the workpiece in the closed dies. A detailed description of the finite-element formulation has already been published [10], [11]. Due to the axial symmetry of the process, it suffices to consider a quarter of the workpiece and the forging dies in a three-dimensional model (Figure 3). A simple plasticity model accounting for thermal strain and isotropic hardening is used, where the yield stress is a function of the effective plastic strain and the temperature. In order to account for the cooling effect due to the heat transport, a thermomechanical contact is defined between the workpiece and the forging dies. The process of inductive heating is modelled in a simplified way based on physical considerations. In the area, where the induction coil covers the workpiece (cf. Figure 3), a volumetric heat source is prescribed for a thin surface layer of the workpiece. The parameter of the heat source has been identified based on results for the so-called standard process with a power of inductive heating $P = 42 \text{ kW}$ and a maximum heating time $t_{\max} = 12 \text{ s}$ [1], [10].

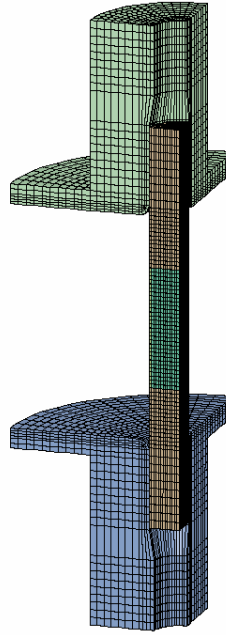


Figure 3: Finite-element mesh for the simulation of the forming process

4 Empirical modelling of temperature measurements

Real-world experiments are conducted in order to analyse the temperature distributions, which can be achieved by different heating strategies as well as identifying systematic deviations of the finite-element analysis (FEA). The power of the inductive heating P with frequency $f_h \approx 15$ kHz is varied between 10 % and 70 % of the maximum power $P_{\max} = 60$ kW. Higher percentages are not considered since the degree of efficiency is too low for these settings. During each experiment, the temperature trajectories are monitored by thermocouples, which are positioned at 12 distinct positions of the workpiece (cf. Figure 1). Since different maximum heating times $t_{\max}$ are realised for all settings of P , replications of some of the measurements are available, which can be used to estimate the variation in the observations. The upper region of the workpiece is not covered by the experiments since the temperature gradients in this region are expected to be small. The factor settings of all real-world experiments are listed in Table 1. For $P = 12$ kW and $P = 30$ kW, no experiments were performed.

The measurements obtained from the experiments are used to compute empirical models by means of Design and Analysis of Computer Experiments (DACE) [4], [5], [6], which predict the temperature trajectories over the heating time for each realised setting of P and each measurement position. Consequently, each model has only the current heating time t as input variable to predict the current temperature T . DACE has been chosen because it is flexible with respect to the distribution of the input variables as well as the complexity of the modelled response. However, since for each setting of P multiple measurements exist and the thermocouples offer a measurement frequency $f_m = 60$ Hz, the number of input values is too high to allow an efficient use of DACE due to the internal matrix inversions and decompositions [5]. Furthermore, the replications show a high variation in the temperature measurements (cf. Figure 4), which are contradictory to the assumption of deterministic output made in DACE.

Table 1: Factor settings of the real-world experiments

P [kW]	6	6	6	18	18	18	18	24	24	24	36	36	36	36	42	42
t_{max} [s]	24	32	48	6	12	24	32	6	12	18	3	6	9	12	12	12

A known concept of integrating white noise into DACE is called nugget effect. It traces back to the Kriging literature [7]. The nugget effect still leads to a perfect correlation of each observation with itself, but a damped correlation with other observations, even if those have the same parameter vector. The damping factor g can be empirically estimated with the other parameters of the DACE model using maximum-likelihood estimation (MLE) [8].

In order to find a model, which reflects the trend as well as the variation in the measurements, a representative subset of the measurements has to be chosen. For this purpose, a random sampling of $n = 100$ observations without replacement is realised. This is appropriate since the sample size n is sufficiently large and each element has an equal probability of selection, thus, leading to an unbiased sample of the population of measurements. The chosen samples are used to compute DACE models with constant regression function, Gaussian correlation function, and nugget effect. For each data set, the log-transformed response is also modelled. The calculation of the model parameters and the choice of the model are based on MLE.

The models are validated by computing predictions for the observations, which have not been used to fit the model. These validations provide an average error over all empirical models of $11.8\text{ }^{\circ}\text{C}$, which is smaller than one percent of the temperature range. Furthermore, a Shapiro-Wilk test is used to test the normality of the standardised residuals. The null hypothesis has to be rejected ($p \approx 0$) since the nugget effect balances the prediction between different temperature trajectories for repeated measurements, which leads to clusters of residuals. The number of runs is too low for the central limit theorem to hold.

5 Design and metamodeling of the finite-element-analysis experiments

The metamodel of the FEA is computed to predict the temperature distribution over the whole workpiece with respect to the power of the inductive heating P and the current heating time t . To accomplish this, two factors encoding the position in the rotational symmetry axis also have to be considered as inputs of the metamodel (cf. left panel of Figure 1), where the height is now considered in the interval between 0...100 mm. The observations for the calculation of the metamodel are provided by computing the temperature distributions corresponding to $P = 6...42\text{ kW}$ in steps of 6 kW for the corresponding maximum heating times $t_{\max,P}$ of Table 1. For $P = 12\text{ kW}$ and $P = 50\text{ kW}$, $t_{\max,12} = 40\text{ s}$ and $t_{\max,50} = 15\text{ s}$ have been realised, respectively. Each of the seven runs can provide the temperature trajectories of each node in the front slice of the net shown in Figure 3, leading to a total amount of 205,842 observations. Thus, another point selection has to be performed in order to allow computing DACE metamodels.

The sample is used to compute global DACE metamodels with constant regression function for the output of the FEA based on MLE. No nugget effect is allowed since the output of the FEA is deterministic. The factor levels of P are specified by means of the performed simulation runs. Thus, only the two-dimensional node positions and the time t can be designed. According to literature [6], [12], different Maximin-distance Latin-hypercube designs (LHD) of size $11d-1 = 32$ are realised for each factor level of P , which are calculated using the algorithm of Jin et al. [13]. Additionally, the 16 corner points of the four-dimensional factor space are evaluated since LHDs tend to focus on the inside of the factor space. This approach results in $n = 240$ observations, which is close to the maximum number to be handled by the DACE toolbox [5]. Due to the limited resolution of the net, the node next to the desired position is chosen.

Again, the DACE metamodels are validated by means of the observations not used to fit the models. The Gaussian correlation function provides an average error of $11.6\text{ }^{\circ}\text{C}$. The use of the Kriging (or power exponential) correlation function can improve the fit to an average error of $7.2\text{ }^{\circ}\text{C}$, which is smaller than one percent of the temperature range. Again, Shapiro-Wilk tests on the standardised residuals strongly indicate that the distribution is not normal ($p \approx 0$ for both models). This may be caused by a violation of the stationarity assumption made in DACE. However, since the uncertainty estimation is not required for the further analysis, the Kriging metamodel is considered in the following section.

6 Combined DACE metamodeling of the forming process

The main idea of the two-stage metamodel is adapted from Kennedy and O'Hagan [14]. They propose using output of different computer simulations with an increasing degree of complexity to compute a metamodel for the most complex simulation model. More precisely, a hierarchy of sub-models is constructed with

respect to increasing complexity. Each sub-model uses only the information of the sub-model one level below, for which the systematic deviations are modelled in terms of a Gaussian process. More details and a formal derivation can be found in the original work [14].

According to this procedure, the real-world measurements represent the upper level, and a DACE model for the systematic deviations of the FEA from these measurements is computed. This DACE model uses a constant regression function and a Kriging correlation function since the smoothness of the response surface can not be assumed a priori. Furthermore, a nugget effect is allowed due to the measurement error in the real-world experiments. In order to compute deviations, replications of the designs already realised in the experiments are necessary, leading to 60 factor combinations (5 settings of P and 12 positions). Since the time step Δt of the simulation is big compared to the 60 Hz measurements of the real-world experiment, each Δt the deviation of the temperature predicted by the empirical DACE model for the measurement position and the corresponding node in the FEA is computed. This procedure results in 2,964 observations of the deviation, 1,354 of which are outside the 95% CIE of the empirical model. The range of the deviations is $[-49\text{ }^{\circ}\text{C}, 484\text{ }^{\circ}\text{C}]$.

2,964 samples are way too many to efficiently compute a DACE model. Thus, a smaller subset of meaningful samples has to be identified. Since the systematic deviations are assumed to show a complex nonlinear behaviour, which depends on the position as well as on the power of the inductive heating, a sequential sample selection is performed, which aims at identifying the most important information in the data. To accomplish this, an initial model is computed for a design containing only the observations at $t = 0\text{ s}$ and $t = t_{\max,P}$ for each of the 60 factor combinations. Afterwards, the observation having the highest prediction error with respect to the current model is selected and the model is updated. This procedure is iterated until $n = 251$ observations have been selected¹.

The validation by means of the deviations, which are not incorporated into the model, results in an average error of $11.4\text{ }^{\circ}\text{C}$. Due to the sequential sampling criterion, the maximum error is only $43.4\text{ }^{\circ}\text{C}$, which is smaller than five percent of the range of deviations. The Shapiro-Wilk test on the standardized residuals again indicates a violation of the stationarity assumption, which results in nonnormally distributed residuals ($p \approx 2 \cdot 10^{-13}$).

7 Results

The results of the different measurements and models are shown in Figure 4. The varying settings of the maximum heating time $t_{\max}$ result in multiple measurements. The gap in the lower measurement of the left plot is caused by a temporary failure of the thermocouple. Due to the nugget effect, the uncertainty of the empirical models of the process reduces to the variation in the series of measurements. As depicted by the predictions shown, two kinds of such variation occur. In the left plot, both series of measurements show the same trend, but have a constant offset. In the right plot, the measurements systematically diverge for $t > 9\text{ s}$. Both situations can be reflected by the confidence-interval estimates (CIE) of the empirical DACE models by using either the original or log-transformed inputs.

The evaluations of the FEA can be predicted accurately by the DACE metamodel, although most of the evaluations are not used for the fitting. In both situations, the FEA produces an approximately linear increase in temperature, whereas the real-world measurements show a nonlinear behaviour due to a demagnetisation of the material with increasing temperature, which results in a changeover of the character of inductive heating. This effect is not considered in the FEA, in which the inductive heating is modelled by a constant volumetric heat source, whose value was calibrated to the highest heating power $P = 42\text{ kW}$. However, for $P = 24\text{ kW}$, the temperature is systematically predicted too low by the FEA, i.e., the assumption of a linear

¹One may ask why this technique has not been used to select the samples in section 4 and 5. In section 4, a nonbiased subset was required to identify the trend and the variance in the data. In section 5, the number of observations was too high to efficiently realise this approach. Nevertheless, the prediction quality of the resulting models showed that these sampling techniques were appropriate.

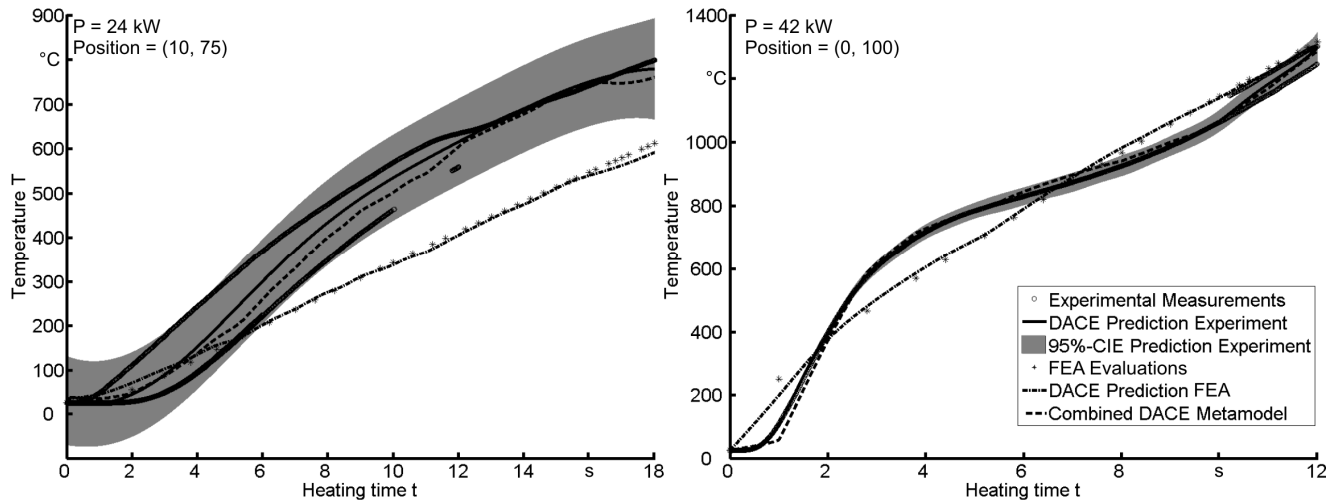


Figure 4: Comparison of the different predictions and measurements for $P = 24 \text{ kW}$ at position $(10, 75)$ (left, cf. Figure 1) and $P = 42 \text{ kW}$ at position $(0, 100)$ (right, cf. Figure 1)

dependence of the energy released by the volumetric heat source on the power of the inductive heating P seems not to be valid due to a lower degree of efficiency during inductive heating for higher settings of P . The combined model is capable of compensating the systematic deviations of the FEA resulting in predictions within the 95 % CIE of the empirical models and in an adequate description of the nonlinear temperature increase. In Figure 5, the improvements of the combined DACE metamodel (right) compared to a DACE model, which is based just on the real-world measurements (left), are depicted. Due to the higher resolution of sampling points in the subspace of possible positions, a prediction of the nonlinear temperature distribution over the whole workpiece geometry is possible (right). In contrast, the regular and sparse distribution of measurement positions in the lower half of the workpiece results in a singular Gaussian process model with a very limited amount of information (left).

8 Conclusions and Outlook

In this work, a two-stage metamodel of an inductive heating process has been presented. This model combines the high resolution of an FEA with the freedom from systematic modelling error of real-world measurements. The calculation of the required sub-models for the measurements, the FEA, and the

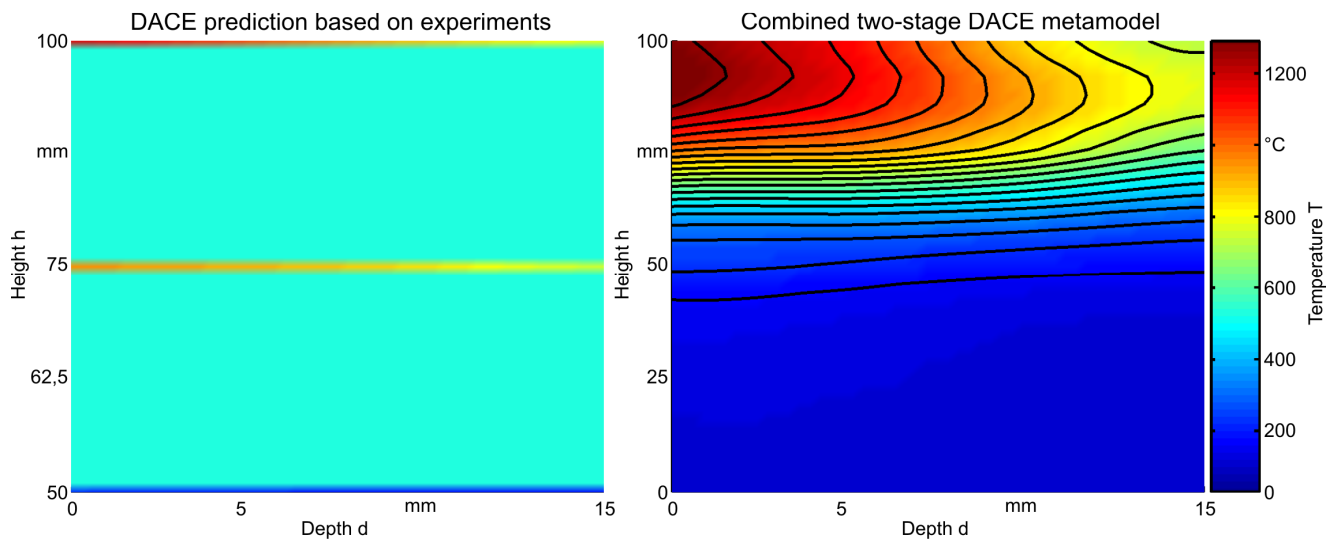


Figure 5: Comparison of the predictions of the temperature distribution after the standard process with $P = 42 \text{ kW}$ and $t = 12 \text{ s}$ based on an empirical DACE model of the corresponding measurements (left) and the combined DACE metamodel (right)

systematic deviations of the FEA are described. In particular, enhancements to the DACE models are applied and sampling techniques to identify meaningful subsets of the observations are presented, which are necessary due to the numerical limitations of the DACE models. All models are validated, and the results of the final metamodel for the process are shown.

The systematic deviations of the FEA hint at possible improvements of the FE model. An implementation of these improvements will also improve the results for the simulation of the whole process. The violation of the assumption of normally distributed residuals remains a problem. It is assumed that this violation is caused by a non-stationary covariance of the observations. A combination of the results of the residual analysis and a corresponding transformation of the factor space seems promising.

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