Identification of the thermal conductivity tensor for transversely isotropic materials

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Abstract
The knowledge of the thermal conductivities is of particular interest for the thermo-mechanical modeling of transversely isotropic composite materials. Hence, the identification of these material parameters by solving an inverse problem is significant, as they cannot be directly measured. In this study, a suitable experimental setup is presented, where infrared thermography is used to measure the surface temperatures of thin specimens. Further, a local identifiability concept is employed to study whether locally unique parameters can be obtained. This leads to a particular step-wise identification concept. The parameter identification is performed applying a nonlinear least-square approach and finite elements. In the step-wise identification process the convection coefficient is required first, and, subsequently, the coefficients of the thermal conductivity tensor are determined. Due to the step-wise identification, the uncertainties of previously identified parameters have to be considered in the subsequent identification steps. The resulting uncertainties are estimated using the Gaussian error propagation concept. It turns out that the thermal conductivities of transversely isotropic materials are generally identifiable from surface temperature data. Furthermore, since all uncertainties have an essential influence on the results of real numerical simulations, their error propagation should be considered in resulting boundary-value problems. Thus, the uncertainty quantification is demonstrated by a validation experiment.

KEYWORDS
material parameter identification, identifiability, finite element method, infrared thermography, composite materials, error propagation, uncertainty quantification

1 | INTRODUCTION

Composite materials have risen in application in recent years and are not anymore high-performance materials with applications in small niches, but highly requested materials for lightweight design in many industries. Hence, the significance of further development and broadening the application fields is of enormous interest in research as well. A crucial point for the application of certain materials is the knowledge about their mechanical and thermal behavior, depending on the field of application. Alongside the pure knowledge, numerical simulations are a key factor for economical and
progressive design and development of composite materials. As robust numerical simulations, especially in the field of continuum mechanics, depend on reliable material parameters, the field of material parameter identification has soared popularity in recent decades.

The identification of material parameters is generally an inverse problem, meaning that the mechanical and/or thermal constitutive (material) model and its solution (analytical, numerical) are known. In contrast, the material parameters within the model have to be identified, see [4,73]. Although first more in-depth studies of parameter identification concepts stem from the 1970s, see, for example, [12] and [10], the further increase of research interest have been associated with the ongoing development of numerical methods to calculate the parameters. Here, the solution of the direct problem using analytically sophisticated approaches or extended numerical solution schemes are applied together with modern experimental techniques (see [50] for the notion of the direct problem). Regarding the optimization schemes, we refer to [9,13,21,45,55,68]. An investigation of optimization schemes is not of interest here, because the applied schemes are fully satisfactory for the current work.

However, we follow a traditional concept based on a nonlinear least-square approach, where finite elements are chosen to solve the direct problem. This approach is denoted as the FEMU approach in recent literature, see, for example, [5,64]. The spatial discretization using finite elements yields—depending on the PDE and the constitutive models—systems of algebraic, ordinary-differential, or differential-algebraic equations. A first finite element based parameter identification procedure is originally introduced by [41]. The identification of material parameters by means of finite elements is mainly driven by [51,53] for mechanical, as well as for thermomechanical constitutive equations by [49]. Further contributions are given in the theses of [42,61,67] or by [11,30,43,44]. Much more publications have been published using finite elements in combination with full-field deformation data. A more general background is provided by [68], where the application of least-square methods in combination with Gauss-Newton like schemes on systems of differential and differential-algebraic equations is discussed. This is the case for finite elements solving the transient heat equation.

Rose and Menzel [64] present and evaluate a comprehensive framework of thermo-mechanically coupled material models for parameter identification issues. Therein, the identification of mechanical and thermal material parameters is not only based on force data obtained from the testing machine, but also experimental displacement data received from digital image correlation measurements and temperature data measured with infrared thermography. Especially the process of bringing together the displacement and temperature values is covered.

In the context of material parameter identification, the question arises whether the material parameters are sufficiently identifiable with the experimental data at hand. Therefore, the concept of local identifiability, as proposed by [12] and [10], can be followed. The identifiability investigations give a certain insight into the optimization problem and show whether uniqueness of a solution in the vicinity of the obtained parameters is guaranteed (this does not address the question whether a global minimum is obtained). As stated by [52] there are two possible reasons for non-uniqueness of parameters—linear dependencies of the parameters and experimental data that does not address the parameters sufficiently. To circumvent non-uniqueness caused by parameter covariance, [40] suggest to either reduce the parametrization of the material model or increase the information obtained from experiments. Further approaches are the introduction of identifiability indices to quantify the inverse problem of material parameter identification, see [6,60] for studies in the context of nanoindentation tests. The presented identifiability index is based on the eigenvalues of the respective Hessian matrix of the optimization problem in the FEMU context. In the field of solid mechanics, exemplary studies regarding the local identifiability are conducted by [27] and [70]. However, thermal material parameters are only studied in the context of thermo-mechanical material models, but not for the purely thermal case.

It is important to use quality measures to distinguish whether a solution obtained from the optimizing scheme is suitable or not. We apply the confidence interval of the identified parameters as quality measure of the parameters, and, of course, the coefficient of determination $R^2$ to assess the quality of the fit. To consider the measurement uncertainty during the experiments and the uncertainty due to the subsequent use of previously identified parameters, we follow the concept of error propagation. A general discussion about uncertainties and error propagation can be found in [7,74]. The maximum expectable error results from the linear error propagation concept. However, as we assume that the errors may compensate each other to a certain extent, we draw on the so-called Gaussian error propagation.

Before the determination of thermophysical parameters from full-field information is investigated, conventional procedures will be discussed first. There are many different methods to determine the thermophysical parameters of materials, see [14] for a survey. In general, they are commonly divided into three groups—stationary and transient methods in the time-domain and periodic methods in the frequency-domain. The laser-flash method, compare [56], is a generally applied contactless method to determine the thermal diffusivity, which then enables the computation of the thermal conductivity. The specimen is subjected to a short laser impulse on one side, whereas the temperature change on the rear
side is measured. The classical laser flash method is only able to measure the thermal diffusivity in the thickness direction of the specimen. For composite materials, such as the carbon fiber reinforced polymer at hand, this implies that the thermal diffusivity is only measured in the perpendicular direction to the built-up layers and therefore restricts the use of the data, for example, for numerical simulations. Further, the hot-disk method is realized that determines the thermal conductivity based on a so-called transient plane source method, see originally [26]. There, the heat equation is evaluated locally at a dot-shaped heat source, see [32]. For frequency-domain methods, we exemplarily refer to [48], where the determination of the thermal conductivity with the hot wire 3ω method at composite materials is presented.

There are numerous studies that relate to the determination of the thermal conductivity. Herein, only a short overview regarding the application to anisotropic solid materials is given. A discussion especially on the determination of the transverse thermal conductivity for carbon fiber reinforced composites is given by [63]. Therein, the authors compare different micromechanical approaches to results from numerical simulations as well as experimental data obtained from the guarded hot plate method and the transient hot-strip experimental procedure. Huang and Yan [33] propose the application of the conjugate gradient method to simultaneously determine the temperature-dependent thermal conductivity and heat capacity. The proposed concept includes the transformation of the inverse problem and a transient function estimation. Another method to experimentally determine the thermal conductivity of fiber-reinforced composites is presented by [72]. Thereby, the authors applied thermocouples to measure the temperature at certain points of a specimen, since there was no optical access for applying non-contact temperature measurement methods. Advantages of the described setup are the minimization of the influence of convection and radiation, achieved by using vacuum cavities and the placement of the specimens. The experimental setup proposed by [76] enables the authors to identify the components of the thermal conductivity tensor and the heat capacity from experimental measurements solving the inverse heat conduction problem. A non-destructive technique to determine the components of the thermal conductivity tensor of orthotropic solid bodies is shown in [1]. Therein, the authors discuss the experimental procedure as well as the formulation and solution of the inverse problem to obtain the three principal thermal conductivities of orthotropic materials with the restriction to small anisotropy. The experimental procedure included a laser source to apply a short laser impulse on the specimen’s surface. In contrast to the mentioned standard laser flash method, the temperature change was measured on the same side of the specimen using an infrared camera. The procedure was verified on steel specimens treated as anisotropic material as well as on carbonaceous material. In further studies, we refer to [2], the aforementioned procedure is applied to carbon fiber reinforced polymers that inherit a larger anisotropy. Philippi et al. [57] present originally a new experimental setup based on the common laser flash-method, but here applied to orthotropic materials. Thereby, in contrast to the classical method, three-dimensional heat transfer was induced due to the application of a geometrical nonuniform heat impulse. The temperature measurement was done with an infrared camera. The obtained temperature fields were used within an estimator to determine, among other parameters, the thermal diffusivity components of the material, see [65] as well, as the authors studied the performance of different estimators. Rassy et al. [24] propose a way to directly identify the thermal diffusivity tensor of orthotropic materials for carbon fiber composites that allows the calculation of the thermal conductivity with known density and heat capacity of the material. Therefore, the authors applied a further improved 3D laser flash method.

The primary aim of this work is the evaluation of a simple experimental setup to measure suitable temperature data and subsequently identify the components of the thermal conductivity tensor of transversely isotropic materials. Thereby, the experimental setup comprises a heat plate and an infrared thermography camera. In contrast to other approaches, such as [1], the proposal here does not require a laser in the experimental setup. Thus, further computationally expensive simulations can be spared to incorporate the surrounding air around the laser spot as it was done by [2]. Opposed to [76], a very simple experimental setup without applying a vacuum chamber is used. Nevertheless, full-field temperature data for the parameter identification procedure can be applied instead of temperatures at certain locations, compare [72]. Further, studies regarding the concept of local identifiability are performed to show which material parameters are identifiable with the measured experimental data. Based on the results of these investigations, a sequential identification procedure is followed to identify the thermal conductivities of transversely isotropic specimens. Since sequential identifications are prone to errors, we use Gaussian error propagation to evaluate the quality of the identified material parameters. To solve the inverse problem, we draw on a nonlinear least-square method that minimizes the difference between the simulation data (model response) and the measured experimental data. The resulting system of nonlinear equations is then solved by means of a trust-region-algorithm. Other methods to deal with the inverse problem, instead using a nonlinear least-squares method, are the application of genetic algorithms [19] or neural networks [20].

In the following, we start with the explanation of the experimental setup as well as the process for extracting the specimens temperature from infrared thermography measurements. Then, the transversely isotropic heat conduction is
shortly recapped. Further, we summarize the applied identification procedure, where we employ a nonlinear least-squares approach and finite elements. Suitable quality measures to evaluate the identified parameters are shown. Also, the question of identifiability of different parameter sets is studied and a suitable identification procedure for the thermal conductivities of transversely isotropic material is deduced. It turns out that a sequential identification procedure is a convenient approach. Thereby, we employ the Gaussian error propagation concept throughout from the parameter identification to the results of subsequent numerical simulations. The work is concluded with a discussion of the identified parameters and the applied identification procedure.

The notation in use is defined in the following manner: geometrical vectors are symbolized by \( \vec{a} \) and second-order tensors by bold-faced Roman letters \( \mathbf{A} \). Furthermore, we introduce column vectors and matrices symbolized by bold-faced italic letters \( \mathbf{A} \).

2 EXPERIMENTAL INVESTIGATION

This work aims at the material parameter identification of the thermal conductivity for a transversely isotropic material. Consequently, suitable experimental data is required. We applied infrared thermography to measure the surface temperatures of thin specimens under specific boundary conditions. In this section, we present the entire experimental setup and proceed with the description of the specimen’s surface temperature extraction from the thermograms.

2.1 Experimental setup

The studies in this work were performed with specimens made from a composite material with a unidirectional carbon fiber-reinforcement and a steel. The steel specimens are treated as isotropic material (the reason is explained later on), while the composite material is transversely isotropic. The fiber volume percentage of the composite material was approximately 50%. The chosen fibers were high performance carbon fibers of type Tenax HTA40, see [77] for details. As matrix material served the cured epoxy resin Araldite LY 556 with anhydride hardener Aradur 917 and imidazole accelerator DY 070. The mixing ratio by weight of the three components is 100:90:1. Further details can be obtained from the data sheet of the manufacturer, see [34].

To provide the experimental data for the following material parameter identification, we drew on an experimental setup that comprised, in contrast to [2,24], no laser source, but a simple heat plate. The heat plate was made of copper, whereas the energy source was a silicon heating pad and the temperature control was realized with a PT 100 resistance temperature detector. We set the heat plate to have a constant surface temperature of 100°C during the experiments. To measure the temperature of the specimens, we applied infrared thermography as a contactless temperature measurement method. Herein, we used the infrared thermography camera VarioCAM HD (InfraTec GmbH, Dresden, Germany). A crucial factor for the heat exchange between heat plate and specimen was the positioning of the specimen. Therefore, we drew on thin yarns, which were glued to the specimen and attached to holders mounted on a movable carrier, to achieve a plane and uniform contact between heat plate and specimen. In addition, a thermo paste was applied in the contact area to increase the heat conduction. A schematic drawing of the experimental setup is given in Figure 1A, the real setup from the viewpoint of the thermography camera is shown in Figure 1B.

The fundamental measurement principle of the infrared thermography is that the radiation of the surface is measured by the camera detector in a pixel-wise manner. Afterwards, the surface temperature can be calculated from the detected radiances. A major drawback of infrared thermography is that only surface temperatures can be measured. Therefore, the emissivity \( \varepsilon \) of the surface is essential among other parameters. Due to the significant influence of the emissivity on the experimental measured temperatures, it is intended to be precisely known. High emissivities close to one are to aim at to reduce interfering effects on the measurement, for example, through reflection of the radiation of surrounding bodies or fluctuations of the surrounding fluid temperature. The manufacturer of the chosen thermography camera recommends the application of the TETENAL camera varnish, see [36], with a known emissivity \( \varepsilon = 0.96 \) in the employed spectral range between 7.5 \( \mu \)m and 14 \( \mu \)m. The temperature of surrounding surfaces \( \Theta_{\infty} \) and the temperature of the surrounding medium \( \Theta_{\infty} \) were determined with a reference measurement and were constant 22.5°C during the experiments. See [47] and the literature cited therein, for a comprehensive overview of the theory of thermography, the measurement principle, and the influence of interfering parameters.
FIGURE 1  Experimental setup to measure the surface temperature of thin quadratic specimens (front view). A Schematic drawing. B Real experimental setup

FIGURE 2  Specimen for surface temperature measurements. (A) Geometry (measures in mm), (B) Painted specimen for infrared thermography

The technical data of the applied thermography system can be found in [37,47]. In contrast to the setup in [47], we used a normal lens with focal length 30 mm, field of view 32.4° × 24.6° and instantaneous field of view 0.57 mrad. The measuring distance of 0.3 m resulted in a pixel width of approximately 0.17 mm. The measuring distance is a negligible factor since the applied thermography system exploits a long-wave atmospheric window in the aforementioned spectral range, where the transmittance of air as surrounding medium is very close to one. Therefore, also the influence of the convection at the front surface of the heat plate can be neglected regarding the temperature measurement. Since the measured radiation is averaged in every pixel for the following temperature calculation, it is to strive for a low pixel width to achieve a high local resolution. This was also crucial for the parameter identification as well as for the extraction of the boundary of the specimen, as described in the following Section 2.2.

As mentioned before, we were only able to measure surface temperatures. Therefore, we utilized thin specimens with quadratic shape and an edge length of 50 mm. The thickness $d$ of the steel specimens was 1.5 and 2.5 mm for the composite material, see Figure 2A. A painted specimen is shown in Figure 2B.

2.2 Extraction of specimens temperature

The total field of view of the thermography camera was set to be slightly exceeding the specimen to sufficiently detect the specimen’s boundary. An exemplary thermogram of the measurements is shown in Figure 3A. It is in evidence that the specimen’s surface temperature was larger than the surrounding environment. The finite element model subsequently
described in Section 4.4 covers only the specimen itself. Therefore, we needed to extract the specimen’s temperature from the thermogram. This was done with an edge detection method in MATLAB using the “sobel edge detection”. The detected contour of the specimen is shown in Figure 3B. It can be seen that the contour comprised also reflections on the heat plate (top left corner in Figure 3B) as well as the glue dots that were applied to fix the specimen. To extract these spurious contour segments, we exploited the known edge lengths of 50 mm to fit the actual edges of the specimen, see the red dashed lines in Figure 3B.

The temperature data from the experiment and the simulations were in general not available at the same spatial points. The temperature values as degrees of freedom were known at the nodal positions in the finite element model. Whereas the experimental temperature values were pixel-wise scattered and needed to be interpolated onto the positions of the nodes in the mesh to ensure a valid comparison of the temperature values during the parameter identification procedure. The contour detection, together with the known edge length of the specimen, enabled the introduction of a scaling factor between pixels in the thermograms and length dimensions. To ensure the procedure, the determined scaling factor was verified with the pixel width resulting from the applied lens and measuring distance. A coordinate system was introduced in the bottom left corner of the specimen, Figure 3B. This was necessary for the following interpolation of the experimental temperature values. Thereby, we performed a linear interpolation of the temperature values to the nodal positions in the finite element mesh employing the MATLAB function scatteredInterpolant. The reader is referred to [64] for a detailed discussion on the interpolation of the experimental data and a related ansatz for the introduction of a coordinate system in the context of thermography measurements.

3 TRANSVERSELY ISOTROPIC HEAT CONDUCTION

The heat conduction equation under consideration reads

\[ c_p \dot{\Theta} = -\frac{1}{\rho} \text{div} \tilde{q} + r_\Theta, \]

where \( c_p \) is the heat capacity, \( \Theta \) the absolute temperature, \( \rho \) the mass density, \( \tilde{q} \) the heat flux vector, and \( r_\Theta \) a volumetric heat source. In this work, we restrict ourselves to the stationary case with the result that the term on the left-hand side vanishes. Moreover, the volumetric heat source \( r_\Theta \) is assumed to be zero,

\[ 0 = \text{div} \tilde{q}. \]

Here, Fourier’s model is assumed for the anisotropic case defining the heat flux vector

\[ \tilde{q} = -\kappa_\Theta(\Theta) \text{grad} \Theta. \]
For the case of isotropy, the second-order thermal conductivity tensor $\kappa_\Theta$ simplifies to a scalar value $\kappa_\Theta$ since the thermal conductivity is equal in all directions. With the case of a transversely isotropic material at hand, the thermal conductivity toward the fiber direction is different to the thermal conductivities orthogonal to the fiber directions. The notation is as follows, $\kappa_{\Theta,a} = \vec{a} \cdot \kappa_\Theta \vec{a} = \mathbf{M} \cdot \kappa_\Theta$ is the thermal conductivity along the fiber direction $\vec{a}$, $|\vec{a}| = 1$, and $\kappa_{\Theta,n}$ the thermal conductivity normal to the fiber direction. Hence, the thermal conductivity tensor can be formulated as

$$
\kappa_\Theta = (\kappa_{\Theta,a} - \kappa_{\Theta,n})\vec{a} \otimes \vec{a} + \kappa_{\Theta,n} \mathbf{I} = (\kappa_{\Theta,a} - \kappa_{\Theta,n})\mathbf{M} + \kappa_{\Theta,n} \mathbf{I},
$$

see [3]. Therein, $\mathbf{M} = \vec{a} \otimes \vec{a}$ denotes the structural tensor and $\mathbf{I}$ the second-order identity tensor. Since for the thermal conductivities $\kappa_{\Theta,a} \geq 0$ and $\kappa_{\Theta,n} \geq 0$ holds, see [31], the thermal conductivity tensor $\kappa_\Theta$ is a positive semi-definite tensor.

To solve the partial differential equation (2), the spatial discretization using finite elements is performed. This is briefly recapped in the following. The system of nonlinear equations is derived by changing the tensorial notation to the matrix notation. The stationary form of the heat equation (2) reads

$$
0 = \text{div} \, \mathbf{q}(\mathbf{x}),
$$

with the heat flux (3)

$$
\mathbf{q}(\mathbf{x}) = -\kappa_\Theta(\Theta) \, \text{grad} \, \Theta(\mathbf{x}).
$$

Further, we specify Dirichlet boundary conditions $\Theta(\mathbf{x})$ on $A^\Theta$ and Neumann boundary conditions $\mathbf{q}(\mathbf{x})$ on $A^\vartheta$, $A = A^\Theta \cup A^\vartheta$,

$$
\Theta(\mathbf{x}) = \Theta^\Theta(\mathbf{x}) \, \text{on } A^\Theta, \quad \mathbf{q}(\mathbf{x}) = \mathbf{q}^\vartheta(\mathbf{x}) \, \text{on } A^\vartheta.
$$

The Neumann boundary conditions are related to the heat flux. Since the heat flux is temperature dependent (mixed boundary conditions caused by convection and radiation), it is called Robin boundary condition, [25]. The respective heat fluxes for convection $\mathbf{q}_{\text{conv}}^\text{rad}$ and radiation $\mathbf{q}_{\text{rad}}(\Theta)$ read

$$
\mathbf{q}_{\text{conv}} = h(\Theta - \Theta_{\text{of}}) \, \text{grad} \, \Theta, \quad \mathbf{q}_{\text{rad}}(\Theta) = \varepsilon \sigma (\Theta^4 - \Theta_{\text{of}}^4).
$$

Therein, $h$ is the convection coefficient, and $\Theta_{\text{of}}$ the absolute temperature of the surrounding fluid. The emissivity $\varepsilon$, as introduced in Section 2.1, is needed for describing the radiative heat transfer. Further, $\sigma = 5.67 \times 10^{-8}$ Wm$^{-2}$ K$^{-4}$ is the Stefan-Boltzmann constant and $\Theta_{\text{of}}$ the absolute temperature of the surrounding region. Multiplying the stationary heat equation (5) with test functions $\delta \Theta(\mathbf{x})$—the virtual temperatures—and integrating over the volume $V$ together with employing the divergence theorem, leads to the weak form of the stationary heat equation

$$
0 = \int_{A^\vartheta} \mathbf{q}(\Theta) \delta \Theta \, dA + \int_V (\text{grad} \, \delta \Theta)^T \kappa_\Theta(\Theta) \, \text{grad} \, \Theta dV.
$$

For the notion of virtual temperature, it is referred to [8] (“virtual” in the sense of the thermal counterpart of the virtual displacement; this should not be misunderstood with the virtual temperatures defined in the meteorological society). The virtual temperatures are assumed to be zero at the Dirichlet boundary conditions, $\delta \Theta = 0$ on $A^\Theta$. When applying the finite element method, an approach for temperatures and virtual temperatures is used, $\Theta(\mathbf{x}) \approx \Theta^h(\mathbf{x}) = N^T(\mathbf{x}) \Theta + \overline{N}^T(\mathbf{x}) \overline{\Theta}$ and $\delta \Theta(\mathbf{x}) \approx \delta \Theta^h(\mathbf{x}) = N^T(\mathbf{x}) \delta \Theta$, where $\Theta \in \mathbb{R}^{n_\Theta}$ are the unknown nodal temperatures, $\overline{\Theta} \in \mathbb{R}^{n_\vartheta}$ the prescribed nodal temperatures and $\delta \Theta \in \mathbb{R}^{n_\Theta}$ the virtual nodal temperatures. $\mathbf{N} \in \mathbb{R}^{n_\Theta}$ and $\overline{\mathbf{N}} \in \mathbb{R}^{n_\vartheta}$ are the vectors of shape functions assigned to the particular nodal degrees of freedom.

The respective spatial derivatives—required for the gradients—are symbolized by the matrices $\mathbf{B} \in \mathbb{R}^{3 \times n_\Theta}$ and $\overline{\mathbf{B}} \in \mathbb{R}^{3 \times n_\vartheta}$, see [59] for a detailed explanation. Inserting the quantities into the weak form (9) and exploiting the arbitrariness of the virtual nodal temperatures $\delta \Theta$ leads to a system of nonlinear equations

$$
\mathbf{g}(\Theta) = 0
$$
with

\[ g(\Theta) = K(\Theta)\Theta + \bar{K}(\Theta)\bar{\Theta} + p_\Theta(\Theta). \]  

(11)

Therein, the temperature-dependent heat flux that results from the mixed boundary conditions is abbreviated,

\[ p_\Theta(\Theta) = \int_{A_\gamma} N(x) \bar{q}(\Theta^h) \, dA. \]  

(12)

whereas the matrices

\[ K(\Theta) = \int_V B^T(x) \kappa_\Theta(\Theta^h) B(x) \, dV \quad \bar{K}(\Theta) = \int_V B^T(x) \kappa_\Theta(\Theta^h) \bar{B}(x) \, dV \]  

(13)

are related to the thermal conductivity. This system represents a system of linear equations if the thermal conductivity tensor is temperature independent, and there is only convection, see Equation (8). If radiation is considered, a system of nonlinear equations occur.

## 4 PARAMETER IDENTIFICATION

In the following, the parameter identification procedure using a nonlinear least-squares (NLS) approach is recapped and quality measures for the identified values are given. Further, the theory of error propagation is introduced because we apply the concept of Gaussian error propagation for uncertainty quantification. Then, the applied finite element model of the specimens is explained and summarized. The chosen experimental data were the surface temperatures of thin quadratic specimens obtained from full-field temperature measurements using infrared thermography. Although this means that at many spatially distributed locations the temperature values are known and therefore much information is provided for the identification process, it is uncertain whether all material parameters are properly addressed by the experiments. This question leads to the concept of identifiability, see in general [10,12] and for relations to solid mechanics [27]. The section closes with an investigation of the identifiability of certain parameters. Here, the convection coefficient \( h \) and the thermal conductivity \( \kappa_\Theta \) for the case of an isotropic material and both thermal conductivities \( \kappa_{\Theta,a} \) and \( \kappa_{\Theta,n} \) for transversely isotropic materials are studied. In this work, we restrict ourselves to the stationary case and therefore only the stationary heat transfer problem is treated for the investigations. It is noteworthy that, of course, only the thermal conductivities are material parameters, whereas the convection coefficient is a parameter that stems from the experimental setup and is, in contrast to the emissivity, not precisely known. Further, reference values for the thermal conductivities based on analytical equations (estimations) are given.

### 4.1 Identification procedure

We consider the nonlinear least-squares approach with an objective function of the form

\[ f(\kappa) = \frac{1}{2} \{ \begin{array}{c} r(\kappa) \end{array} \}^T \{ \begin{array}{c} r(\kappa) \end{array} \} = \frac{1}{2} \{ s(\kappa) - d \}^T \{ s(\kappa) - d \} \to \min, \]  

(14)

to identify the parameters, see [27] for an extended discussion. \( r(\kappa) = s(\kappa) - d \) defines the residuum between the model \( s(\kappa) \) and the experimental data \( d \in \mathbb{R}^{n_D}. n_D \) is the total number of experimental data. The response of the model \( s(\kappa) \in \mathbb{R}^{n_D} \) depends on the parameters \( \kappa \in \mathbb{R}^{n_\kappa} \) with the number of parameters \( n_\kappa \). As described in Section 2.2, the measured temperatures of the thermography comprise also the surrounding of the tested specimen. Hence, only a subset of all obtained temperatures \( \Theta^\text{exp} \in \mathbb{R}^{n_\Theta} \) should be compared to the simulation data. Thus, the matrix \( \tilde{M} \) extracts only the required subset of experimental temperatures, \( \tilde{\Theta}^\text{exp} = \tilde{M} \Theta^\text{exp}, \tilde{\Theta}^\text{exp} \in \mathbb{R}^{n_\Theta} \). To evaluate the experimental data \( d = \tilde{\Theta}^\text{exp} \) and the model response \( s(\kappa) \) at the same points, we perform a spatial interpolation of the temperature subset \( \tilde{\Theta}^\text{exp} \) to the nodal positions in the finite element model.
The so-called normal equation
\[
\frac{df(\kappa)}{d\kappa}\bigg|_{\kappa=\kappa^*} = J^T(\kappa^*)(s(\kappa^*) - d) = 0
\] (15)
is obtained through application of the necessary condition of a local minimum (vanishing gradient of the objective function). It represents a system of nonlinear equations, where \( \kappa^* \) defines the solution obtained by an optimization tool. We abbreviate the Jacobian
\[
J = \frac{dr(\kappa)}{d\kappa} = \frac{ds(\kappa)}{d\kappa},
\] (16)
\( J \in \mathbb{R}^{n_d \times n_k} \), which is equal to the functional matrix or sensitivity matrix since unweighted residuals are applied. In this work, the simulation data vector \( s \) results from the nonlinear system (10) and only contains the nodal temperatures \( \Theta_{FE} \) on the surface, where a comparison to the experimental data is possible. Thus, the derivatives with respect to the parameter vector \( \kappa \) are required. There are different approaches to obtain the sensitivities. Generally, local and global sensitivity analysis can be distinguished, we refer to [66] for an overview regarding global sensitivity analysis. Among others the Sobol sensitivity analysis can be used as a global approach, see [62] for a certain application. In contrast, local sensitivity analysis comprises the internal numerical differentiation (IND) and external numerical differentiation (END), [28,29]. Here, we follow the external numerical differentiation concept, that is, the computation of the sensitivities (16) by means of the central difference method,
\[
\frac{ds(\kappa)}{d\kappa} = \sum_{i=1}^{n_d} \sum_{j=1}^{n_k} \Theta_{i}^{FE}(\kappa + \Delta \kappa_j e_j) - \Theta_{i}^{FE}(\kappa - \Delta \kappa_j e_j) \frac{2\Delta \kappa_j}{e_j e_j^T},
\] (17)
with the vectors \( e_i \in \mathbb{R}^{n_d} \) and \( e_j \in \mathbb{R}^{n_k} \), where all entries are zero except the one in row \( i \) or \( j \) alternatively. END possesses the advantage that the finite element program can be treated as a black-box solver, and that the sensitivities must not be provided by analytical derivations. In particular, we solve the system of nonlinear equations (15) with a trust-region algorithm that is implemented in the MATLAB subroutine \texttt{lsqnonlin}, see [16,17]. As there are numerous methods to solve this problem, the reader is also referred to [9,13,21,55,68].

Since the nonlinear least-square problem is based on thermography data and the finite element method, the abbreviation NLS-TG/FEM approach is chosen.

### 4.2 Quality measures

The aforementioned optimizing schemes, here the trust-region algorithm, will provide a solution \( \kappa^* \) of the problem (15). Thus, the question about the quality of the identified parameters arises. As proposed by [10,12], the concept of local identifiability addresses the issue of whether there is a unique local minimum. Therefore, the Hessian matrix \( H \) is needed,
\[
H(\kappa) = \frac{d^2f(\kappa)}{d\kappa d\kappa}\bigg|_{\kappa=\kappa^*} = \left[ \frac{\partial^2 f(\kappa)}{\partial \kappa_i \partial \kappa_j} \right]_{\kappa=\kappa^*} = \left[ \sum_{k=1}^{n_k} \left( \frac{\partial^2 s_k(\kappa)}{\partial \kappa_i \partial \kappa_j} (s_k(\kappa) - d_k) + \frac{\partial s_k(\kappa)}{\partial \kappa_i} \frac{\partial s_k(\kappa)}{\partial \kappa_j} \right) \right]_{\kappa=\kappa^*}, \] (18)
see also [39] for further details. A common approximation of Equation (18) is
\[
H \approx J^T J = \left[ \frac{\partial s_k(\kappa)}{\partial \kappa_i} \frac{\partial s_k(\kappa)}{\partial \kappa_j} \right]_{\kappa=\kappa^*},
\] (19)
which is reasonable for a good fit (\( s_k(\kappa) - d_k \approx 0 \)), see [58] for a detailed discussion. The influence of the aforementioned approximation of the Hessian is studied on an example in Appendix A. In this work, we employ the Hessian (18) to compute the remaining quality measures. Since we have only one parameter, \( n_k = 1 \), in our sequential identification procedure, there is no real computational effort. However, it should be noted that for more than one parameter mixed second derivatives occur and the computational effort increases significantly. In the case of accomplishing the necessary condition (13) and for nonvanishing, positive definite sub-determinants of the Hessian, there exists a unique local minimum.
It is recommended that the identifiability studies should be done with synthetic data in reidentification processes to prevent that scattering of real experimental data is influencing the results (generate data with given parameters by the finite element program and reidentify the parameters). A noteworthy drawback of performing identifiability studies is that the sub-determinants of the Hessian are never exactly zero and hence the evaluation is experience-based as the scale of the values depends also on the problem under consideration. An alternative to using the determinant of the Hessian is suggested in [50] by computing the eigenvalues. There, the local identifiability concept is called stability investigation.

A commonly applied quality measure is the coefficient of determination $R^2$,

$$R^2 = 1 - \frac{\sum_{i=1}^{n_d} (d_i - s_i)^2}{\sum_{i=1}^{n_d} (d_i - \bar{d})^2}, \quad \text{with} \quad \bar{d} = \frac{1}{n_d} \sum_{i=1}^{n_d} d_i$$

that gives only an estimation of how good the model data reflects the experimental data. Values close to one imply a good fit. It is important to note that there are some drawbacks in employing the coefficient of determination, see [22, sect. 11.2] and the references given therein. Hence, the $R^2$-value does not represent the quality of the found parameters. In contrast, a suitable measure for the parameter quality is the confidence interval

$$\kappa_{\text{conf}} = \kappa^* \pm \Delta \kappa \quad \text{with} \quad \Delta \kappa_i = \sqrt{P_{ii}}, \quad i = 1, \ldots, n_\kappa.$$

where $\kappa^*$ are the identified parameters in the local minimum obtained from the numerical optimization scheme and $\Delta \kappa$ the respective uncertainties. Here, the uncertainties are equal to the standard deviation of the parameters as they are obtained from the diagonal elements of the covariance matrix,

$$P = s^2 H^{-1}(\kappa^*).$$

The unknown variance of the residuals can be estimated with

$$s^2 = \frac{1}{n_D - n_\kappa} r^T(\kappa^*) r(\kappa^*),$$

see also [44]. According to [10] there are some assumptions for the application of Equation (22) and (23). It is assumed that the errors in the measurements are additive. Further, the residuals are supposed to have zero mean, a common unknown variance, and are uncorrelated. Additionally, the independent variables are expected to be errorless and the parameter vector $\kappa$ to be constant, whereby no prior information is used.

The correlation matrix

$$C = [c_{ij}] \quad \text{with} \quad c_{ij} = \frac{P_{ij}}{\sqrt{P_{ii} P_{jj}}}, \quad i,j = 1, \ldots, n_\kappa.$$

is not immediately a quality measure, but gives a suggestion whether and how the material parameters are influencing each other. Thereby, one should not instantly conclude from (statistical) correlation to causality. Off-diagonal values close to $\pm 1$ mean a strong positive or negative linear correlation between the material parameters, whereas values close to zero stand for no correlation. An alternative correlation matrix is discussed in [50], which is drawn on in real applications in [23,38]. However, this is not followed here.

### 4.3 Error propagation

In general, every measurement is influenced by measurement errors. Since the material parameter identification is based on experimental data—no matter what measurement methods are drawn on, for example, tensile or torsion tests, full-field measurement methods—the concept of error propagation can be applied. For a general discussion about uncertainties as well as different philosophies for the error propagation, the reader is referred to [74] and [7]. With the function $F(\kappa)$, where $\kappa \in \mathbb{R}^{n_\kappa}$ and $n_\kappa$ is the number of influencing parameters, the error propagation gives the uncertainty $\Delta F$, which is then used in the confidence interval $F \pm \Delta F$. Therefore, the known estimated uncertainty $\Delta \kappa$ of the influencing parameters is needed. Mainly, two different strategies can be distinguished, linear and Gaussian error propagation.
In linear error propagation, it is assumed that all errors influencing the function value and therefore the maximum expectable error is obtained,

\[
\Delta F = \sum_{i=1}^{n_p} \left( \left| \frac{\partial F}{\partial x_i} \right| \Delta x_i \right).
\] (25)

In contrast, the Gaussian error propagation—although also a linear error propagation concept—considers that the errors may compensate each other to a certain extent and therefore are added in quadrature. Hence, the uncertainty from Gaussian error propagation,

\[
\Delta F = \sqrt{\sum_{i=1}^{n_p} \left( \frac{\partial F}{\partial x_i} \Delta x_i \right)^2},
\] (26)

is always smaller than the one obtained from linear error propagation (25), compare [74, sect. 3.11]. It has to be considered that Equation (26) is only applicable if the errors are random and the influencing parameters \( x \) are independent. If the last condition is not given, the covariances \( P_{ij} \) between the parameters have to be considered as well,

\[
\Delta F = \sqrt{\sum_{i=1}^{n_p} \left( \frac{\partial F}{\partial x_i} \right)^2 \Delta x_i^2 + \sum_{i=1}^{n_p} \sum_{j=1}^{n_p} \left( \frac{\partial F}{\partial x_i} \frac{\partial F}{\partial x_j} P_{ij} \right), \quad i \neq j},
\] (27)

see also [7, sect. 4.3] and [74, sect. 9.2] for further explanations regarding dependent parameters. In this work, we draw on the Gaussian error propagation and compute the partial derivatives needed by means of numerical differentiation.

### 4.4 Finite element model

To provide the simulation data for the described parameter identification scheme, we drew on a finite element model of the specimen in Figure 2A. Thereby, the adequate modeling of the experimental setup had to be done carefully, on the one hand, to have a realistic model, and, on the other hand, to provide simple boundary conditions. Due to the optical accessibility of the front surface for the thermographic measurement, heat transfer through convection and radiation had to be considered. Hence, these boundary conditions can be described with Equation (8)1 for convection and Equation (8)2 for radiation. The emissivity \( \varepsilon = 0.96 \) in Equation (8)2 was known due to the applied varnish on the specimen’s surface, see Section 2.1. In contrast, the convection coefficient \( h \) for the natural convection boundary condition (8)1 was unknown. In general, the convection coefficient can be seen as a function of the surface temperature, the temperature of the surrounding fluid \( \Theta_{\infty} \), the fluid medium itself and the geometry of the surface, see [35].

There are analytical formulae to estimate the convection coefficient, see for details [75]. In our case of the vertical wall with natural convection, the estimation formulae lead after some calculations to

\[
h = 0.517 \text{ W m}^{-2} \text{ K}^{-1} \left( 0.825 + 1.564 \text{ K}^{-1/6} \Delta \Theta^{1/6} \right)^2.
\] (28)

Therein, the temperature of the surrounding fluid \( \Theta_{\text{of}} = 295.65 \text{ K} = 22.5^\circ \text{C} \) and ambient air as the surrounding medium (properties from [71]) are considered. Further, the exact dimensions of the plate, compare Section 2.1, are taken into consideration through a mean Nusselt number, which was originally introduced by [15]. The convection coefficient depends on the temperature difference \( \Delta \Theta \) between surface and surrounding medium. Since the specimen’s temperature decreased with increasing distance to the heat plate, see Figure 3A, a spatially varying convection coefficient results from Equation (28). In order to circumvent this property, we simplified the computation of the temperature difference \( \Delta \Theta \) and used only the mean value of all surface temperatures,

\[
\Delta \Theta = \bar{\Theta}^\text{exp} - \Theta_{\text{of}} \quad \text{with} \quad \bar{\Theta}^\text{exp} = \sum_{i=1}^{n_\text{a}} \bar{\Theta}_i^\text{exp}.
\] (29)
An alternative way to determine the convection coefficient is the identification from the measured experimental data. This is studied in Section 4.5.

In addition to the radiative and convective heat transfer boundary conditions on the front surface, we apply a temperature boundary condition (Dirichlet boundary condition) on the left side of the finite element model to consider the heat plate as an energy source. As mentioned in Section 2.1, the heat plate is set to have a temperature of 100°C during the experiment. To consider the non-ideal heat exchange at the contact interface between heat plate and specimen, the temperature boundary condition is set to the mean value \( \Theta_{pl} \) on the left edge that is identified for the respective specimen as shown in Figure 3B. Further, we apply a symmetry boundary condition in thickness direction for minimizing the computational costs and model only half of the specimen’s thickness. This means that no normal heat flux occurs on the backside of the model and therefore the adiabatic condition \( \tilde{q} = 0 \) is applied. Because of the small specimens thickness, we neglect the convective and radiative heat transfer at these small sides. The boundary conditions for the model are compiled in Figure 4A. The spatial discretization of the described finite element model is done with 20-noded hexahedral elements that are suitable for purely heat transfer problems. We use four elements in thickness direction and 25 elements along each edge of the quadratic geometry. The discretized model is shown in Figure 4B. A mesh convergence study was done to avoid an influence of the discretization on the identified parameters. Because of the different thickness of the steel and composite specimens, two geometrical models were set up. The numerical simulations were done with our in-house finite element program Tasafem.

4.5 Investigations on identifiability

In order to obtain reliable parameters, an investigation on the identifiability of the parameters with the present experimental data is necessary. The first option is to consider the underlying equations by evaluating the Hessian matrix of the objective function (14). This can be done either analytically or numerically with synthetic experimental data to prevent influences from the scattering of real experimental data.

In terms of the heat transfer problem, there are several material parameters of interest, such as the convection coefficient \( h \), the emissivity \( \epsilon \), or the two entries of the thermal conductivity tensor \( \kappa_{\Theta} \). In our case, the emissivity \( \epsilon \) is assumed to be known from the experimental setup. The thermal conductivity tensor \( \kappa_{\Theta} \) reduces to a scalar value \( \kappa_{\Theta} \) for isotropic materials. First, the question of local identifiability is discussed for simultaneous identification of the thermal conductivity \( \kappa_{\Theta} \) and the convection coefficient \( h \) in the case of isotropy. Then, the identification of both thermal conductivities \( \kappa_{\Theta,a} \) and \( \kappa_{\Theta,n} \) in the case of a transversely isotropic material is investigated. Analytical and numerical consideration applying the finite element method are considered, see Section 4.4.

4.5.1 Identifiability of convection coefficient and thermal conductivity (isotropy)

First, we consider the identification of the convection coefficient \( h \) and the thermal conductivity parameter \( \kappa_{\Theta} \) for the case of isotropy. For this case the stationary heat equation can be reduced to a one-dimensional approximation and the local identifiability study can be performed analytically. Thus, the parameters under consideration are \( \kappa^T = \{ \kappa_{\Theta}, h \} \). The
temperature distribution \( \Theta(x) \) in Equation (B12), compare Appendix B, describing the heated specimen, can be used to provide the simulation data \( s(\alpha) \). Further, it is assumed that exact experimental data \( d \) is given at two points \( x_1 = L/4 \) and \( x_2 = 3L/4 \) with the temperatures \( \Theta_1 \) and \( \Theta_2 \). Then, the Jacobian (16) reads

\[
J(\alpha) = \begin{bmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{bmatrix} = \begin{bmatrix} \frac{\partial \Theta(x_1, \kappa_\Theta, h)}{\partial \kappa_\Theta} & \frac{\partial \Theta(x_1, \kappa_\Theta, h)}{\partial h} \\ \frac{\partial \Theta(x_2, \kappa_\Theta, h)}{\partial \kappa_\Theta} & \frac{\partial \Theta(x_2, \kappa_\Theta, h)}{\partial h} \end{bmatrix},
\]

whereas the parameters \( \kappa^T = \{ \kappa_\Theta, h \} \) are exploited and no weighting factors are considered. The partial derivatives can be computed as

\[
\frac{\partial \Theta(x, \kappa_\Theta, h)}{\partial \kappa_\Theta} = \hat{\Theta} [(x - L) \beta \sinh (\alpha (L - x)) + L \beta \cosh (\alpha (L - x)) \tanh (\alpha L)] / \cosh (\alpha L),
\]

\[
\frac{\partial \Theta(x, \kappa_\Theta, h)}{\partial h} = \hat{\Theta} [(L - x) \gamma \sinh (\alpha (L - x)) - L \gamma \cosh (\alpha (L - x)) \tanh (\alpha L)] / \cosh (\alpha L),
\]

with the abbreviations

\[
\alpha = \sqrt{\frac{2h}{\kappa_\Theta d}}, \quad \beta = \sqrt{\frac{h}{2\kappa_\Theta^3 d}}, \quad \gamma = \sqrt{\frac{1}{2h\kappa_\Theta d}}.
\]

As known, a unique, local minimum of the optimization problem exists for non-vanishing sub-determinants of the Hessian, which is then positive definite. Since we use exact experimental data, which is equal to the model data in this identifiability investigation, that is, \( s(\alpha) - d = 0 \), there is no difference in using the Hessian (18) or the approximation (19). Therefore, we employ \( H = J^T J \). Further, formulating the determinant of the Hessian with the Jacobian components leads to

\[
\det H = (J_{12}J_{21} - J_{11}J_{22})^2.
\]

Insertion of Equations (31) and (32) yields \( \det H = 0 \). Thus, the simultaneous identification of the thermal conductivity \( \kappa_\Theta \) and the convection coefficient \( h \) cannot be performed with only surface temperature data at hand. In that case, local identifiability is not guaranteed.

To illustrate the performed study, the parameters are set to \( L = 50 \text{ mm}, d = 1.5 \text{ mm}, \hat{\Theta} = 353 \text{ K}, \kappa_\Theta = 50 \text{ W K}^{-1} \text{ m}^{-1} \) and \( h = 7 \text{ W K}^{-1} \text{ m}^{-2} \). Figure 5A,B visualize that a long valley with combinations of \( \kappa_\Theta \) and \( h \) exists that each minimizes the objective function. Therefore, an infinite number of solutions exists. Thus, applying the NLS-TG/FEM approach cannot provide unique parameters (or they are very sensitive). This implies that one of the parameters \( h \) or \( \kappa_\Theta \) must be determined by another experiment. Later on, the convection parameter \( h \) is determined for a plate with known thermal conductivity \( \kappa_\Theta \). In this regard, the convection parameter \( h \) is assumed to be known in the following considerations.

### 4.5.2 Identifiability of thermal conductivity tensor (transversal isotropy)

This work primarily addresses the parameter identification of the components in the thermal conductivity tensor for transversely isotropic material. Thus, the question of local identifiability of both components, \( \kappa_{\Theta,a} \) and \( \kappa_{\Theta,n} \), \( \kappa^T = \{ \kappa_{\Theta,a}, \kappa_{\Theta,n} \} \), is studied in the following. The experimental data comprises surface temperatures obtained from infrared thermography, see Section 2.2. Unfortunately, the identifiability study was not analytically possible, so we applied the numerical optimization scheme NLS-TG/FEM as proposed in Section 4.1 and used the finite element model described in Section 4.4. As already mentioned, numerical identifiability studies are performed with synthetic generated experimental data in a re-identification procedure.

We choose \( \kappa_{\Theta,a} = 10 \text{ W m}^{-1} \text{ K}^{-1} \) and \( \kappa_{\Theta,n} = 1 \text{ W m}^{-1} \text{ K}^{-1} \) and generate synthetic experimental data with the aforementioned finite element model, whereas the fiber direction was horizontal \( \hat{a} = \hat{e}_x \). The reidentification led to \( \kappa_{\Theta,a} = 10 \text{ W m}^{-1} \text{ K}^{-1} \) and \( \kappa_{\Theta,n} = 1 \text{ W m}^{-1} \text{ K}^{-1} \), whereas the determinant of the Hessian was small but nonzero, \( \det H \approx 10^{-3} \) indicating difficulties in the identification. Further, the correlation coefficient between both thermal conductivities was obtained to \( c_{12} = -0.004 \). So, in general, both thermal conductivities can be identified with the present experimental setup.
A more detailed insight into the synthetic data exhibited that the main heat conduction occurred, as expected, in horizontal direction. Further, the thermal conductivity \( \kappa_{\theta,n} \), which is normal to the fiber direction, was mainly influenced by a small temperature gradient in thickness direction of the finite element model as there was no temperature gradient in the synthetic experimental data in vertical direction.

However, if we consider real experimental data from thermography measurements, a small temperature gradient even in vertical direction due to non-perfect alignment at the heat plate is present. Hence, the influence on the simultaneous identification of both thermal conductivities is of particular interest. Therefore, we repeated the identification with real experimental data. The applied optimizing scheme provided the parameters \( \kappa_{\theta,a} = 6.185 \text{ W m}^{-1} \text{ K}^{-1} \) and \( \kappa_{\theta,n} = -5.173 \text{ W m}^{-1} \text{ K}^{-1} \) from one experiment. Since negative values for the thermal conductivity are physically not reasonable, it can be concluded that a simultaneous identification of both thermal conductivities will not be achieved with real experimental data as some imperfections in the alignment are not preventable.

To circumvent the simultaneous identification of the thermal conductivities \( \kappa_{\theta,a} \) and \( \kappa_{\theta,n} \), we performed two experiments - one with the fiber direction of the specimen in horizontal direction (\( \vec{a} = \vec{e}_x \)) and one with the specimen rotated by ninety degrees (vertical fiber direction, \( \vec{a} = \vec{e}_y \)). Then, we sequentially identified both thermal conductivity values by keeping one value constant and identifying the other one since there is no strong linear correlation between both parameters. For the sake of completeness, it is noteworthy that the results from the previous section can be transferred and therefore a simultaneous identification of the convection coefficient \( h \) and both thermal conductivities \( \kappa_{\theta,a} \) and \( \kappa_{\theta,n} \) is not possible.

### 4.6 Reference values for transversely isotropic material

The identified parameters for the thermal conductivities \( \kappa_{\theta,a} \) and \( \kappa_{\theta,n} \) can be compared to parameters based on analytical equations. The thermal conductivity in fiber direction \( \kappa_{\theta,a} \) can be obtained from the rule of mixtures by

\[
\kappa_{\theta,a} = \kappa_{\theta,f//} \varphi + \kappa_{\theta,m} (1 - \varphi),
\]

where \( \kappa_{\theta,f//} \) denotes the thermal conductivity of the fibers in axial direction, \( \varphi \) the fiber volume percentage and \( \kappa_{\theta,m} \) the thermal conductivity of the pure matrix material. In order to calculate the thermal conductivity normal to the fiber direction \( \kappa_{\theta,n} \) different equations exist, see the discussion in [63]. Here, we draw on the so-called self-consistent equation,

\[
\kappa_{\theta,n} = \frac{\kappa_{\theta,f//} + \kappa_{\theta,m} + (\kappa_{\theta,f//} - \kappa_{\theta,m}) \varphi}{\kappa_{\theta,f//} + \kappa_{\theta,m} - (\kappa_{\theta,f//} - \kappa_{\theta,m}) \varphi} \kappa_{\theta,m},
\]

\( \kappa_{\theta,f//} \) defines the thermal conductivity of the fibers normal to the fiber axis.
The chosen composite material has a fiber volume percentage of $\varphi = 50\%$. The manufacturer of the carbon fibers provides the thermal conductivity along the fiber axis $\kappa_{\theta,\parallel} = 17$ Wm$^{-1}$ K, see [77]. Since no information on the thermal conductivity of the pure fibers normal to fiber axis is given, we drew on the value $\kappa_{\theta,\perp} = 1.7$ Wm$^{-1}$ K from [69] as a general value for carbon fibers. The thermal conductivity of the matrix material in the cured state was determined in [46] to $\kappa_{\theta,m} = 0.187$ Wm$^{-1}$ K. Hence, the obtained reference values from Equations (35) and (36) are $\kappa_{\theta,a} = 8.59$ Wm$^{-1}$ K and $\kappa_{\theta,n} = 0.44$ Wm$^{-1}$ K, which are discussed in the application of the NLS-TG/FEM approach later on.

### 5 Sequential Identification of Thermal Conductivity Tensor

In this section, we present a sequential identification of the convection coefficient $h$ as well as the thermal conductivities $\kappa_{\theta,a}$ and $\kappa_{\theta,n}$ of the composite material. Since this is a step-by-step identification process, the uncertainties of the previously determined parameters affect the calculation of the parameters currently under investigation. This is considered using the Gaussian error propagation concept, see Section 4.3. To identify the convection coefficient, a specimen made from isotropic material (steel) with known thermal conductivity is drawn on, which was obtained from thermophysical experiments. Then, the identified convection coefficient is used to identify the thermal conductivity $\kappa_{\theta,a}$ of the composite material based on experimental data, where the fiber direction is equal to the horizontal direction ($\vec{a} = \vec{e}_x$). As mentioned before, the thermal conductivity $\kappa_{\theta,n}$ is kept constant for the identification of $\kappa_{\theta,a}$. In a subsequent step, the thermal conductivity $\kappa_{\theta,n}$ is identifiable from an experiment, where the fiber direction is equal to the vertical direction ($\vec{a} = \vec{e}_y$). The section closes with a discussion on the sequential identification procedure.

#### 5.1 Identification of convection coefficient $h$ using steel

In the first step, we determined the thermal conductivity of a steel specimen that was subsequently used to identify the convection coefficient $h$. The thermal conductivity $\kappa_{\theta}$ cannot be directly measured, but can be calculated from different thermophysical parameters,

$$\kappa_{\theta}(\Theta) = \rho(\Theta) \alpha(\Theta) c_p(\Theta). \tag{37}$$

The density $\rho$ of the steel was obtained from volume and weight measurements to 7.905 g cm$^{-3}$. We neglect the temperature-dependence of the density in the following. Further, the thermal diffusivity $\alpha$ was studied at certain temperatures using the laser flash analysis (LFA) as introduced by [56]. Therefore, the samples were varnished with a thin graphite layer to increase the laser absorption. The curves of the detected signals after the laser pulse were fitted with the applied Cowan model, see [18]. The experimental data in Figure 6A was then approximated with a polynomial of second order. In order to finally obtain the thermal conductivity $\kappa_{\theta}$ from Equation (37), the specific heat capacity $c_p$ was investigated by temperature modulated differential scanning calorimetry (DSC) measurements, see Figure 6B. Ultimately, the thermal conductivity $\kappa_{\theta}$ for the investigated steel was calculated, Figure 6C. The thermal conductivity $\kappa_{\theta} = 70.507$ Wm$^{-1}$ K$^{-1}$ was evaluated for the temperature of the surrounding fluid during the experiments, $\Theta_{ref} = 22.5\,^\circ$C.

Since the described sequential identification procedure is followed, the error propagation has to be considered in each step. The influencing parameters for the thermal conductivity $\kappa_{\theta}$ are the density $\rho$, the temperature conductivity $\alpha$, and the heat capacity $c_p$, $\vec{x}^T = \{ \rho, \alpha, c_p \}$ according to Equation (37). Since these parameters result from the three aforementioned measurement principles, it is assumed that there is no influence among themselves. Therefore, Equation (26) is applied that gives the uncertainty in the thermal conductivity $\kappa_{\theta}$,

$$\Delta \kappa_{\theta} = \sqrt{\left( \frac{\partial \kappa_{\theta}}{\partial \rho} \Delta \rho \right)^2 + \left( \frac{\partial \kappa_{\theta}}{\partial \alpha} \Delta \alpha \right)^2 + \left( \frac{\partial \kappa_{\theta}}{\partial c_p} \Delta c_p \right)^2} = 2.907 \text{ W m}^{-1} \text{ K}^{-1}. \tag{38}$$
The partial derivatives can be computed from Equation (37). The accuracy of the density determination is assumed to be 2% as a precision scale and a caliper with an accuracy of 0.01 mm were used. The laser flash apparatus LFA 427 (Netzsch-Gerätebau GmbH, Germany) and the differential scanning calorimeter Netzsch DSC F204 Phoenix (Netzsch Gerätebau GmbH, Germany) gave the remaining accuracies of 3% and 2%, see also [54]. These accuracies were then used to determine the necessary uncertainties. Evaluating Equation (38) leads to $\Delta \kappa_\Theta = 2.907 \text{ Wm}^{-1} \text{ K}^{-1}$, and, consequently, to $\kappa_\Theta = 70.507 \pm 2.907 \text{ Wm}^{-1} \text{ K}^{-1}$ for the thermal conductivity of the chosen steel.

In the next step, the convection coefficient $h$ was identified using thermography data measured with the experimental setup in Section 2.1. The NLS-TG/FEM scheme provides the solution $h^* = \{h^*\}$. Evaluating the quality measures results in the confidence interval $h = h^* \pm \Delta h^* = 7.885 \pm 0.441 \text{ Wm}^{-1} \text{ K}^{-1}$. Here, as stated in Section 4.2, we compute the Hessian (18) and afterwards the uncertainty. The identified value is obtained with the previously calculated thermal conductivity $\kappa_\Theta$ of the steel specimen and the given quantities of the emissivity $\varepsilon = 0.96$, ambient temperature $\Theta_\infty = 22.5^\circ\text{C}$ and temperature at the left edge of the specimen $\Theta_{pl} = 97.354^\circ\text{C}$.

Although the experiments were performed carefully, some measurement errors are not preventable. Therefore, different factors have to be considered that influence the measurements and the subsequent parameter identification. The transmittance of the surrounding medium is negligible. As a result, we consider the influence of the emissivity $\varepsilon$, the ambient temperature $\Theta_\infty$ and the temperature of the left edge of the specimen $\Theta_{pl}$, which serves as a Dirichlet boundary condition in the finite element model. Further, the error propagation from previously determined parameters is incorporated to estimate the uncertainty of the identified parameter. Additionally, it is assumed that the ambient temperature $\Theta_\infty$ equals the temperature of surrounding surfaces $\Theta_{osf}$ and the surrounding fluid temperature $\Theta_{osf}$, $\Theta_\infty = \Theta_{osf} = \Theta_{osf}$.

In this work, the uncertainty $\Delta h^*$—stemming from the NLS-TG/FEM scheme—is considered in the error propagation besides the uncertainties of the prescribed values in the finite element simulation to estimate the overall uncertainty. The factors mentioned afore result in the overall uncertainty $\Delta h$ of the convection coefficient, where the influencing parameters are $x = \{h^*, \kappa_\Theta, \varepsilon, \Theta_\infty, \Theta_{pl}\}$.

$$\Delta h = \sqrt{\left(\frac{\partial h}{\partial h^*} \Delta h^*\right)^2 + \left(\frac{\partial h}{\partial \kappa_\Theta} \Delta \kappa_\Theta\right)^2 + \left(\frac{\partial h}{\partial \varepsilon} \Delta \varepsilon\right)^2 + \left(\frac{\partial h}{\partial \Theta_\infty} \Delta \Theta_\infty\right)^2 + \left(\frac{\partial h}{\partial \Theta_{pl}} \Delta \Theta_{pl}\right)^2} = 0.938 \text{ Wm}^{-2} \text{ K}^{-1}. \quad (39)$$

We simplify the partial derivative to $\partial h/\partial h^* = 1$. The other partial derivatives are obtained from numerical differentiation by means of central differences, where for each partial derivative the entire parameter identification using the NLS-TG/FEM approach in Section 4.1 is performed two times. The uncertainties $\Delta h^* = 0.441 \text{ Wm}^{-2} \text{ K}^{-1}$ and $\Delta \kappa_\Theta$ from Equation (38) are known from the NLS-TG/FEM identification and the error propagation evaluation in Section 5.1 respectively. The uncertainty $\Delta \Theta_{pl}$ is set to the standard deviation of the experimental temperature values on the left edge of the specimen and therefore varying for every set of experimental data. Further, the uncertainties $\Delta \varepsilon = 0.02$ ($\approx 2\%$) and
\[ \Delta \Theta_{\infty} = 1 \text{ K are assumed. The uncertainty in the emissivity } \epsilon \text{ results from the fact that we have to rely on the information given by the manufacturer, where some dispersion may occur.} \]

Evaluating Equation (39) results in \( \Delta h = 0.938 \text{ Wm}^{-2} \text{ K}^{-1}. \) It is in evidence that the uncertainty of the identified value \( \delta h^* \) is approximately doubled due to the consideration of error propagation. The main influencing factors are the remaining uncertainty \( \Delta h^* \) after the numerical optimization, the uncertainty \( \Delta \kappa_{\Theta} \) in the thermal conductivity of the steel and the influence from the Dirichlet boundary condition \( \Theta_{pl} \). In contrast, variations in the emissivity or the ambient temperature are not significant for the identified convection coefficient. Hence, the convection coefficient \( h = 7.885 \pm 0.938 \text{ Wm}^{-2} \text{ K}^{-1} \) was used in the subsequent identification processes.

According to Section 4.4, the convection coefficient \( h \) can also be roughly estimated from analytical considerations. The mean experimental surface temperature of the steel specimen is determined from the thermography data to \( \Theta_{\exp} = 78.215^\circ\text{C}. \) Consequently, the temperature difference \( \Delta \Theta = 55.715^\circ\text{C} \) results from Equation (29). Further, evaluating Equation (28) leads to \( h_{\text{analyt.}} = 7.794 \text{ Wm}^{-2} \text{ K}^{-1}. \) Hence, the identified convection coefficient \( h = 7.885 \text{ Wm}^{-2} \text{ K}^{-1} \) from the NLS-TG/FEM approach is reasonably close to the value obtained from analytical equations. Since the convection coefficient is only required to subsequently identify the thermal conductivities, it can be sufficiently determined from analytical equations instead of being identified from specimens with known thermal conductivity as performed above.

### 5.2 Identification of thermal conductivity \( \kappa_{\Theta,a} \)

In the next step, experimental data obtained from a specimen with horizontal fiber direction \( \bar{a} = \bar{e}_x \) is used. The given quantities are the identified convection coefficient \( h \), the emissivity \( \epsilon \), the ambient temperature \( \Theta_{\infty} \), and the temperature at the Dirichlet boundary condition \( \Theta_{pl} \). As studied in Section 4.5, the thermal conductivity in fiber direction \( \kappa_{\Theta,a} \) can be uniquely identified with known convection coefficient \( h \). The thermal conductivity normal to the fiber direction \( \kappa_{\Theta,n} \) was set to the reference value from Section 4.6, \( \kappa_{\Theta,n} = 0.44 \text{ Wm}^{-1} \text{ K}^{-1}. \) Since the linear correlation between both thermal conductivities is not strong (correlation coefficient \( r = -0.004 \)), the influence of the chosen value for \( \kappa_{\Theta,n} \) on the identification of the thermal conductivity \( \kappa_{\Theta,a} \) is assumed to be negligible.

The NLS-TG/FEM identification procedure of Section 4.1 computes \( \kappa_{\Theta,a} = \kappa_{\Theta,a}^* \pm \Delta \kappa_{\Theta,a}^* = 6.250 \pm 0.152 \text{ Wm}^{-1} \text{ K}^{-1}. \) Since the experimental data was obtained from a different experiment than in the previous section, possible influences of the emissivity and ambient temperature had to be considered again in the uncertainty determination. Due to the sequential parameter identification procedure, the parameters \( \mathbf{x}^T = \{ \kappa_{\Theta,a}, h, \epsilon, \Theta_{\infty}, \Theta_{pl} \} \) are not influencing each other and the error propagation formula in Equation (26) can still be used. This leads to the uncertainty

\[
\Delta \kappa_{\Theta,a} = \sqrt{\left( \frac{\partial \kappa_{\Theta,a}}{\partial \Delta \kappa_{\Theta,a}} \Delta \kappa_{\Theta,a} \right)^2 + \left( \frac{\partial \kappa_{\Theta,a}}{\partial h} \Delta h \right)^2 + \left( \frac{\partial \kappa_{\Theta,a}}{\partial \epsilon} \Delta \epsilon \right)^2 + \left( \frac{\partial \kappa_{\Theta,a}}{\partial \Theta_{\infty}} \Delta \Theta_{\infty} \right)^2 + \left( \frac{\partial \kappa_{\Theta,a}}{\partial \Theta_{pl}} \Delta \Theta_{pl} \right)^2} = 0.505 \text{ Wm}^{-1} \text{ K}^{-1}
\]

(40)

of the thermal conductivity \( \kappa_{\Theta,a} \). As before, the influence of variations in the emissivity is nearly negligible for the uncertainty in the thermal conductivity. Although it is important to note that this only holds for the radiative boundary condition in the finite element model and not for the measurement of the experimental temperature data. Also, the error propagation from the identified convection coefficient \( h \) is significant. In contrast to the uncertainty determination of the convection coefficient, the uncertainty of the thermal conductivity is much more sensitive to the ambient temperature. Again, it is clearly visible that the error propagation significantly increases the uncertainty of the identified value.

### 5.3 Identification of thermal conductivity \( \kappa_{\Theta,n} \)

In analogy to the procedure in the previous section, the thermal conductivity normal to the fiber direction \( \kappa_{\Theta,n} \) can be identified using the NLS-TG/FEM approach. The experimental data was obtained from an experiment, where the fibers were in the vertical direction \( \bar{a} = \bar{e}_y \) and hence are parallel to the heat plate. The NLS-TG/FEM procedure provides \( \kappa_{\Theta,n} = \kappa_{\Theta,n}^* \pm \Delta \kappa_{\Theta,n}^* = 1.787 \pm 0.086 \text{ Wm}^{-1} \text{ K}^{-1}. \) To determine the uncertainty \( \Delta \kappa_{\Theta,n} \), we had to consider also the influence of the previously identified thermal conductivity in fiber direction \( \kappa_{\Theta,a} \) due to the sequential identification procedure. Thus, the
TABLE 1  Confidence intervals of the identified parameters within the sequential identification procedure

| Parameter                      | Value ± uncertainty | Dimension       | Uncertainty in % |
|--------------------------------|---------------------|-----------------|-----------------|
| Thermal conductivity (steel)   | \( \kappa_\Theta \) | \( 70.507 \pm 2.907 \) W m\(^{-1}\) K\(^{-1}\) | 4.12            |
| Convection coefficient         | \( h \)            | \( 7.885 \pm 0.938 \) W m\(^{-1}\) K\(^{-1}\) | 11.90           |
| Thermal conductivity           | \( \kappa_{\Theta,a} \) | \( 6.250 \pm 0.505 \) W m\(^{-1}\) K\(^{-1}\) | 8.08            |
| Thermal conductivity           | \( \kappa_{\Theta,h} \) | \( 1.787 \pm 0.214 \) W m\(^{-1}\) K\(^{-1}\) | 11.98           |

influencing parameters are \( \mathbf{x}^T = \{ \kappa_{\Theta,a}^*, \kappa_{\Theta,h}, \epsilon, \Theta_\infty, \Theta_{pl} \} \).

\[
\Delta \kappa_{\Theta,h} = \sqrt{\left( \frac{\partial \kappa_{\Theta,h}}{\partial \kappa_{\Theta,a}} \Delta \kappa_{\Theta,a} \right)^2 + \left( \frac{\partial \kappa_{\Theta,h}}{\partial h} \Delta h \right)^2 + \left( \frac{\partial \kappa_{\Theta,h}}{\partial \epsilon} \Delta \epsilon \right)^2 + \left( \frac{\partial \kappa_{\Theta,h}}{\partial \Theta_\infty} \Delta \Theta_\infty \right)^2 + \left( \frac{\partial \kappa_{\Theta,h}}{\partial \Theta_{pl}} \Delta \Theta_{pl} \right)^2}
\]

\[
= 0.214 \text{ W m}^{-1} \text{ K}^{-1}.
\]

As it was before, the main uncertainty contributions stem from the convection coefficient and the ambient temperature, whereas the influence of the uncertainty of the thermal conductivity \( \kappa_{\Theta,a} \) is negligible. This also supports the executed sequential parameter identification procedure.

5.4 Discussion

The identified parameters using the NLS-TG/FEM procedure and the corresponding uncertainties stemming from the error propagation concept are compiled in Table 1.

Through the sequential identification procedure it becomes obvious that following an error propagation concept significantly increases the uncertainty of the identified parameters. Thereby, the sensitivity of the parameters to certain factors may vary. Exemplarily, it can be seen that for the problem under consideration the convection coefficient is quite insensitive to the ambient temperature, which, however, does not hold for the thermal conductivities. It should be mentioned that the computed sensitivities and uncertainties of the parameters are only valid for the problem at hand. Changes in the setup—such as the specimen’s geometry or different temperature levels—may result in different values. Further, the uncertainties of the identified parameters are influencing the results of following numerical simulations and can lead to significant uncertainties, for example, in the temperatures.

In Section 4.6 the thermal conductivities \( \kappa_{\Theta,a} = 8.59 \text{ W m}^{-1} \text{ K}^{-1} \) and \( \kappa_{\Theta,h} = 0.44 \text{ W m}^{-1} \text{ K}^{-1} \) were obtained as some reference values from the rule of mixtures and the self-consistent equation. In comparison to the identified values (\( \kappa_{\Theta,a} = 6.250 \text{ W m}^{-1} \text{ K}^{-1} \) and \( \kappa_{\Theta,h} = 1.787 \text{ W m}^{-1} \text{ K}^{-1} \)), the thermal conductivity in fiber direction is lower, whereas the thermal conductivity normal to the fiber direction is larger than the reference value. The differences to the reference values may occur due to perturbations from the manufacturing process of the composite specimens (e.g., fiber alignment, fiber volume percentage) and experimental disturbances, like the alignment of the specimen in front of the heat plate. Further, the thermal conductivity of the fibers normal to the fiber axis \( \kappa_{\Theta,f,\perp} \) was not precisely known and therefore was estimated from a general reference, compare Section 4.6.

6 VALIDATION AND UNCERTAINTY QUANTIFICATION FOR A PLATE WITH A HOLE

To study the influence of the uncertainties on the prediction computation, a validation example was carried out. Here, a plate with horizontal fiber direction \( \vec{a} = \vec{e}_x \), analogously to the previous specimens with a hole (diameter 6 mm, center 10 mm from left edge) was drilled after the manufacturing process. The experiment was performed with the same setup as before. Figure 7A shows the experimental temperature distribution in the stationary case. The finite element simulation
FIGURE 7  Temperature distributions of a plate with a hole. (A) Experiment, (B) simulation, (C) relative error

FIGURE 8  Uncertainty contributions of different parameters. (A) Convection coefficient $h$, (C) thermal conductivity $\kappa_{\Theta,a}$, (C) thermal conductivity $\kappa_{\Theta,n}$, (D) overall relative temperature uncertainty

concerned determines the temperature distribution in Figure 7B. The simulation was done with the identified values for the convection coefficient and the thermal conductivities as shown in Table 1. A relative error

$$
\varepsilon_{\Theta} = \left| \Theta^{\text{FE}} - \hat{\Theta}^{\text{exp}} \right| \times 100,
$$

between the particular simulated temperatures $\Theta^{\text{FE}}$ and the projected experimental temperatures $\hat{\Theta}^{\text{exp}}$ is introduced that is presented in Figure 7C. It is noteworthy that the valley of very small relative errors stems from a sign conversion in the
temperature difference. The asymmetry at the horizontal axis in the center of the relative error is caused by the nonideal contact between specimen and heat plate. The relative errors are mainly lower than 5%, whereby the error increases to up a overall maximum of 44% at the boundary of the specimen and behind the hole due to the edge detection scheme.

Commonly, the parameter identification is only a step toward the implementation of a certain material behavior for further numerical simulations. Here, however, the parameters $x^T = \{ h, \kappa_{\theta,a}, \kappa_{\theta,n} \}$—together with their uncertainties—are influencing the results of the numerical simulations as well. In our case, the uncertainties of the parameters result in an uncertainty of the nodal temperatures of the finite element model,

$$
\Delta \Theta^{FE(k)} = \sqrt{\delta h^{(k)} + \delta \kappa_{\theta,a}^{(k)} + \delta \kappa_{\theta,n}^{(k)}} = \sqrt{\left( \frac{\partial \Theta^{FE(k)}}{\partial h} \Delta h \right)^2 + \left( \frac{\partial \Theta^{FE(k)}}{\partial \kappa_{\theta,a}} \Delta \kappa_{\theta,a} \right)^2 + \left( \frac{\partial \Theta^{FE(k)}}{\partial \kappa_{\theta,n}} \Delta \kappa_{\theta,n} \right)^2} \quad k = 1, \ldots, n_{\text{nodes}},
$$

(43)

where $n_{\text{nodes}}$ is the number of nodes of the finite element model. In order to investigate the individual uncertainty contributions, the contribution of the convection coefficient $\delta h$, the thermal conductivity in fiber direction $\delta \kappa_{\theta,a}$, and normal to the fiber direction $\delta \kappa_{\theta,n}$ are abbreviated. The spatial distributions of these uncertainties are shown in Figure 8A–C. It is in evidence that the main influence on the uncertainty $\Delta \Theta^{FE(k)}$ of the nodal temperatures is the uncertainty in the thermal conductivity in fiber direction. Figure 8D shows the spatial distribution of the relative uncertainty $\Delta \Theta^{FE(k)}/\Theta^{FE(k)}$ in the nodal temperatures. Further, the uncertainty in the thermal conductivity normal to the fiber direction $\Delta \kappa_{\theta,n}$ shows a small influence only behind the hole (with respect to the heat conduction direction). The convection coefficient $h$ leads to an increase in the temperature uncertainty with increasing distance from the temperature boundary condition on the left end of the model. Certainly, the main uncertainty contribution of the convection coefficient occurs at the right end of the specimen centered in the vertical direction. The maximum relative uncertainty in the temperatures of the spatial domain reaches up to 4.5%, which corresponds to a maximum uncertainty $\Delta \Theta^{FE(k)} = 1.8^\circ C$.

### 7 | CONCLUSIONS

The thermal conductivities of transversely isotropic composite materials are of particular interest for the thermo-mechanical modeling of these materials and corresponding simulations. Therefore, the parameter identification procedure based on experimental data should yield reliable values. In the work at hand, the focus lies on the parameter identification of both thermal conductivities $\kappa_{\theta,a}$ and $\kappa_{\theta,n}$, whereby the experimental data is obtained from infrared thermography measurements. We restricted ourselves to the stationary case, which simplifies the underlying equations and enables identifiability studies that were performed partly also with analytical equations.

The heat transfer through convection and radiation during the experiments has to be considered in the finite element model for the parameter identification as well. Although the emissivity of the specimen’s surface was known through application of a varnish, the convection coefficient remains unknown. Identifiability considerations show that a simultaneous identification of the convection coefficient and the thermal conductivity is not possible with only surface temperature data, even for the case of an isotropic material. Hence, thermophysical experiments were applied to determine the thermal conductivity of an isotropic steel, which was then used to identify the convection coefficient to calibrate the environment for the following experiments with composite material. It was shown that the identified convection coefficient was reasonably close to analytical calculations. Therefore, the analytical values can be sufficiently employed for identifying the thermal conductivities. With the identified convection coefficient, the thermal conductivity components of the transversely isotropic material were identified from two separate experiments. The fiber direction in the experiments was aligned in a way that heat conduction only occurs in the direction along or normal to the fibers respectively. However, it should be mentioned that other orientations of the fiber direction in the specimens are possible to obtain the thermal conductivities.

Further, the propagation of errors was followed to determine the uncertainties of the identified parameters. It is shown that especially the use of previously identified parameters is a significant source increase uncertainties compared to the solely application of numerical optimization schemes.

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APPENDIX A. EFFECT OF APPROXIMATING THE HESSIAN ON THE UNCERTAINTY

The Hessian matrix $H$ is required to compute different quality measures that are commonly used to evaluate the solution of the identification procedure, see Section 4.2. Especially the uncertainty is of particular interest to conduct error propagation. The full Hessian matrix (18) is often approximated by Equation (19). This approximation is assumed to be justified for a good fit between the model response $s(\kappa^*)$ with the identified parameters $\kappa^*$ and the experimental data $d$ that results in disappearance of the first term in Equation (18), $(s(\kappa^*) - d \approx 0)$. However, the influence of this approximation on the deduced uncertainty should be studied.

To compute the full Hessian (18), the second derivatives of the model response with respect to the parameters are needed, $\frac{\partial^2 s_k(\kappa)}{\partial \kappa_i \partial \kappa_j}$, $k = 1, \ldots, n_k$, $i, j = 1, \ldots, n_k$. Since this is very complex from an implementation point of view, numerical differentiation is drawn on to obtain the second derivatives. In general, the required difference quotients can be obtained by performing Taylor series expansion, see exemplarily [21,58]. It is necessary to distinguish between second derivatives with respect to a particular parameter and mixed second derivatives. For the case $i = j$, the difference quotients read in component representation

$$
\frac{\partial^2 s_k(\kappa)}{\partial \kappa_i^2} = \frac{\Theta^\text{FE}_k(\kappa + \Delta \kappa_i \vec{e}_i) - 2\Theta^\text{FE}_k(\kappa) + \Theta^\text{FE}_k(\kappa - \Delta \kappa_i \vec{e}_i)}{\Delta \kappa_i^2}.
$$

(A1)

Otherwise, $i \neq j$ yields

$$
\frac{\partial^2 s_k(\kappa)}{\partial \kappa_i \partial \kappa_j} = \frac{\Theta^\text{FE}_k(\kappa + \Delta \kappa_i \vec{e}_i + \Delta \kappa_j \vec{e}_j) - \Theta^\text{FE}_k(\kappa + \Delta \kappa_i \vec{e}_i - \Delta \kappa_j \vec{e}_j) - \Theta^\text{FE}_k(\kappa - \Delta \kappa_i \vec{e}_i + \Delta \kappa_j \vec{e}_j) + \Theta^\text{FE}_k(\kappa - \Delta \kappa_i \vec{e}_i - \Delta \kappa_j \vec{e}_j)}{4\Delta \kappa_i \Delta \kappa_j},
$$

(A2)

with the vectors $\vec{e}_i \in \mathbb{R}^{n_k}$ and $\vec{e}_j \in \mathbb{R}^{n_k}$ having the property that all entries are zero except the one in row $i$ or $j$.

The influence on the uncertainty due to approximating the Hessian should be exemplarily shown for the parameter identification of the convection coefficient $h$ using the steel specimen as shown in Section 5.1. It is in evidence that the required difference quotients depend on the number of optimized parameters. Here, we have only one parameter, $n_k = 1$. Therefore, no mixed second derivatives occur. The choice of $\Delta \kappa_i$ in the difference quotient (A1) was done according to common recommendations, see [21,58] for more in-depth discussions. In our case, $\Delta \kappa_i = \sqrt{4\epsilon_m n_k}$ was used, whereby $\epsilon_m$ is the machine accuracy, $\epsilon_m \approx 10^{-16}$, and $n_k$ the respective material parameter. Table A1 shows the values of the Hessian $H$ and the uncertainty $\Delta h$ for applying the full Hessian (18) as well as the approximation (19). The discrepancy in the
TABLE A1  Quality measures evaluated with full Hessian matrix (18) and approximation (19)

| Quality measure | Hessian (18) | Approx. Hessian (19) | Dimension       |
|-----------------|-------------|----------------------|-----------------|
| Hessian matrix  | $1.085 \times 10^9$ | $1.106 \times 10^9$ | m$^4$ K$^4$ W$^{-2}$ |
| Uncertainty     | $0.441$     | $0.430$              | W m$^{-2}$ K$^{-1}$ |

Hessian as well as the uncertainty $\Delta \kappa_1$ due to the approximation is about 2% in this example. The magnitude of deviation can be transferred to the other identifications in this work as well.

APPENDIX B. TEMPERATURE DISTRIBUTION FOR ONE-DIMENSIONAL HEAT CONDUCTION AND CONVECTION

The temperature distribution in the stationary case is studied for a brick-shaped volume with a square front surface of length $L$ and the thickness $d$, compare Figure B1. To distinguish the heat flux density $q = -\mathbf{v} \cdot \mathbf{n}$ from the one-dimensional heat flux, the notation $Q$ for the one-dimensional heat flux is chosen. In the one-dimensional case the conductive heat flux $Q_{\text{cond}}$ in y- and z-direction is neglected. Furthermore, we assume $L \gg d$ and take only the convective heat flux $Q_{\text{conv}}$ on the front and back surface into account. The heat balance for the small volume element in Figure B1 reads,

$$Q_{\text{cond},x} - dQ_{\text{conv}} - Q_{\text{cond},x+dx} = 0.$$  \hfill (B1)

Heat flux into the volume element in Figure B1 is taken into account with a positive sign, whereas heat flux out of the volume is considered with a negative sign. The conductive heat flux $Q_{\text{cond},x}$ is given by Fourier’s law,

$$Q_{\text{cond},x} = -\kappa_\Theta A_x \frac{\partial \Theta}{\partial x},$$  \hfill (B2)

whereby $\kappa_\Theta$ is the thermal conductivity and $A_x = Ld$ the surface, where conductive heat transfer occurs. The convective heat flux $Q_{\text{conv}}$ reads in general

$$Q_{\text{conv}} = hA_s(\Theta - \Theta_{\text{ref}}),$$  \hfill (B3)

with the quantities of the convection coefficient $h$, the surface $A_s = 2Lx$, where convective heat transfer appears, and the temperature of the surrounding fluid $\Theta_{\text{ref}}$. In order to substitute $dQ_{\text{conv}}$ in Equation (B1), the infinitesimal convective heat flux $dQ_{\text{conv}}$ is required,

$$\frac{dQ_{\text{conv}}}{dx} = h(\Theta - \Theta_{\text{ref}}) \frac{dA_s}{dx} \rightarrow dQ_{\text{conv}} = hdA_s(\Theta - \Theta_{\text{ref}}).$$  \hfill (B4)

whereby it is exploited that only the convective heat transfer surface $A_s$ is depending on $x$. Further, reformulating Equation (B1) and performing Taylor expansion to substitute $Q_{\text{cond},x+dx}$ leads to,

$$0 = -\kappa_\Theta A_x \frac{d^2 \Theta}{dx^2} + h \frac{dA_s}{dx}(\Theta - \Theta_{\text{ref}}).$$  \hfill (B5)

According to [35], it is beneficial to introduce the abbreviation

$$\vartheta = \Theta - \Theta_{\text{ref}}.$$  \hfill (B6)

leading to the linear, homogeneous differential equation of second-order with constant coefficients

$$0 = -\kappa_\Theta A_x \frac{d^2 \vartheta}{dx^2} + h \frac{dA_s}{dx} \vartheta.$$  \hfill (B7)
In the case that heat transfer through radiation is considered, a nonlinear, inhomogeneous differential equation is obtained. A general solution of Equation (B7) is

$$\theta(x) = C_1 e^{cx} + C_2 e^{-cx} \quad \text{with} \quad c = \sqrt{\frac{2h}{\kappa\Omega d}}.$$  \hspace{1cm} (B8)

On the left hand side of the body in Figure B1 the Dirichlet boundary condition

$$\theta(x = 0) = \hat{\Theta}$$ \hspace{1cm} (B9)

is assumed, whereas on the right-hand side the convective heat loss is negligible and therefore the adiabatic boundary condition

$$\left.\frac{d\theta}{dx}\right|_{x=L} = 0$$ \hspace{1cm} (B10)

is applied. Accordingly, the temperature distribution

$$\theta(x) = \frac{\cosh \left( \sqrt{\frac{2h}{\kappa\Omega d}} [L - x] \right)}{\cosh \left( \sqrt{\frac{2h}{\kappa\Omega d} L} \right)} \hat{\Theta}$$ \hspace{1cm} (B11)

is obtained, or by exploiting Equation (B6)

$$\Theta(x) = \frac{\cosh \left( \sqrt{\frac{2h}{\kappa\Omega d}} [L - x] \right)}{\cosh \left( \sqrt{\frac{2h}{\kappa\Omega d} L} \right)} \hat{\Theta} + \Theta_{\text{ref.}}.$$ \hspace{1cm} (B12)

A more detailed description by accounting different boundary conditions and shapes of the volume under consideration is given by [35].