„Improving the temperature predictions of subsurface thermal models by using high-quality input data. Part 1: Uncertainty analysis of the thermal-conductivity parameterization“

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Keywords

Thermal modelling, thermal conductivity, parameterization, sensitivity analysis, uncertainty analysis

Highlights

- Effect of TC input examined for thermal modelling studies.
- Uncertainty analysis for modelled temperatures is performed.
- Borehole parameterization prevails over literature parameterization.
- Considering facies effects significantly reduces temperature uncertainty.
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Graphical abstract

ABSTRACT

The subsurface temperature field and the geothermal conditions in sedimentary basins are frequently examined by using numerical thermal models. For those models, detailed knowledge of rock thermal properties are paramount for a reliable parameterization of layer properties and boundary conditions. Despite the state-of-the-art in other research fields (e.g. hydrogeological ground-water models) where the spatial permeability variations within geological layers is often considered, parameterization of the major rock thermal properties (in particular thermal conductivity, to minor extent radiogenic heat production and specific heat capacity) is almost always conducted by applying constant parameters for each modelled layer. Moreover, initial parameter values are usually obtained from only few core measurements and/or literature values, which raise questions for their representativeness. Only some rare studies have considered detailed lithological composition or well log information, still with constant layer properties.

This study presents a thermal-modelling scenario analysis in which we demonstrate how the use of both different parameter input type (from literature, lithology and well logs) and parameter input style (constant or spatially varying layer values) affects model temperature predictions in sedimentary basins. It is a case study located in the Danish-German border region at the northern margin of the North German Basin. To conduct the scenario analysis, rock thermal properties are determined from lithological descriptions and standard petrophysical well logs for several boreholes in the area of study. Statistical values of rock thermal properties are derived for each geological formation at each well location and, furthermore, for the entire dataset. The thermal model is validated against known observed temperatures of good quality.

Results clearly show that the use of location-specific well-log derived rock thermal properties and the integration of laterally varying input data (reflecting changes of lithofacies) significantly improves the temperature prediction. The parameterization from boreholes always prevails over the parameterization based on literature values, and it allows for reducing uncertainty of model temperatures by up to 80%.

1. Introduction

Where thermal conduction is accepted to be present as main heat-transport mechanism, terrestrial heat-flow (physically: heat-flow density) and the configuration of rock thermal properties mainly determine the heat budget and the stratification of the temperatures of the

subsurface. According to the general heat equation, thermal conductivity (TC) and, to a minor extent, radiogenic heat production (RHP) are the most important rock thermal properties forming the steady-state temperature field (beside the heat flow). Where no direct observations are available, numerical modelling of the geological system and the processes acting therein is a proven technique to examine the thermal field on various scales and in different resolutions. Numerous modelling studies have been undertaken to investigate the thermal field in sedimentary basins worldwide, often in context of the exploration and exploitation of hydrocarbons or geothermal energy. For the North German Basin (NGB), where the present work is located, more than 25 studies covering a broad range of scientific issues have been published in the past two decades (*cf.* Fuchs and Balling, 2016, (part 2, this issue) for a more detailed review on modelling studies in the NGB). Obviously, TC is important in geothermal studies. However, this importance is generally not reflected in how this parameter is treated in model parameterization.

Following the most common modelling concept, the subsurface is simplified to geological (stratigraphic, structural) units (formations, layers) for which thermal boundary conditions and representative laterally constant rock thermal properties are set. The underlying assumptions are that rock thermal properties do not vary significantly on a local or even regional scale, and that it is possible to derive values representative for the geological formation in the modelled area. In the past, the simplification to structural units with constant parameter values was mainly driven by general computational limits, which forced researchers to develop time-efficient model designs, and by an overall lack of knowledge on the thermal specifications of the subsurface rocks. Today, this simplified concept possesses two fundamental drawbacks.

First, the assumption of neglecting lateral changes in lithology (facies) and thus rock thermal properties is not tenable anymore since this effect is basically long known (e.g. Chapman et al., 1984) but also repeatedly documented in recent petrophysical studies (e.g. Norden and Förster, 2006; Schütz et al., 2012b; Homuth et al., 2014; Fuchs et al., 2015). The effect of facies-dependent TC variability is further consolidated by the detailed analysis of temperature logs (e.g. Fuchs and Förster, 2010; Sippel et al., 2013; Schütz et al., 2012a, 2014; Fuchs et al., 2015) as well as modelling results (e.g. Ollinger et al., 2010) which demonstrated that considering lateral varying TC values results in an improved fit between measured and modelled temperatures.

Second, calculating representative layer values (formation scale) requires reliable data of the thermal properties of rock formations. Such data can be obtained with high accuracy by

laboratory measurements on drill-core samples, which are certainly expensive to extract, rarely available, limited to borehole locations, and often restricted to specific geological targets. Moreover, calculating representative formation values from a number of measurements carried out on sampled rocks, that do not necessarily reflect neither the local lithological composition of a geological formation, nor of which lateral heterogeneity, can be afflicted with large uncertainties (upscaling problem).

The approach most often applied to circumnavigate this problem, is to attribute rock thermal properties of stratigraphic formations (model layers) according to known values of their dominant lithology. For the NGB, Scheck (1997) started the parameterization of the first modern 3D thermal model following the above approach by applying laboratory TC data (dry measured, non-in-situ) compiled by Hurtig and Schlosser (1976). Unfortunately, the documentation therein is quite poor: original lab workers, location and type of the rock samples as well as laboratory methods (treatment, preparation and measurement technique) are not reported. Moreover, most values documented for the stratigraphic units in Scheck's work are not reproducible from the Hurtig-and-Schlosser data.

Useful alternatives, like the application of geophysical measurements that easily allow calculation of representative formation values from borehole TC profiles in sedimentary settings, have recently been successfully developed (Hartmann et al., 2005; Fuchs and Förster, 2014; Fuchs et al., 2015). These thermal parameter profiles nowadays allow the precise modelling of borehole temperatures (e.g. errors < 3 °C in the latter reference). Additional alternatives to the parameterization with a 'representative' constant layer value are introduced, for instance, by Vogt et al. (2010) and Mottaghy et al. (2011). The authors used a stochastic modelling approach (realizations of TC probability distributions) combined with a constraining post-processing (calibration on temperatures) to reduce temperature uncertainties. They demonstrated that a stochastically simulated, spatial TC distribution can reduce the temperature uncertainty of a specific target location significantly by around 50% (from 25 to 12 °C at 2300 m depth). Nevertheless, these alternative studies are exceptional cases. The majority of modelling studies are still using the time-saving conservative approach outlined above. Consequently, the parameter set defined by Scheck (1997) started to become very popular. A series of subsequent modelling studies has continuously implemented this 'first' parameter set as representative for the specific stratigraphic units. To date, a surprisingly high 70% of the parameterized layers in subsequent modelling studies (in the NGB) implemented these values. It has also to be considered that, despite of some rare studies (e.g. Vosteen et al., 2004), the

majority of heat-transfer studies has not been calibrated to real observations. A quantification of the fit between modelled and measured temperatures is presented only in a few studies.

Beyond these fundamental parameterization issues, another problem comes into play. Where temperatures predicted by purely conductive models show inconvenient misfits compared to measured temperatures, the influence of convective processes as additionally relevant heat-transport mechanism is often assumed to be present. In many studies located in the NGB, advective or convective flow processes are frequently attributed to a permeable Mesozoic and Cenozoic stratigraphy, interrupted by an impervious Triassic Muschelkalk (Magri et al., 2005; Magri et al., 2008; Cacace et al., 2010; Noack et al., 2010; Kaiser et al., 2011; Sippel et al., 2013; Kaiser et al., 2013; Noack et al., 2013; Scheck-Wenderoth et al., 2014). Depending on the layer thickness and the allocated permeability (which for specific geological units is often also transferred from one study to another), fluid flow is frequently claimed to contribute considerably to the thermal regime, mainly above the Muschelkalk. This is remarkable as, consolidated basins like the NGB typically have small inclination of the sedimentary layers (Ziegler, 1992) and considerable contrasts in the vertical component of hydraulic conductivity between the different deposited rock types. Due to lack of data, it still remains unclear if vertical fluid flow realistically affects the heat transfer through the rock layers on a regional or basin scale. Well-constrained counter arguments in this ‘debate’ are provided by the analysis of continuous borehole temperature logs available for the NGB. The majority of these logs measured under thermal equilibrium, displayed in e.g. Förster (2001), Fuchs and Förster (2010), and Fuchs and Förster (2014), show no thermal evidence for large-scaled fluid flow cells in Cenozoic and Mesozoic depths. Even, small disturbances related to specific highly permeable sandstone aquifers are rarely observed from these logs.

Therefore, the questions arise: (1) Are poor temperature forecasts of conductive models due to the poor parameterization approach of the rock TC? (2) Is the proposed positive impact of convective flow in coupled models (which is almost never quantified in current studies) simply caused by a compensation of the oversimplified conductive modelling approach? In the present study, part 1, we examine the effect of different TC parameterization approaches on the fit between modelled and measured temperatures. For that purpose, a regional 3D steady-state conductive thermal model is developed for a region in the NGB. In our uncertainty analysis, parameter sets stemming from different sources (literature, analysis of bore logs and well logs) and of varying resolution (constant and lateral varying formation values) are tested. The major research questions that we will answer in this paper are: (1) How big is the effect of the TC parameterization approach (source and quality) on the uncertainty of modelled temperatures in

sedimentary settings, and (2) can the prediction uncertainty be reduced by considering the spatial variation of formation TC values which can be observed from boreholes?

This paper includes the description of the background data (Section 2), details of the modelling methods and procedures applied (Section 3) and a numerical uncertainty analysis to identify the most-promising TC parameterization approach (Section 4). A detailed heat-flow study and new detailed subsurface temperature maps of the area of study (Danish-German border region in the NGB) derived based on the outcome of this study (part 1) are presented and discussed in part 2 (Fuchs and Balling, 2016; this issue).

2. Background data

This study benefits from a large amount of borehole data available from a total of 224 deep wells in the study area. Boreholes were drilled between 1951 and 2012 and reach depths between 780 and 6105 m below sea level (mbsl) (67 out of the 213 wells reach depth > 2000 mbsl). The majority of the boreholes (approx. 180) are concentrated in the Southern and Southeastern part of the study area, close to potential geological traps for oil and gas near the salt structures in the *Glückstadt-Graben* area. All wells were screened for lithological, stratigraphical, petrophysical and geophysical borehole data to select these boreholes with the most promising amount of high-quality data. Finally, 75 wells were selected: 21 from the Danish part and another 54 from the German part (*cf.* Fig. 1). For all wells, lithological and stratigraphical information were available either from the completion or from the mud reports. These reports were provided by pdf-scans. For Danish wells, digital log data (las format) were provided by the Geological Survey of Denmark and Greenland (GEUS) covering a broad spectrum of standard well logs. For German wells, digital log data were available only for explored geological reservoirs of some few wells. Thus, pdf-scans of paper-printed log data were provided for 47 of the 54 wells by the State Agency for Agriculture, Environment and Rural Areas Schleswig-Holstein (LLUR). Lithological and, to some extent, stratigraphic information, in particular for the German boreholes, was provided as tiff-scans. Therefore, use of lithological, stratigraphical, and well logging data, in particular for the German part, demands a time-consuming digitization during the first part of the study. Well logs were semi-automatically digitized using NeuraLog[®] and saved as las files. Lithological and stratigraphical data were digitized manually.

Figure 1. Map of the study area, including the northern part of the *Glückstadt Graben* located in the North-German Basin. This area is characterized by numerous salt structures. Only boreholes that provide data for the parameterization of *scenarios C* and *D*, or reliable temperatures included in the uncertainty analysis, are displayed.

2.1. Structural data – 3D geological model

A 3D structural subsurface model of the study area generated by using GOCAD[®] (Mallet, 2002) is introduced by Kirsch et al. (2015). This geological model is based on the Geotectonic Atlas of NW-Germany (Baldschuhn et al., 1996) and the detailed reinterpretation of selected seismic data (c. 315 sections in the study area by using Petrel[®]) and geological information obtained from boreholes (c. 224). The main focus was on a cross-border correlations of German and Danish seismic sections and the evaluation of the data shown in the Geotectonic Atlas, in particular with respect to the numerous salt structures. For this purpose, lithological descriptions from bore logs are correlated with stratigraphy, well-log and seismic data. Finally, a 3D

structural model consisting of 12 basic units down to the base of the Zechstein, fully consistent with data from seismic profiles and boreholes, is now available. In the present study, additional pre-Zechstein data from Maystrenko and Scheck-Wenderoth (2013) have been used to form the sedimentary and the crystalline basis of the final geological model. For the thermal model, all 14 stratigraphic units, including depth ranges, are summarized in Table 1.

Table 1. Thickness and elevation of modelled geological units.

Geological unit	Top			Thickness	Numerical FEFLOW layer
	highest	low est	median	min - max	
	[meter below sea level]			[m]	
1 Quaternary/Tertiary	-74	3	-4	30 - 5,008	1-2
2 Upper Cretaceous, Base Chalk	10	5,063	492	0 - 2,325	3-5
3 Low er Cretaceous	138	5,693	1,127	0 - 790	6-8
4 Upper Jurassic	237	5,762	1,196	0 - 287	9-11
5 Middle Jurassic	1,819	4,248	3,722	0 - 1,457	12-14
6 Low er Jurassic	1,276	4,369	2,273	0 - 2,950	15-17
7 Upper Keuper (Rhaetian/Gassum)	693	5,033	1,504	0 - 815	18-20
8 Low er Keuper	688	5,297	1,281	0 - 4,725	21-23
9 Upper Buntsandstein/Muschelkalk	776	6,311	1,644	0 - 2,085	24-26
10 Middle Buntsandstein	904	7,191	2,092	0 - 2,084	27-29
11 Low er Buntsandstein	943	9,320	2,494	0 - 915	30-32
12 Zechstein	138	10,118	2,514	80 - 6,950	33-35
13 Sedimentary Pre-Zechstein	1,624	10,310	3,740	0 - 8,195	36-38
14 Crystalline Basement	1,290	16,319	5,965	3,746 - 18,705	39-43

Due to the presence of the deep-reaching *Glückstadt Graben* in the Southeast and the shallow crystalline of the *Ringkøbing-Fyn High* in the North, geological units show large variations in thickness and depth. Within the study area, the thickness of sedimentary rocks accumulated in the graben structure ranges between c. 2 km in the North (close to the *Ringkøbing-Fyn High*) and c. 15 km in the Southeast (close to the maximum depth of the *Glückstadt Graben*). The base of Zechstein evaporates is located at depth between c. 2 and 10 km, whereas the top sometimes is very close to the surface. Consequently, the top and thickness of the crystalline crust is varying vice versa. To establish a convenient lower thermal boundary condition, the final geological model was extended to a depth of 20 km, which left place for a minimum of 5 km of crystalline crust below the maximum depth of the *Glückstadt Graben*. Further details of the local geological settings are given in part 2 (Fuchs and Balling, 2016; this issue)

2.2. Petrophysical data

Well-logging data from varying ages and of varying quality were available for more than 68 wells in the study area. Wells in the German part, mainly drilled for oil and gas exploration between 1951 and 1984, have often been logged with self-potential (SP) and resistivity logs

only. Modern well logs (mainly gamma-ray log and sonic log) are available for fewer wells. Logging data in Danish wells have been measured between 1951 and 2012 and cover a broad spectrum of standard well logs (usually self-potential, resistivity, gamma ray, density log, sonic log, neutron-neutron log, photoelectric factor, caliper log; rarely: photoelectric-factor log). Thus, the database for well-log based predictions of rock thermal properties is heterogeneous. For the majority of logging data made available by GEUS and LLUR, the application of corrections (following Serra, 1984) due to borehole or environmental effects (in particular considering the effect of borehole breakouts) was needed. All logs in this study were sampled to fixed 0.25m intervals.

Profiles of bulk TC were calculated for each borehole with reliable well-logging data using the prediction equations for sedimentary rocks developed by Fuchs et al. (2015). This new procedure, extended from the original concept of Fuchs and Förster (2014), allows the estimation of TC for each combination of up to five standard well log response values and derived predictors used in the present study (volume fraction of shale, interval sonic transit time, neutron porosity, bulk density, photoelectric factor). Depending on the number, combination and quality of well logs available, the selected prediction equation was varied along the borehole to minimize the expected prediction error as documented in Fuchs et al. (2015). This approach is validated for sedimentary rocks which cover 13 out of the 14 modelled layers. According to the general lack of information on the crystalline crust, we applied the same approach for the rocks of unit 14. The calculated formation value is reasonable and within the range expected from literature.

Where spectral gamma-ray logs are available, radiogenic heat production (RHP) of the rocks is calculated from the measured contents of Th, U, K and the density of a rock using relationships given in Rybach (1986). Where only standard gamma-ray logs are available, RHP is estimated applying the empirical equations from Bückner and Rybach (1996). Depending on data quality, both methods allow the determination of RHP with an uncertainty typically lower 10%.

Where available, data from sonic log and density log are used to estimate the porosity. Finally, all intervals with parameter determinations are merged to a 'best profile' of TC, SHC, RHP and, if applicable, porosity for each borehole (Fig. 1).

2.3. *Measured temperatures*

In contrast to the large amount of geological and standard well logging data, reliable temperature data from boreholes in the study area are scarce. One continuous profile with

equilibrium temperatures (10 cm reading steps, logged more than two years after end drilling activities; to a depth of 1177 m [MD]) is available for the Sønderborg-1 borehole (Balling and Bording, 2013), located in the northeastern part of the study area. Moreover, 148 bottom-hole-temperature values (BHT) are available from a total of 44 wells (Germany: 78 values in 27 wells, Denmark: 70 values in 17 wells), mainly for a depth range between 1000 and 3000 mbsl. BHT data compiled for this study are taken from Poulsen et al. (2012a) and Kühne (2006) for the Danish and the German part, respectively. Depending on the number of BHTs in each borehole and the data (shut-in time, radius) given in the original well reports, available BHT's have been corrected by applying the most suitable method under given conditions. While most of the Danish BHT data have been corrected by the cylindrical source method (19 CMI-corrected BHT values; correction procedure described in Poulsen et al., 2012b), only few of the German BHT data allowed the application of a correction scheme. For 10 values in 7 wells, an empirical approach was applied based on the cylindrical source method and possible also with single BHT values (correction performed by Schulz and Werner, 1987). Only for one well in the German part, Schleswig Z1, the Horner-plot method was applied (7 values).

In this study, temperature data are primarily used for calibration and validation of the numerically modelled temperatures. In this procedure, quality of the measured temperature data is mandatory for the quality of the final predicted temperatures. Therefore, we included only logged temperature data (Sønderborg well, 23 values sampled along the ~1200 m profile) and corrected BHT values ($n = 36$, 21 wells) in the final temperature data set and ignored uncorrected BHT's. This new temperature data set comprises values ranging between 11 °C and 172 °C for depth levels between 60 m and 6065 mbsl. Finally, temperature data were randomly subdivided into a calibration set (70% of data; $n = 41$) and a validation set (30% of data, $n = 18$). According to the data and correction type, each temperature value is attributed with a weight factor that reflects the quality of the data using a modified classification originally introduced by Schulz and Werner (1987), where temperature log = 1, BHT CMI corrected = 0.9, BHT Horner corrected = 0.8, BHT empirical corrected = 0.4). This weight factor was applied in the calibration procedure.

3. Model set up, workflow and governing equations

For the present uncertainty analysis, a 3D conductive steady-state thermal model was developed. This model is based on the input of structural information from the detailed 3D

geological model (Section 2.1), petrophysical rock properties determined for these structural units (Section 2.2) and reliable boundary conditions (Section 3.2) constrained by measurements (surface temperature and interval heat flow). To examine the effect of the TC input on the temperature fit, different TC parameter sets (scenarios) are defined, whereas all remaining parameters and boundary conditions are kept constant. Property values assigned and methods applied for the different scenarios are documented in Section 3.3.

For the 3D heat transport simulation (forward modeling), the commercial FEM software FEFLOW® (Diersch, 2014) was utilized. The basic three-dimensional heat equation for the energy transport, considering heat conduction as only heat driving process, is written as:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + H, \quad (1)$$

where ρ in the rock density [kg m^{-3}], c is the SHC [J (kg K)^{-1}], $\frac{\partial T}{\partial t}$ is the temperature change with time, λ is the rock TC [W (m K)^{-1}], H is the RHP [W m^{-3}], and $\frac{\partial T}{\partial x}$, $\frac{\partial T}{\partial y}$, $\frac{\partial T}{\partial z}$ are the temperature gradients in x, y, and z directions, respectively. Since we assume conduction as main heat-driving process, and steady-state conditions ($\frac{\partial T}{\partial t} = 0$), the temperature solution depends only on rock TC and RHP and the given boundary conditions.

The general importance of calibrating numerical models for heat transfer problems is widely known and different techniques has been applied in the past (e.g. Wang, 1989; Shen et al., 1990; Vosteen et al., 2004; Rath et al., 2006). In model runs of the present study, where initial rock TC is calibrated by implementing temperature observations, (constraining method), the FEFLOW Parameter estimation program FePest® is used. FePest implements the model-independent parameter estimation software PEST, originally developed by John Doherty (Doherty, 2002) for groundwater problems. PEST is based on a non-linear parameter estimation technique of the Gauss-Levenberg-Marquardt algorithm (GLMA). In this approach, TC is iteratively (incrementally) adjusted within given limits until the objective function comprising the sum of weighted squared deviations between measured temperatures (calibration data set) and their respective model outcomes is minimized. The direction and magnitude of the adjustment are expressed by a parameter upgrade vector. The optimal direction of this vector is identified by an interpolation between the gradient-descent method (linear behavior of objective function) and the Gauss-Newton method (non-linearity) and is controlled by a scaling parameter. PEST dynamically updates lambda depending on the progress in reducing the objective function. Further details are given e.g. in Doherty (2015).

For all initial and calibrated model runs, deviations between modelled and measured temperatures are calculated for the calibration, the validation, and the full temperature data set, respectively. Arithmetic mean error (ame), standard deviation (sd), median and root mean square error (rmse) are calculated for all three data sets and compared for each model run. Further details on the applied statistical calculations are documented, for instance, in Deutsch and Journal (1998). A comparison of mean deviations between modelled and measured temperatures is performed using the student's *t*-test for paired samples ($n = 59$). A level of 5% ($\alpha = 0.05$) is chosen as threshold for statistical significance. For p values $< \alpha$, the null hypothesis (mean temperature uncertainties are equal) is rejected in favor of the alternative hypothesis (mean uncertainties are significantly different). Compared groups have been initially tested for normal distribution using the Kolmogorov–Smirnov test and for equality of variances using the Levene test.

3.1. Structure and mesh generation

The geological structure has been integrated in the thermal model, by defining 14 structural layers (units). Thirteen layers define sedimentary units from the Quaternary down to the sedimentary Pre-Zechstein, below which the model contains the crystalline rocks of the upper crust. For details on the geology, see information given in part 2 of this study (Fuchs and Balling, 2016; this issue) and P. Balling et al. (2013). In setting the model lower depth limit, care must be taken to the structural configuration of the crust, strongly influenced by the deep *Glückstadt Graben* located in the Southern part of the study area. To avoid uncertainties related to the deeper crustal and upper mantle configuration, the Moho or the lithosphere–asthenosphere as boundary levels (e.g. Scheck, 1997; Marotta et al., 2000; Norden et al., 2008; Cacace et al., 2010; Noack et al., 2012), we use a depth of 20 km for the lower model boundary. This is between Moho and top of the crystalline crust, where we find (from modelling) that thermal anomalies caused by the deep reaching graben structure are not significant anymore. Furthermore, the 20 km depth level is sufficiently shallow to avoid a further subdivision of the crystalline crust.

Due to lack of detailed knowledge, faults are not independently parameterized as geological features and are here considered as structural offset only. To keep the relation between vertical and lateral extent of the meshed elements within reasonable limits, the crystalline crust is subdivided into four numerical layers. Moreover, above and below individual layers, a 1m thin ‘buffer zone’ was included as extra numerical FEFLOW layer. This procedure limits a common

model bias to the thin buffer layers, as the temperature calculation at the nodes based on the rock thermal properties averaged from all neighbor model elements. So, in total, the 14 geological units are represented by 43 numerical FEFLOW layers, and 44 slices. Where geological units show discontinuities ('geological holes' with areas of zero thickness), for instance Mesozoic and Cenozoic layers at salt diapirs and walls, a minimum thickness of 0.1 m is automatically assigned to assure continuum conditions. Here, parameters are adopted from the original geological unit.

For meshing, the FEFLOW internal Grid-builder routine (anisotropy = 1, gradation = 5) is used. The generated model consists of 3,719,715 three-dimensional prismatic mesh elements and 1,913,692 nodes. The horizontal resolution, and thus the horizontal element size, varies within the model area. The average distance between nodes generally ranges between c. 1.5 km for offshore areas and c. 0.75 km for onshore areas. Where salt structures are present (annulus + 2 km buffer), the grid is further refined resulting in an average node distance of c. 0.3 km. This allows consideration of structural details of the salt features. Based on the size of the model area (c. 14,000 km²), the average horizontal element size is 0.16 km². The vertical resolution varies according to the variable thickness of the structural units.

3.2. Thermal boundary conditions

Different types of thermal boundaries are set for the model topography (upper thermal boundary, constant temperature) and for the maximum depth of 20 km (lower thermal boundary, constant heat-flow). For setting the surface conditions, it has to be considered that almost one third of the study area is covered by shallow sea water from the North Sea and Baltic Sea. According to data from Becker and Schulz (2000) as well as Siegel and Gerth (2014), the long-term annual mean surface temperature averages c. 10 °C for the North Sea and c. 8 °C for the Baltic Sea, which differs only slightly from the long-term annual onshore mean surface temperature of 8.9 °C (1981-2010; DWD, 2014). Bottom water temperatures are recorded to be slightly lower. For the upper model boundary (i.e. model topography), a constant temperature of 9 °C is applied.

The lower thermal boundary is defined by a constant basal heat flow at the constant depth of 20 km (Neumann boundary condition). The applied lower boundary heat flow of 49.2 ± 4.1 mW/m² is derived from borehole interval heat flow values determined at 7 locations and considering the RHP from those intervals down to the 20 km depth level. Further details regarding the heat-flow analysis and the calculation of basal and surface heat flow are provided

in part 2 of this study (Fuchs and Balling, 2016; this issue). The lateral boundaries are ‘no-flow boundaries’.

3.3. Scenarios and parameterization

To examine the effect of source and quality of the thermal parameterization on the fit between modelled and measured temperatures, five main scenarios were developed, each containing several models (Table 2). Model names can be read abbreviated as ‘Letter of scenario’ + ‘_’ + ‘Type of TC distribution’ + ‘_’ + ‘model run’.

Table 2. Summary of the numerical models included in the scenario analysis.

Scenario	Source	Determination of TC	TC distribution	Model run	Model name
A	literature	Values from Scheck (1997)	constant	initial	A_con_i
			constant	calibrated	A_con_c
B	literature	Values from Balling et al. (2013)	constant	initial	B_con_i
			constant	calibrated	B_con_c
C	lithological analysis	Lithological composition from bore logs, application of mixing model including end-member values and porosity	constant	initial	C_con_i
			constant	calibrated	C_con_c
			lateral varying	initial	C_var_i
			lateral varying	calibrated	C_var_c
D	well-log analysis	Well-log based prediction using equations from Fuchs et al. (2015)	constant	initial	D_con_i
			constant	calibrated	D_con_c
			lateral varying	initial	D_var_i
			lateral varying	calibrated	D_var_c
E	random	Assuming constant values of 2.0, 2.5 and 3.0 W/(mK) for the complete model domain	constant	initial	E_2.0_i
			constant	calibrated	E_2.0_c
			constant	initial	E_2.5_i
			constant	calibrated	E_2.5_c
			constant	initial	E_3.0_i
			constant	calibrated	E_3.0_c

Abbreviations: *i* = initial, *c* = calibrated, *con* = constant layer values, *var* = lateral varying layer values

TC and RHP for different stratigraphic units in *scenario A* are taken from literature (Scheck, 1997). Where layers are finer resolved in the present model compared with Scheck’s model (e.g. Upper, Middle, and Lower Jurassic instead of Jurassic only), the literature value for the larger unit (e.g. Jurassic) is assigned to each of the modelled layers. Where one of our model layers covers two of Scheck’s layers (e.g. ‘Sedimentary Pre-Zechstein’ including Lower Permian and Rotliegend), the arithmetic mean value of the literature data is assigned to our model layer. For RHP of the crystalline crust, we used the value of 2.0 $\mu\text{W}/\text{m}^3$, proposed for the differentiated crust in Scheck’s model 2B. The model of Scheck (1997) was developed for the Northeast German Basin (NEGB) and resulted in a general misfit of c. 5 °C when compared with borehole temperature measurements (Scheck-Wenderoth, personal communication, 2015).

For *scenario B*, TC and RHP values reported for a thermal model of the Glückstadt Graben by P. Balling et al. (2013) were used. The implemented TC and RHP parameters have been calibrated on temperature data by Balling and coworkers (data from ‘final calculation best-fit model’) and thus should be optimized for the specific conditions of the *Glückstadt-Graben* area. Where the structural subdivision differs compared with the present study, the process of parameter allocation is performed similar to scenario A. The original misfit (rmse) compared with measured temperatures (6 wells, $n = 56$) averages at c. 10 °C (Phillip Balling, personal communication, 2014).

The TC parameterization of *scenario C* is based on the detailed analysis of lithological bore logs as described in Norden et al. (2012). For each bore log, the lithological descriptions are classified into 9 main lithotypes (anhydrite, dolomite, rock salt, limestone and chalk, sandstone, siltstone, claystone and shale, marlstone and mudstone, other). The lithological composition (thickness weighted) for the upper 13 modelled geological units (all above the crystalline crust) is derived from 42 boreholes in the study area. Assuming matrix TC values for each lithotype and well-log-derived mean porosity values, the geometric-mean model (Lichtenecker, 1924) is applied to compute a bulk formation TC representative for each borehole location:

$$\lambda_b = \prod_{i=1}^n \lambda_i^{\phi} \quad (2)$$

Herein, λ is the TC of the i th component (mineral fraction/lithotype considered for matrix or water filled pore space) and ϕ is the fractional proportion of the i th component. Lithotype-specific matrix TC values (anhydrite: 4.0 W/(mK), dolomite: 3.5 W/(mK), rock salt: 5.2 W/(mK), limestone and chalk: 3.1 W/(mK), sandstone: 6.5 W/(mK), siltstone: 2.7 W/(mK), claystone and shale: 2.1 W/(mK), marlstone and mudstone: 2.1 W/(mK), other: 3.0 W/(mK) are compiled from regional petrophysical studies and textbooks (Brigaud et al., 1990; Norden and Förster, 2006; Fuchs and Förster, 2010; Schön, 2011). RHP is estimated from gamma-log readings as described in Section 2.2.

For *scenario D*, TC and RHP are parameterized based on the detailed analysis of geophysical borehole measurements as described in Section 2.2. This approach was applied on 27 wells, where well-log data of reliable quality were available.

For both *scenarios C* and *D*, the TC parameterization of the crystalline crust (unit 14) was performed in a different way, as the applied well-log based prediction approach is assumed to be valid for sedimentary rocks only. Few observations regarding the nature of the shallow crystalline crust are available and only from the northernmost boreholes in the study area. The

top basement is reached in some boreholes (Borg-1, Brøns-1, Løgumkloster-1, Rødekro-1, and Varnæs-1) and seems to reveal Ordovician to upper Paleozoic metamorphic rocks that are classified as microcrystalline slate or schist. Due to the lack of any local rock material and laboratory measurement, mineral composition and rock thermal properties for the crystalline crust are not determined. Furthermore, these rocks are unlikely to be representative for the entire upper crust. We have applied a TC value of 3.1 W/(mK) for the crystalline basement (unit 14), which is found to be a reasonable estimate both for slates (Schintgen et al., 2015) and for the upper crystalline crust (Balling, 1995; Norden et al., 2012) in adjacent areas.

For *Scenario E*, TC values invariant for the model domain are assumed. This approach reflects the assumption of a constant temperature gradient with depth, often used as ‘rule of thumb’, totally ignoring what is known from structure, lithological variability and rock thermal properties. Values of 2.0, 2.5 and 3.0 W/(mK) have been tested uniformly for all geological units in different model runs, representing temperature gradients of approx. 40.0, 32.0, and 26 °C/km.

For *scenario A, B and E*, layer values are assigned as constant values only. A spatial (lateral) variation using literature or random values is obviously not possible. Consequently, statistical parameters which could later define reasonable limits for the parameter variation within the calibration process (using FePest) are not available either. For these scenarios, TC is allowed to vary within $\pm 30\%$ from the initial formation value. Although effect of temperature, pressure and anisotropy on the in-situ TC is known to exist, we did not include any such empirical corrections into our scenarios in order to relate the observed temperature uncertainty directly to the model-specific TC parameterization. For the same reason, we did not include the palaeoclimatic effect in this study. A borehole-specific parameterization example for *scenarios A–D* is given in Fig. 2.

For *scenario C and D*, statistical parameters like the arithmetic mean (am), standard deviation (sd), minimum (min) and maximum (max) values, 25% and 75% quantiles ($Q_{0.25}$, $Q_{0.75}$), and the 95% confidence interval ($CI_{0.95}$) are calculated for each geological unit at each borehole location (see averaged values for the complete model area in Fig. 3). For models with a laterally constant TC (C_con_i, C_con_c, D_con_i, D_con_c), representative formation values averaged (am) from all considered borehole location are calculated and listed in Table 3. The optimization range for the calibration procedure is defined by the averaged standard deviation for all implemented borehole location. For models with spatially distributed values (C_var_i, C_var_c, D_var_i, D_var_c), TC is regionalized for each formation based on the borehole

information by using an ordinary kriging procedure (Krige, 1951), which is implemented as FEFLOW routine. For the TC optimization (calibration) of these models, TC is allowed to vary within one standard deviation as determined for each formation interval at each borehole location.

The mean values and range of the thermal-parameter sets in each scenario are documented (or summarized) in Table 3 and Fig. 4. A borehole-specific parameterization example is given in Fig. 2. An example for the spatial variability of TC derived from well-specific formation values within the study area is given in Fig. 3. The internal Kriging algorithm (ordinary) in FEFLOW is used to regionalize the borehole values within each modelled unit.

Unit	TC in W/(mK)					RHP in $\mu\text{W}/\text{m}^3$				
	Scenario					Scenario				
	A	B	C	D	E	A	B	C	D	E
1	1.5	1.5	2.62 ± 0.15	2.52 ± 0.45		0.7	0.7	0.81		
2	1.9	2.1	3.13 ± 0.25	3.08 ± 0.35		0.3	0.3	0.32		
3	2.0	1.5	2.64 ± 0.17	2.32 ± 0.49		1.4	1.4	1.14		
4	2.0	1.8	2.44 ± 0.24	2.44 ± 0.47		1.4	1.4	0.9		
5	2.0	1.8	2.6 ± 0.24	1.93 ± 0.34		1.4	1.4	1.18		
6	2.0	1.8	2.44 ± 0.06	1.68 ± 0.59		1.4	1.4	1.5		
7	2.3	2.4	2.6 ± 0.22	2.22 ± 0.54		1.4	1.4	0.9		
8	2.3	2.4	2.5 ± 0.31	2.22 ± 0.47		1.4	1.4	1.27		
9	1.925	1.75	2.74 ± 0.32	2.49 ± 0.49		0.65	0.95	1.12		
10	2.0	1.6	2.45 ± 0.23	2.36 ± 0.50		1.0	1.5	1.41		
11	2.0	1.6	2.41 ± 0.31	2.35 ± 0.54		1.0	1.5	1.44		
12	3.5	3.5	4.42 ± 0.67	4.41 ± 0.91		0.09	0.09	0.38		
13	2.45	2.45	2.4	2.56 ± 0.55		1.5	1.5	1.2		
14	3.1	2.8	3.1	3.1		2.0	1.2	2		

Table 3. Basic parameter sets of rock thermal properties for all scenarios. Listed TC values are used only in models that are parameterized with laterally constant values. RHP values are representative formation values implemented in all models.

Figure 2. Borehole example for TC formation values applied for different scenarios. Yellow and brownish colors are clastic rocks; blue and pale colors are carbonates; green and purple colors are evaporates. Black thin line and grey-shaded envelope characterize mean value and error range of the well-log based TC prediction.

Figure 3. Formation TC for the example of the Lower Cretaceous. Left: Spatial variability of formation TC, right: deviations of regional values from overall formation mean TC value listed in Table 2.

Figure 4. Variability of mean formation TC values applied for different scenarios. Box plot is defined by: colored box = inner 50%, light color below median, dark color = above median; whiskers define min and maximum mean values. Scenario A: red segment; scenario B: green segment; scenario C: non-filled box plot with black frame; scenario D: blue-filled box plot without frame.

4. Thermal modelling results

Figure 5 shows the deviations between measured and modelled temperatures for the different scenarios.

Figure 5. Deviations between measured and modelled temperatures for the different scenarios. Box plot is defined by inner 50% (box) and minimum/maximum values (whiskers). Values in the lower table are the p -values calculated in the paired t -test. For p -values $< \alpha = 0.05$, the mean values of the calculated temperature uncertainties for models compared are significantly different at the 5% significance level.

4.1. Initial models

Scenario A (model *A_con_i*) shows a wide absolute error distribution for the predicted temperatures ranging between 2.5 and 61.6 °C, which accumulates to a high uncertainty averaging 30.6 °C (rmse). The uncertainties of *scenario B* (*B_con_i*) show a range between 0,

and 38.4 °C (ame) which accumulates to an rmse of 14.3 °C. The application of *scenario C* (C_con_i , C_var_i) results in an rms error of 6.1 and 6.5 °C for constant and laterally varying TC values. The absolute error distribution range between 0.1–17.4 °C and 0.1–19.0 °C, respectively. For *scenario D*, temperature uncertainties range between 0.1–23.3 °C and 0.0–13.7 °C, resulting in an rms error of 6.6 and 4.5 °C for constant (D_con_i) and laterally varying TC values (D_var_i). The three different random TC parameterizations of *scenario E* cause different temperature uncertainties. They show a broad error distribution (0.1–46.8 °C and 0.1–32.7 °C) for constant model TC values of 2.0 and 3.0 W/(mK) ($E_2.0_i$ and $E_3.0_i$). For a model TC value of 2.5 W/(mK) ($E_2.5_i$), errors range between 0.1 and 18.2 °C. rms errors are 16.7, 14.1 and 7.3 °C.

Scenario A shows significantly higher uncertainties than *scenario B* ($p < 0.000$), and both show significantly higher uncertainties than *scenarios C* and *D* (all p values < 0.000). Between *scenarios C* and *D*, no significant differences can be observed for constant TC values ($p = 0.130$), but for spatially distributed TC values ($p = 0.000$). Models of *scenario E* show heterogeneous results. Model $E_2.0_i$ shows significantly different uncertainties compared with all other scenarios with constant TC values, while models $E_2.5_i$ and $E_3.0_i$ show partly significant and partly non-significant differences. Lowest uncertainties are observed for model $E_2.5_i$ resulting in significantly lower uncertainties compared with uncertainties of *scenarios A* and *B*.

Differences between constant and lateral varying models show inconsistent results for *scenarios C* and *D*. Differences compared for models C_con_i (rmse = 6.7 °C) and C_var_i (rmse = 6.1 °C) of *scenario C* are insignificant ($p = 0.109$), while differences compared for models of *scenario D* (D_con_i : rmse = 6.6 °C; and D_var_i : rmse = 4.5 °C) are highly significant ($p < 0.000$).

4.2. Calibrated models

For all scenarios (constant and lateral varying), the calibrated models show significantly lower uncertainties than the initial models. Modelled temperatures for the calibrated model runs consistently show rmse below 6 °C. rmse values are 5.8 °C (A_con_c), 5.4 °C (B_con_c), 5.3 °C (C_con_c), 5.2 °C (C_var_c), 5.4 °C (D_con_c), 3.3 °C (D_var_c), and 4.6 °C (all models of *scenario E*) respectively. Maximum absolute errors are usually between 10 and 15 °C; an exception is model C_con_c . For *scenarios C* and *D* which based on borehole parameterization, temperature models with laterally varying TC values show significantly

lower uncertainties than models with lateral constant TC values (p -values are <0.001 when comparing: C_con_c C_var_c for *scenario C* and D_con_c and D_var_c for *scenario D*). The calibrated *scenario D* (model D_var_c ; laterally variable well log input) shows significantly lower temperature uncertainties than all other models (p -value always ≤ 0.002). The initial *scenario D* (model D_var_i) is still as good as the calibrated models of the *scenarios A* and *B* (no significant differences, p -value always >0.07).

5. Discussion

5.1. General results

The type of parameterization has a significant influence on the quality of the modelled temperatures. Comparison of the initial (laterally constant TC) model runs illustrates that the parameterization based on borehole data (*scenarios C* and *D*) clearly prevails over parameterization from literature values (*scenarios A* and *B*). In our study, the uncertainty in modelled temperatures can be reduced using TC derived from borehole data by values ranging between c. 25% (lithotypes analysis versus area-specific literature values from *scenario B*) and c. 80% (well-log analysis versus basin-specific literature values from *scenario A*). This observation is of particular importance if no or few temperatures are available for the model calibration. In this case, the quality of the TC parameterization explicitly determines the quality of the modelled temperatures. Even the use of a random TC parameterization (constant value for the full model domain; *scenario E*) that yields constant temperature gradients can result in a smaller temperature uncertainty than the use of literature values which originally stem from the same sedimentary basin, but from a different area. Accordingly, values derived from geophysical well logs or lithological bore logs are clearly preferable to formation specific literature values for the TC parameterization of thermal models.

For quite some time, the Gauss-Levenberg-Marquardt algorithm (GLMA) in FePest is known to be an effective method for calibrating groundwater models. Applying this constraining post-processing method for calibrating the TC data by including measured temperatures turns out to be a very suitable approach for geothermal models as well. Its application consistently results in smaller temperature uncertainties compared with the initial model runs, both when TC is laterally constant and variable. It has to be considered that applying this approach on models with a spatial TC distribution (depending on the number of pilot points with TC control)

increases the number of model runs and thus the modelling time significantly (e.g. model D_var_c: 4182 model runs in 38 h, 12 cores, parallelization mode).

The calibrated models with constant formation TC values (*scenarios A–D*) show uncertainties (rmse) ranging between 5 and 6 °C, which is good in terms of predicting subsurface temperatures. As a precondition to achieve the observed small uncertainties, we combined a geological model with a high structural resolution (many structural layers) for the depth sections where most temperature data for calibration are available (mainly upper 3 km). In cases where the geological structures are less well resolved and/or if only few or poor temperature data are available, modelled temperatures are expected to show larger uncertainties. We note that all calibrated models of *scenario E* show slightly smaller uncertainties of 4.6 °C compared with the other scenarios. As the calibrated model here represents the optimized configuration of the formation TC for the full model domain, this uncertainty value has to be seen as the minimum threshold that can be achieved with the given temperature data set and constant formation TC values. This value of roughly 5 °C can be assumed to cover the combined uncertainties resulting from geological structure, temperature data and the applied parameter set. The RHP and the thermal boundary conditions also have an impact on the model temperature solution. In general, including those, with lateral variability, into the calibration process most likely will result in a further improvements in particular when significant variations may occur. However, for this TC sensitivity analysis, RHP and the thermal boundary conditions have not been included as parameter to be adjusted in the calibration process.

By comparing uncertainties of the calibrated ‘literature scenarios’ (with laterally constant values) (A + B) with those from the borehole scenarios (C + D), one should be aware that, during the calibration process, TC is allowed to vary within $\pm 30\%$ in *scenarios A* and *B*, whereas it is allowed to vary within $\pm 1\sigma$ (sd) in *scenarios C* and *D*. As can be calculated from values in Table 3, standard deviations derived for *scenarios C* and *D* correspond to a TC variability consistently lower than the 30-% threshold. On average, formation of TC values in *scenarios C* and *D* are allowed to vary only around 9 and 21%, respectively, from the initial value. Consequently, application of the averaging value of 15% would have been more realistic bounds compared with the *scenarios C* and *D* and finally would have resulted in larger uncertainties of the calibrated models of *scenario A* and *B*.

5.2. Influence on the TC variability

As can be seen from Fig. 4, TC varies considerably within geological formations in the model area. For well-log derived formation TC values (*scenario D*), variability of the mean formation values (different from the overall mean value of the formation used for laterally constant parameterization) at different locations ranges between 15% (unit 5, Middle Jurassic) and 49% (unit 11, Lower Buntsandstein) with an average value of 35%. For bore-log derived formation TC values (*scenario C*), the variability at different locations show slightly lower values ranging between 4% (unit 6, Lower Jurassic) and 35% (unit 8, Lower Keuper) and averaging at 19%. The observed variability of formation TC is in agreement with the results and conclusions of previous studies on the effect of facies-dependent variations on rock TC in the NGB (e.g. Norden and Förster, 2006; Fuchs and Förster, 2010; Schütz et al., 2012a,b, 2014, 2013; Fuchs et al., 2015).

Consideration of the observed lateral variation of the formation TC in our thermal model, generally results in a significant reduction of the uncertainty of the modelled temperatures. However, when considering initial and calibrated models, it is difficult to come to general conclusions. For *scenario C* (TC derived from lithological bore logs), calibrated models (with spatially distributed TC values) show significant lower uncertainties ($p < 0.000$), but the initial models ($p = 0.109$) do not. For *scenario D* (well-log derived TC), both initial and calibrated models (with variable TC) show significant lower uncertainties (p -values < 0.000) compared with models with constant TC values.

This inconsistency might be caused by the different uncertainties introduced by the determination methods of TC from bore or well logs. The calculation of formation TC values from lithological bore logs (*scenario C*), requires a detailed analysis of the lithological composition for each formation (*cf.* Section 3.4). Analysis results are mainly determined by the quality and the degree of the lithological descriptions documented in the bore logs. Moreover, for same rocks, documented descriptions might differ from borehole to borehole according to the different geologists making these descriptions at different times, their techniques applied and their experience in doing such work. The subsequent implementation of end-member TC values for each of the 9 derived rock types, and the application of appropriate mixing models, is afflicted with additional uncertainties. Considering the range of TC values for specific sedimentary rock types known from textbooks (e.g. Schön, 2011), an uncertainty of at least 10–20% for the matrix TC values seems to be reasonable. The applied geometric-mean model, commonly used in petrophysical and geothermal studies of sedimentary rocks, is known as a good approximation of reality, but it is also known to produce additional uncertainties averaging around 10% (Fuchs et al., 2013). In contrast, use of well-log data allows calculating

representative formation values of TC with a smaller error, generally ranging between 5 and 10% (Fuchs et al., 2015). Taking this into account, smaller errors observed for *scenario D* compared to *scenario C* seems to be reasonable.

The insignificant differences between constant and lateral varying parameterized models for the initial model runs could be possibly explained considering the uncertainty introduced by the *scenario-C* parameterization (using bore logs). Taking the uncertainties of the initially determined TC values into account obviously balance the improvements of considering the lateral TC variability. In contrast, uncertainties of the *scenario-D* parameterization (using well logs) are small, thus the consideration of the spatial TC distribution excels the effect of constant TC parameterization even for the initial model.

The calibrated *scenario C* (model C_var_c; well logs, spatial TC distribution regionalized by kriging) shows a temperature uncertainty (full distribution width) of 12.5 °C (for a depth interval of 6 km) with a mean and a standard deviation of 1.6 ± 2.9 °C. This is remarkably similar to the results of Vogt et al. (2010), where a thermal model with a stochastically simulated spatial TC distribution (based also on well-log data), and constrained by temperature measurements, shows an uncertainty of 12 °C (full distribution width) around a specific depth of 2300 m (sd = 1.8 °C). Using well logs as input data, both regionalization approaches (kriging and stochastic approach) improve the modelling results significantly.

6. CONCLUSIONS

- (1) The source and quality of the TC parameterization clearly determine the uncertainty of the modelled temperatures. The parameterization from boreholes always prevails over the parameterization based on literature values, and it allows reducing the uncertainty of modelled temperatures by up to 80%. Thus we clearly recommend to use bore log data or even better well-log data for the parameterization of the model layer TC.
- (2) Including lateral variability of the formation TC (analyzed from borehole data) does have a highly significant uncertainty-reducing impact on the modelled temperatures. We recommend considering this effect in particular for regional or basin-wide models.
- (3) When models are calculated with laterally constant TC values for model units, the structural resolution and the amount of temperature observations included in the calibration procedure are more important than the quality of the original input data.

- (4) When models are calculated with laterally variable TC values derived from well-logging data, the structural resolution and the number of temperature observations used for the calibration procedure becomes less important.
- (5) Calibrating the model input by using the Gauss-Levenberg-Marquardt algorithm, implemented in FePest considerably improves the fit between modelled and measured temperatures. We conclude that the application of combined numerical forward and inverse calibration procedures, such as Feflow and FePest, are very well suited for solving geothermal heat transport problems.

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