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Effects of Transient Processes for Thermal Simulations of the Central European Basin

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Abstract. Transient processes play a major role in geophysical applications. In this paper, we quantify the significant influence arising from transient processes for conductive heat transfer problems for sedimentary basin systems. We demonstrate how the thermal properties are affected by changing the system from a stationary to an instationary system and what impact transient boundary conditions (derived from paleoclimate information) have. Furthermore, we emphasize the importance of time-stepping approaches and the simulation duration since both factors influence the sensitivities of the thermal properties. We employ global sensitivity analyses to quantify not only the impact arising from the thermal properties but also their parameter correlations. Furthermore, we show how the results of the sensitivity analysis can be used to gain further insights into the complex Central European Basin System. This computationally very demanding workflow becomes feasible through the construction of high precision surrogate models using the reduced basis method.

1 Introduction

A proper quantification of the thermal state of sedimentary basins is of primary interest for subsurface exploration studies. This is especially the case nowadays where systematic efforts are made worldwide to develop concepts of proof for low-carbon energetic solutions. Among others, geothermal resources buried in the underground of sedimentary basins and/or in volcanic areas are harvested either for their direct heating usage or for electricity generation (Fridleifsson, 2001; Fridleifsson et al., 2008; Glassley, 2014). However, the development of geothermal projects requires extensive and site-specific studies of the underground thermal regime, which can only be predicted within a certain degree of confidence due to limitations in available observables. Heat flow measurements, temperature logs, and thermochronological data provide the basic observations to characterize the evolution and spatial distribution of temperatures in the underground. However, these datasets are generally sparse and lacking in coverage to provide enough information for a proper assessment of available geothermal resources (Horváth et al., 2015; Schellschmidt et al., 2002). An alternative is to rely on process-oriented mathematical models that incorporate the details of the subsurface geology and the driving physics responsible for the observations done in the field.

On the scale of the whole lithosphere, heat conduction is the main heat transport mechanism. The effects of fluid mediated processes are usually less relevant if not locally. The regional thermal configuration of a conductive lithosphere reflects to a first-order the available heat in place. The latter depends on the tectonothermal configuration of the plate, which evolved through

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geological times under varying thermal loading conditions as provided by the underlying convective mantle, the amount of heat generated by dissipative processes within the plate (and therefore on the local geology), and, lastly, by the surficial climate conditions (Turcotte and Schubert, 2002). It has been long recognized that the near-surface temperature distribution can maintain a "thermal memory" of the past surface boundary conditions. If conduction is considered as the only active heat transport mechanism, a variation in surface temperature propagates downward with a signal attenuation that scales with the square root of the internal period times the thermal diffusivity of the plate (Turcotte and Schubert, 2002). Given common ranges of thermal rock properties, daily and annual surface temperature variations are damped down to a depth of few tens of meters and therefore believed not to affect the temperature at greater depths. The situation changes when considering long-term variations in surface temperature as occurring over a glacial cycle, which could potentially affect the temperature gradient down to significant depths (kilometers scale) (Turcotte and Schubert, 2002). Despite these observations, commonly, studies of the thermal state of the continental lithosphere consider steady-state conditions, the working assumption being that of instantaneous thermodynamic equilibrium under a spatially variable but constant in time set of loading conditions (Bayer et al., 1997; Noack et al., 2012; Freymark et al., 2017; Fuchs and Balling, 2016; Scheck-Wenderoth and Maystrenko, 2013). Transient effects, as due to fluid mediated processes and, as relevant for the current study, to long term surface temperature variations are generally considered to be of secondary relevance and as such has received so far little attention (Ebigbo et al., 2016; Freymark et al., 2019; Mottaghy et al., 2011; Noack et al., 2013). Corrections to a steady-state geotherm for paleoclimatic effects requires to account for time-varying surface boundary conditions. Such boundary conditions can be derived from available Earth System Models (ESM hereafter). This requires (i) an efficient transfer of information from a global to a (sub)regional resolution as typical for subsurface geothermal studies, and (ii) an analysis of the sensitivity of the parameters at play (i.e. rock thermal properties) within proper confidence intervals. Under steady-state conditions, model validation is generally achieved by manual "tuning" of the rock parameters (thermal conductivity and heat production) within specified ranges. However, the dimension of the parameter space for a transient system poses serious computational limitations. This aspect can explain why the sensitivity of transient processes on the regional thermal characteristics has never been neither investigated nor quantified.

It is the main goal of this study to demonstrate how to properly quantify the thermal state of a conductive lithosphere, including an in-depth and deterministic consideration of the sensitivity of the parameters at play as they can vary within proper confidence intervals. We will describe and discuss an automated, software-based workflow to achieve this goal, which also enables us to take into account transient boundary effects as derived from instance from paleoclimate reconstruction studies. Based on the developed workflow, we will demonstrate the relevance of such transients on the overall parameter sensitivity when compared to an analysis done under the assumption of steady-state thermal equilibrium.

The aim of the study is therefore to investigate the sensitivity of the regional thermal characteristic of a lithospheric plate while moving away from a stationary state representation. The approach enables then to quantify the effects of paleoclimate conditions on the current thermal state of sedimentary basins, with special focus on their influences on the rock thermal properties. The need to consider paleoclimate effects has been long recognized. However, so far, it has only been considered for correction of (1D) vertical temperature gradients (Clauser, 1984), while its influence on the thermal properties, such as thermal conductivity and radiogenic heat production, has never been investigated.

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In this paper, we present a global sensitivity analysis to determine, next to the impact of the thermal properties themselves, also whether the parameter correlations could be affected and to which degree by considering transient processes. Our choice of a global sensitivity analysis stems from the results of previous efforts by one of the co-authors, who has been successful in demonstrating how a local sensitivity analysis likely leads to overestimating the influence of the model properties on the same model response (Degen et al., 2020a).

Given the high computation demands of a global sensitivity analysis, we hereby rely on surrogate models. In this paper, we use the Reduced Basis (RB) method to construct our surrogate model. The RB method is a Model Order Reduction (MOR) technique that aims at significantly reducing the spatial and temporal degrees of freedom of, as applied in this study, finite element problem formulations. The RB method has been widely studied by, for example, Grepl and Patera (2005); Hesthaven et al. (2016); Prud'homme et al. (2002); Quarteroni et al. (2015) for mathematical benchmark examples, and for the first time by Degen et al. (2020b) in a geoscientific context. In this study, we make use of the RB method to guide the construction of the surrogate model since it allows, in contrast to other statistical methods including Kriging and response surfaces (Baş and Boyacı, 2007; Bezerra et al., 2008; Frangos et al., 2010; Khuri and Mukhopadhyay, 2010; Miao et al., 2019; Mo et al., 2019; Myers et al., 2016; Navarro et al., 2018), the retrieval of the entire state variable (i.e. temperature).

Our case study is the Central European Basin System (CEBS), a complex intracontinental basin in northern and Central Europe, being of interest for both past hydrocarbons and, currently low enthalpy geothermal exploration (Maystrenko et al., 2013; Scheck-Wenderoth and Maystrenko, 2013), and Scheck-Wenderoth et al. (2014).

The paper is structured as followed: In Section 2, we briefly introduce the concepts of the global sensitivity study, the governing equations, and the paleotemperature data. The results of the steady-state analyses, the influence of transient boundary conditions, and transient processes are described of Section 3. This is followed by the discussion of the results in Section 4 and a conclusion in Section 5.

2 Materials and Methods

In the following, we briefly introduce the methodology of the sensitivity analyses used throughout this paper. Details regarding the global sensitivity analysis are presented in (Sobol, 2001; Saltelli, 2002; Saltelli et al., 2010), while the study by Wainwright et al. (2014) described a comparison based on either local or global sensitivity analyses. The applicability and benefits of relying on global sensitivity analyses for applied basin-scale thermal models have been discussed in detail in a previous study by (Degen et al., 2020a). In a subsequent paragraph, we also provide the system of partial differential equations used for the forward modeling of the steady-state and transient conductive heat transfer.

2.1 Global Sensitivity Analysis

The global sensitivity analysis is done by relying on the SALib Python library (Herman and Usher, 2017). We make use of the Sobol sensitivity analysis with a Saltelli sampling routine (Sobol, 2001; Saltelli, 2002; Saltelli et al., 2010). This was done because the Sobol sensitivity analysis is variance-based and returns, in contrast to a local analysis, also parameter correlations

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(Sobol, 2001). To avoid statistical errors, as higher first-order than total-order contributions, we use 100,000 realizations per parameter for the steady-state and 10,000 for the transient analyses.

As the quantity of interest, we hereby define the total amount of heat available in the model (steady-state analyses), and the total amount of heat available in the model over all time steps considered (transient analyses). Our choice enables us to quantify the influence of the paleotemperatures on the physical processes being investigated. Worth mentioning at this stage, that the focus of the current study paper is not to provide an overall fit to available measurements. This is why we do not use, as commonly done, the misfit between measurements and simulated temperatures as our quantity of interest. This is also the main reason behind our choice to employ the RB method for the surrogate model construction. Many other methods (Baş and Boyacı, 2007; Bezerra et al., 2008; Frangos et al., 2010; Khuri and Mukhopadhyay, 2010; Miao et al., 2019; Mo et al., 2019; Myers et al., 2016; Navarro et al., 2018) construct surrogate models for the observation space only. This entails that every value outside this space has to be obtained via inter- and extrapolation routines, Therefore these approaches share the disadvantage of not taking the physical laws describing the process of interest into consideration. These limitations would have severely impacted the current study that focuses on understanding the effects of the physical processes of heat transport on the resulting thermal and parameter state of the lithosphere rather than on crude fit of temperature values at certain measurement locations. In other words, our interest here is on the entire temperate state of the plate. Our surrogate model proves useful in our efforts since it is by definition physics-preserving. This to say that we can retrieve temperature values at every location in the model and, thus can determine the relevance of all thermal properties as relevant for the physics at play, steady/transient heat conduction. For further information regarding the global sensitivity analysis, we refer to Sobol (2001) and for the sampling routine to Saltelli (2002); Saltelli et al. (2010). A comparison between local and global sensitivity analyses is provided in Wainwright et al. (2014) for hydrological models and in Degen et al. (2020a) for a basin-scale geothermal model.

2.2 Forward Problem

In order to improve the efficiency of the solvers and to investigate the relative importance of rock thermal properties on the resulting thermal configuration, we make use of adimensional forms of all relevant equations in this study.

In this paper, we consider both steady-state and transient conductive heat transfer simulations. For the steady-state conductive heat transfer, we take the radiogenic heat production as the source term into account (Turcotte and Schubert, 2002). Following the derivation presented in Degen et al. (2020a), we obtain:

$$-\frac{\lambda}{\lambda_{\text{ref}}\, S_{\text{ref}}}\,\frac{\nabla^2}{l_{\text{ref}}^2}\,\left(\frac{T-T_{\text{ref}}}{T_{\text{ref}}}\right) + \frac{S\, l_{\text{ref}}^2}{S_{\text{ref}}\, T_{\text{ref}}\, \lambda_{\text{ref}}} = 0, \tag{1}$$

where λ is the rock thermal conductivity, T the temperature, S the radiogenic heat production, λ_{ref} the reference thermal conductivity, T_{ref} the reference temperature, S_{ref} the reference radiogenic heat production, and l_{ref} the reference length.

Following a similar procedure, we can derive the following adimensional partial differential equation (PDE) for the transient case:

$$-\frac{\alpha}{\alpha_{\text{ref}}\, S_{\text{s,ref}}}\,\frac{\nabla^2}{l_{\text{ref}}^2}\,\left(\frac{T-T_{\text{ref}}}{T_{\text{ref}}}\right) + \frac{S\, l_{\text{ref}}^2}{S_{\text{s,ref}}\, T_{\text{ref}}\, \alpha_{\text{ref}}} = \frac{\partial \frac{T-T_{\text{red}}}{T_{\text{ref}}}}{\frac{t}{t_{\text{ref}}}}, \qquad \text{with } t_{\text{ref}} = \frac{l_{\text{ref}}^2}{S_{s,\text{ref}}\, \alpha_{\text{ref}}} \tag{2}$$

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Here, α is the diffusivity , S_s the specfic radiogenic heat production, t the time, α_{ref} the reference diffusivity, $S_{\text{s,ref}}$ the reference specific heat production, and t_{ref} the reference time.

2.2.1 Surrogate Model Construction

The surrogate model used in this study is based on the RB method. RB is a model order reduction method, aiming at finding low dimensional representations for the high dimensional finite element simulations, which we are considering in this study. In inverse processes, such as global sensitivity study we need to perform the forward simulations many times with varying rock properties. Due to the high number of forward solves, the problem becomes computationally too demanding if we use the high fidelity finite element forward simulation. Instead, the idea is to "train" a model that is representative of a pre-defined range of rock properties. This trained model is a low dimensional representation of our original finite element problem. Note that we simplify the model in the mathematical instead of the physical domain. This means that we avoid introducing errors through, for instance, simplifying the physics or considering a smaller spatial and or temporal domain.

The RB method is subdivided into an offline and online phase. During the offline phase, performed only once, the surrogate model is constructed. All expensive computations take place during this stage only. Based on this offline stage, we can then use the developed surrogate model in outer loop processes, such as global sensitivity analysis. Simulations using this reduced model are part of what is referred to as an online stage. Further information regarding the RB method can be found in (Hesthaven et al., 2016; Prud'homme et al., 2002).

We generate all reduced models with the software package DwarfElephant (Degen et al., 2020b). DwarfElephant is based on the Multiphysics Object-Oriented Simulation Environment (MOOSE), a state-of-the-art finite element solver primarily developed by the Idaho National Laboratory (Alger et al., 2019). The setup and construction of the reduced model are analog to the one described in Degen et al. (2020a) and here omitted for the sake of clarity.

2.3 Paleoclimate Boundary Condition

The paleotemperature data (Fig. 1) that serves as an input for our transient boundary condition investigation has been simulated using the Max-Planck-Institute Earth System Model (MPI-ESM) (Giorgetta et al., 2013). The MPI-ESM uses the exchange of energy, momentum, water, and carbon dioxide to couple the atmosphere, the ocean, and the land surface. For the atmosphere it is based on ECHAM6 (Stevens et al., 2013), for the ocean on MPIOM (Jungclaus et al., 2013), for the ocean's biogeochemistry on HAMOCC (Ilyina et al., 2013), and for the terrestrial biosphere on JSBACH (Giorgetta et al., 2013).

The data has been simulated with truncation of T31, which measures the horizontal resolution of the atmospheric model. For the ocean resolution, the GR30 model has been used. Furthermore, time-dependent topographic changes and river routing were considered in the generation of the paleoclimate temperatures.

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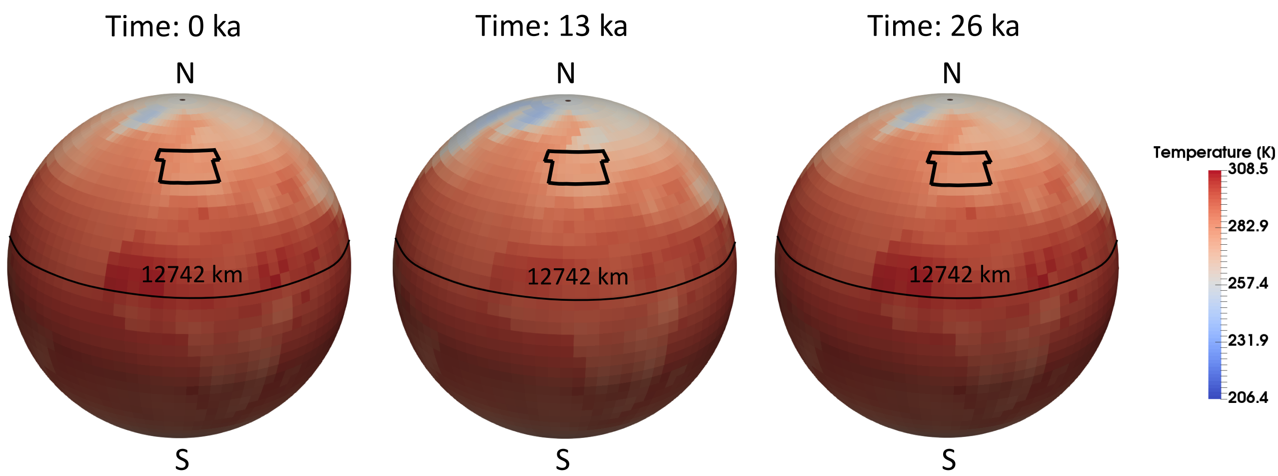

Figure 1. Paleotemperature data from the Max-Planck Institute Earth System Model for the timesteps 0 ka, 13 ka, and 26 ka. The black rectangle represents the outline of the surface temperatures used for the transient simulations of the CEBS model.

3 Central European Basin System

The study area is the Central European Basin System (CEBS) in northern and Central Europe, for which a detailed 3D lithosphere-scale geological model is available (Maystrenko et al., 2013; Scheck-Wenderoth and Maystrenko, 2013; Scheck-Wenderoth et al., 2014). The model has a lateral extent of 1784x1060 km, and covers the whole sedimentary sequence, upper and lower crust and the underlying mantle lithosphere down to the lithosphere-asthenosphere boundary (LAB).

To close the system of equations 1 or 2 requires to assign proper boundary conditions. Throughout, the entire paper, we apply both at the upper and lower model boundaries Dirichlet-type first-order boundary conditions. The lower boundary condition corresponds to the 1300 °C isotherm (Turcotte and Schubert, 2002). Values imposed along the upper boundary differ for each analysis and will be discussed in the respective sections.

3.1 Steady-State

In the following, we illustrate the influence of the thermal properties on the temperature distribution under a steady-state conductive thermal regime. In order to reduce the number of thermal properties that need to be investigated, we make a selection through various global sensitivity analyses for the steady-state conductive heat transfer. Therefore, the obtained results will serve as a basis for the analyses that will be done in the following chapters. As the upper boundary conditions, we choose 8 °C, corresponding to the annual average surface temperature in the region.

First, we focus our investigation on the sedimentary layers. Hence, we only vary the thermal properties for the Cenozoic, Cretaceous, Jurassic, Triassic, Zechstein, Rotliegend, Permo-Carboniferous Volcanics, and Pre-Permian Rocks. All other thermal properties are kept constant, the values of which are derived from previous studies. Fig. 2 shows the respective first- and total

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order indices. We observe that most contributions are first-order contributions and that the parameter correlations are indeed negligible. Overall, we have a higher influence resulting from variations in thermal conductivity than from radiogenic heat production values.

To narrow down the parameter space for further investigations, we make use of the five most influencing thermal conductivity and radiogenic heat production values (blue boxes in Fig. 2). We are interested in including the radiogenic heat production in our analysis despite its minor influence since we aim to investigate conceptual behavior changes induced by including paleo-climate information.

Hence, for the thermal conductivity, we consider the Cenozoic, Cretaceous, Jurassic, Triassic, and Pre-Permian Rocks. The thermal conductivity of the Cenozoic has the highest influence, followed by the thermal conductivity of the Cretaceous. The thermal conductivity of the Pre-Permian Rocks is slightly lower and the lowest sensitivity is found for the Jurassic and Triassic sediments.

In terms of heat production, the most influencing layer is the Pre-Permian Rocks sedimentary layer, followed by the Triassic sequence. The radiogenic heat production of the Cretaceous and the Cenozoic have a similar sensitivity, being significantly lower than for the sedimentary layers discussed above. The lowest sensitivity in terms of radiogenic heat production that we integrate into the analysis is associated with the Jurassic layer.

We repeat the same analysis but considering thermal property variations in the crustal and mantle layers only. Therefore, we keep the thermal properties of the sedimentary layers as fixed and constant. The results are shown in Fig. 3. Overall, we observe analog to the previous analysis that the thermal conductivity has a higher influence than the radiogenic heat production. However, the difference in their influence is significantly lower. Again, the parameter correlations are negligible. For the crustal layers, we chose the three most influencing ones as based on thermal conductivity and radiogenic heat production values for further analyses.

For the thermal conductivity, we consider the Upper Crust Baltica and Avalonia, and the Lithospheric Mantle. Here, the Upper Crust Baltica has the highest influence followed by the Upper Crust Avalonia. The Lithospheric Mantle has the lowest influence.

In the case of the radiogenic heat production, the highest influences are found within the Upper Crust Avalonia, followed by the Upper Crust Baltica. Furthermore, we consider the radiogenic heat production of the Lower Crust for further analyses. So far, our analysis has been based on sub-grouping the relevant units into either sedimentary layers of crustal-mantle domains. Therefore, we did not investigate any possible parameter correlations among them. This is done in the following, where we systematically vary the most prominent thermal properties in both the sediments and the crust-mantle as derived from the previous analysis. The results are shown in Fig. 4.

We observe that the thermal conductivity of the Lithospheric Mantle is the most influencing thermal property, followed by the thermal conductivity of the Triassic sedimentary unit. The latter has a relevance similar in magnitudes to the Upper Crust Baltica and Avalonia. Also important are the thermal conductivities of the Cenozoic and Cretaceous. The two most important layers in terms of radiogenic heat production are the Upper Crust Baltica and Avalonia. Given the results obtained so far, we decided to focus on these eight parameters in the following analyses.

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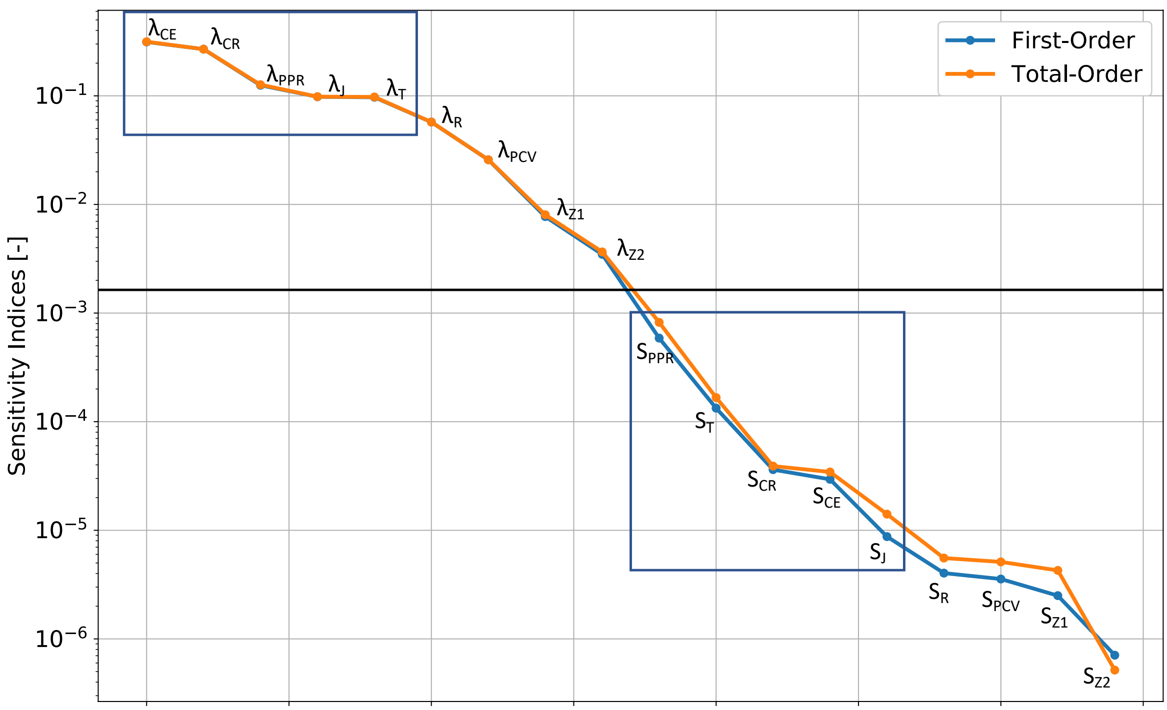

Figure 2. Global sensitivity indices for the analysis focussing on the sedimentary layers of the CEBS. The first-order indices are denoted in blue and the total-order indices in orange.

3.2 Impact of Solver Accuracy

In the previous section, we determined the impact of the various thermal properties for the steady-state case, here considered as the “base” case for all further analyses. In addition, the investigation carried out so far, have enabled us to narrow down the parameter space on which to focus the remaining part of the study.

Before moving to the investigation of the influences of transient processes on the model response, we would like to briefly discuss the relevance of the accuracy chosen for the reduced model. For the steady-state simulations, all reduced models were constructed with an accuracy of $5 \cdot 10^{-4}$. Such a value ensures that the reduced models have a higher accuracy than typical temperature measurements. Since these measurements have been used in previous works (Maystrenko et al., 2013; Scheck-Wenderoth and Maystrenko, 2013; Scheck-Wenderoth et al., 2014) to validate the model, we cannot infer any information below that accuracy. Therefore, for this specific case, the reduced and full model are equivalent to, for instance, parameter estimations and global sensitivity studies.

The RB method considers time as an additional parameter (Hesthaven et al., 2016), which leads to a higher dimensional parameter space moving from a steady-state to a transient analysis. Besides, in a transient study, the system must be solved for each time step. Consequently, if we can assume a similar parameter complexity for the thermal model parameters, both the

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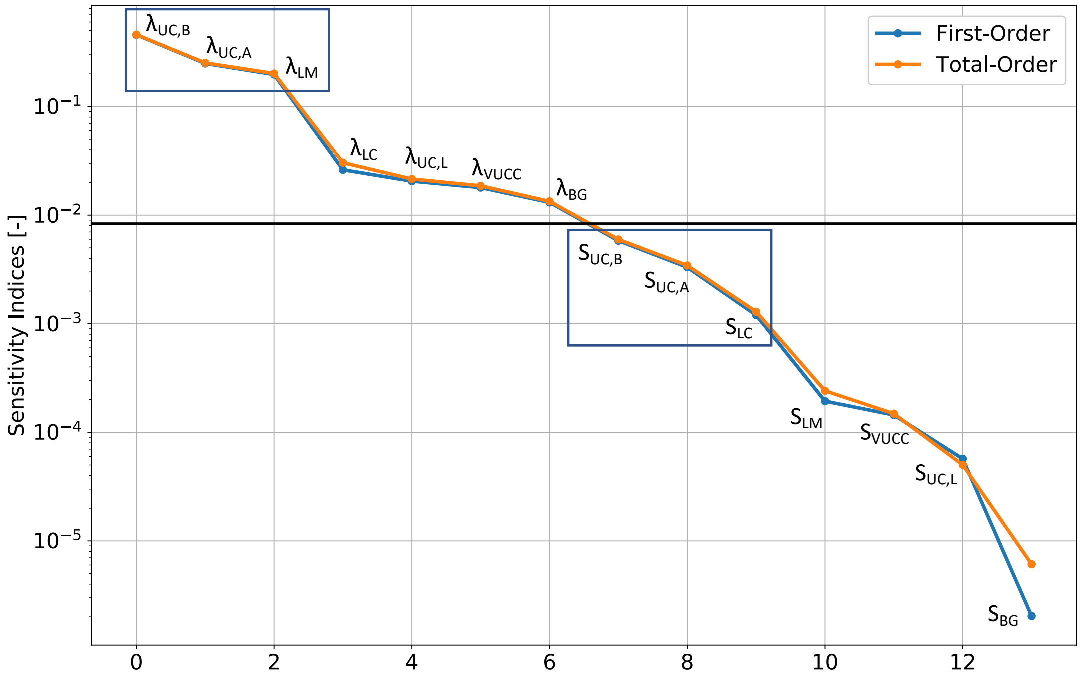

Figure 3. Global sensitivity indices for the analysis focused on the crustal layers of the Central European Basin System. The first-order indices are denoted in blue and the total-order indices in orange.

dimension of the reduced model and the compute time for each individual basis function will increase for the transient case. This, in turn, translates into higher compute time for the sensitivity analyses.

We can compensate for this by relaxing the accuracy used in the reduced models, $4{\cdot}10^{-3}$ for the transient case. By utilizing such an accuracy, we are still able to obtain reduced models that have an error in the same order of magnitude as the temperature measurements, However, with a significantly lower computational cost. We must note that, by doing so, it is also possible that we introduce an additional error source. Sensitivity analyses are based on the relative changes induced by model parameter variations. Since all simulations are similarly affected by the chosen accuracy, we can maintain the relative differences for the different accuracy levels (see Fig. 5). Therefore, the accuracy loss can be considered insignificant.

To prove this point, we perform a sensitivity analysis focused on the sedimentary layers only by varying the adopted accuracy within the above-discussed bounds. As Fig. 5 displays, the results are the same for all accuracies tested of the reduced model. Differences occur but are only limited to the parameters having the lowest sensitivity. However, these parameters must be excluded from the discussion since their errors of the sensitivity analyses are higher than their actual first- and total-order contributions. Also, the observed difference can likely be induced by the Sobol sensitivity analysis itself.

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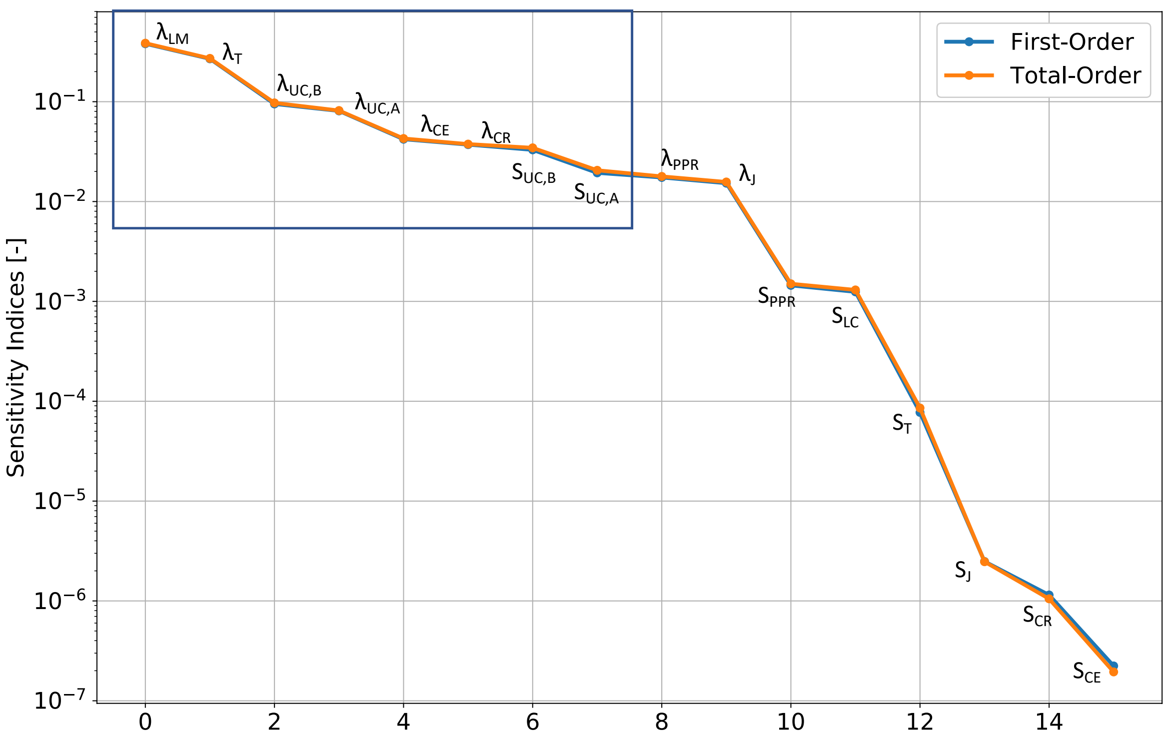

Figure 4. Global sensitivity indices for the analysis combining sedimentary and crustal layers of the Central European Basin System. The first-order indices are denoted in blue and the total-order indices in orange.

Based on what stated above, we can conclude that, for the remaining analyses, we can make use of reduced models with a lower accuracy, thus having faster construction times of the reduced model and a less demanding sensitivity analyses.

3.3 Paleoclimate

To include paleotemperature corrections to the steady-state results presented so far requires to move towards a transient system. Therefore, a first investigation deals with studying the global influence from this system change, by means of a global sensitivity analysis where we consider a transient case, but no paleoclimate influence (Fig. 6 branch 1a).
Only after having been able to quantify the influence of considering transient processes on the sensitivity of the thermal properties, we could investigate the effect of the sensitivity of the system response to adopting transient boundary conditions to incorporate paleotemperature information into basin-scale models (Fig. 6 branch 1b). In the following, we explain in detail how we account for paleoclimate corrections and which impact such corrections have on the respective sensitivities of the thermal rock properties.

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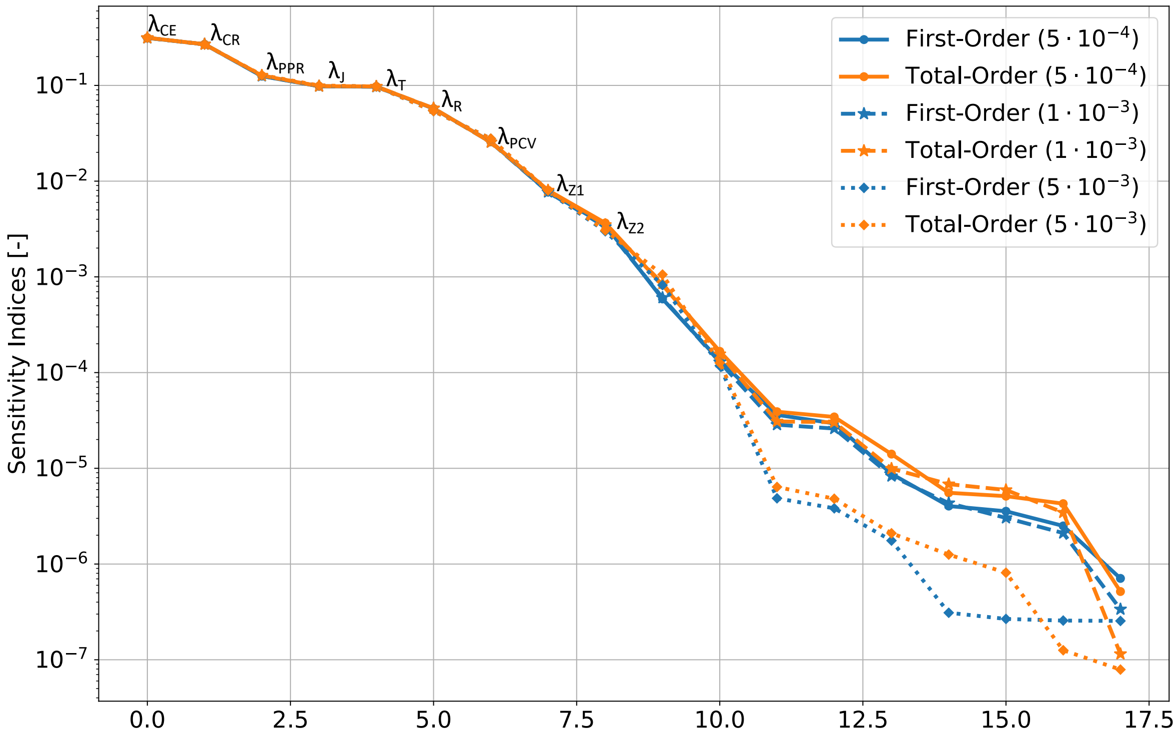

Figure 5. Global sensitivity indices for the analysis focused on the sedimentary layers of the Central European Basin System for an accuracy of the reduced model of $5{\cdot}10^{-4}$ (solid lines), $1{\cdot}10^{-3}$ (dashed lines), and $5{\cdot}10^{-3}$ (doted lines). The first-order indices are denoted in blue and the

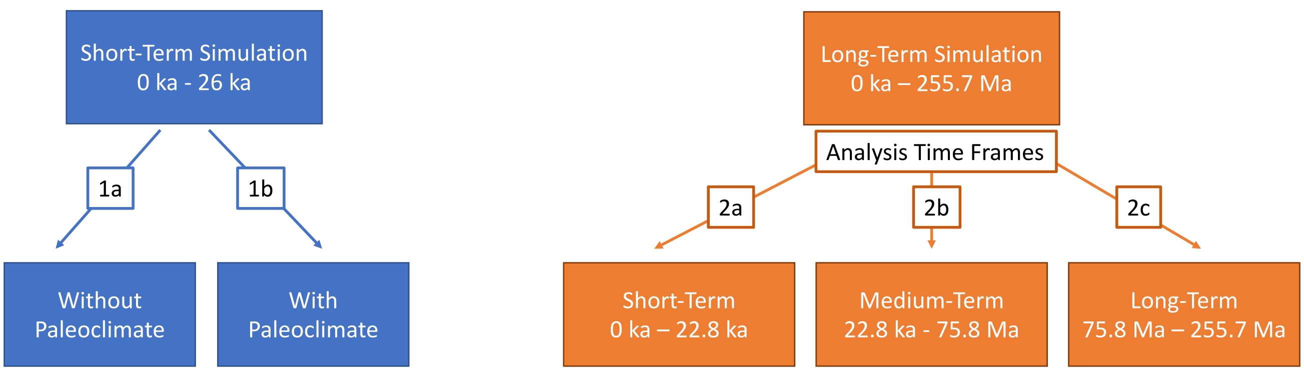

Figure 6. Schematic overview of the transient models.

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3.3.1 Short-Term Transient Processes

For determining the impact of a transient simulation, we make use of a constant upper boundary conditions, Dirichlet type of 1.6 °C (Fig. 6 branch 1a). This corresponds to the average (in space and time) temperature derived from the reconstructed paleotemperatures for the CEBS model area. We, therefore, simulate the system under such thermal loading for 26,000 years which is equal to the time frame for which reconstructed paleotemperatures are available. We adopted a constant time step size of 200 years. As the quantity of interest, we use, as for all following analyses, the total amount of heat in the model cumulative over all time steps.

Fig. 7 compares the sensitivities of the thermal properties for the steady-state and transient system. We observe that both the overall differences in the influence of the individual thermal properties and the parameters correlations increase. The Cenozoic and Cretaceous sedimentary layers gain significantly in importance, while the Triassic sediment maintains an influence similar in magnitudes as for the steady-state case. The Upper Crust is less significant in terms of both the diffusivity and the specific radiogenic heat production. The most extreme change is observed for the diffusivity of the Lithospheric Mantle which, for the steady-state runs, had the highest influence, but for the transient case one of the lowest. To sum up, we can observe a systematic change in the system response with the sedimentary layers gaining in importance, whereas the deeper crustal and mantle becoming less sensitive.

Regarding the correlations, we observe the strongest correlation between the diffusivities of the Cenozoic and Cretaceous sediments, followed by the correlation between the diffusivities of Cretaceous and Triassic sediments. An aspect that is in agreement with the findings described above.

3.3.2 Data Fit

Prerequisite to investigate the influence of paleoclimate corrections on the thermal properties is a proper quantification of the sensitivity of the same thermal properties with respect to changes in the imposed upper boundary conditions. This is indeed needed to rule out possible sources of uncertainty.

To properly quantify the influence on uncertainties in adopted paleotemperatures on the thermal properties of the different layers, we derive a first-order trend in surface temperature over time. These uncertainties are arsing from both temporal and spatial effects. The spatial uncertainties are mainly caused by the low resolution of the paleoclimate data set. For the derivation of the trend, we first focus on the past temperature distribution for all computational points of the global ESM analysis lying inside the CEBS area (black lines of Fig. 8). By inspecting Fig. 8, it can be noticed how all considered points follow a similar trend. Therefore, we can consider the average of all data points as a good representation, and make use of it in the following to derive the paleotemperature trend to be imposed as time-varying boundary condition. We fitted the paleotemperatures by a fourth-order polynomial (black line in Fig. 9), using the Python library SciPy (Jones et al., 2014). The final polynomial fit has the following form:

$$4.3 \cdot 10^{-8} t^4 - 2.7 \cdot 10^{-5} t^3 + 5.4 \cdot 10^{-3} t^2 - 2.8 \cdot 10^{-1} t - 3.6 \quad (3)$$

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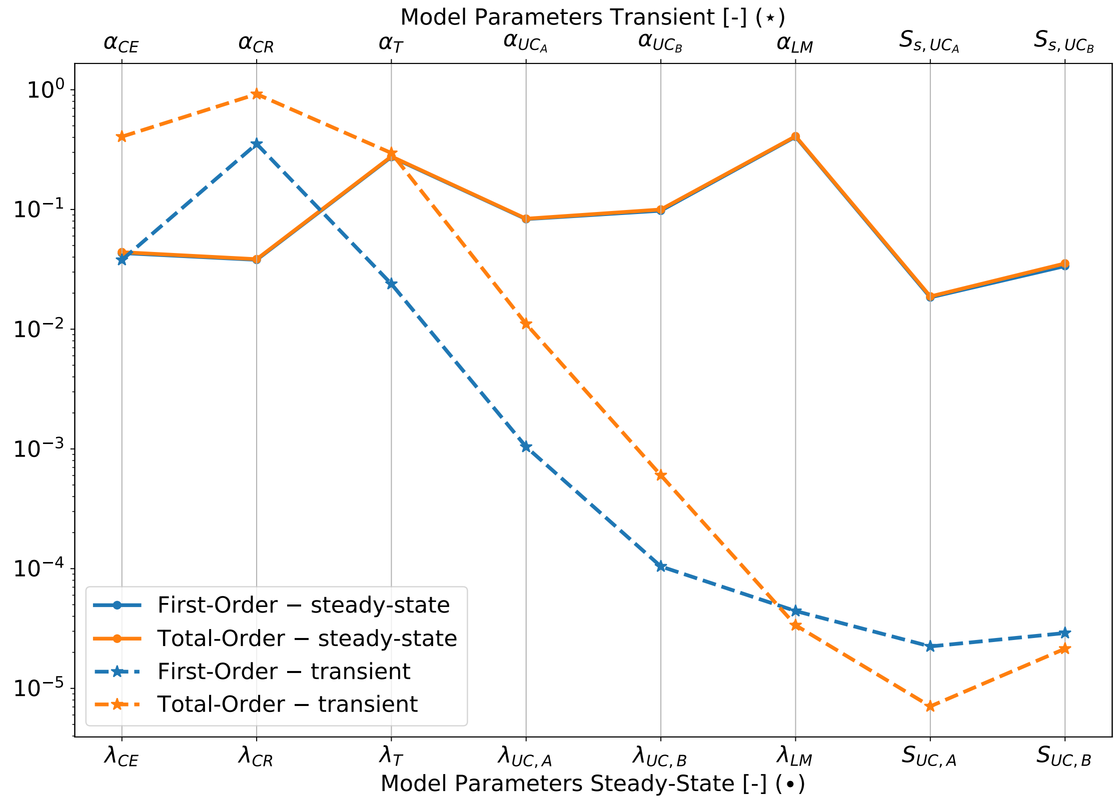

Figure 7. Global sensitivity indices for the analysis with steady-state (solid lines) and transient conditions (dashed lines) of the Central European Basin System. The first-order indices are denoted in blue and the total-order indices in orange.

We have tested additional polynomial degrees and found that, while a third-order polynomial (blue line Fig. 9) cannot recover the paleotemperature pattern, a fifth-order polynomial (green line Fig. 9) does not significantly improve the fit in comparison to the fourth-order polynomial. To investigate how sensitive the thermal properties are for uncertainties of the upper boundary condition, we allow a variation of the upper boundary condition that increases with time. We, therefore, adopted a time increasing scaling factor, under the assumption that the uncertainties in the reconstructed temperatures should decrease while approaching present-day conditions. To derive the magnitude of the scaling parameter, we use the spatial distribution of the surface temperatures over time. In this way, we allow any physically plausible surface temperature variation. The results are shown in Fig. 10. In a subsequent step, the trend has been normalized to the present-day surface temperature and applied to each point of the computational grid separately. This permits us to resolve the spatial distribution of the surface temperature. The displayed temperature lines represent during the glaciation times the temperature on top of the ice sheet. Hence, we would normally need to correct the temperatures to obtain the values at the bottom of the ice sheet. Note that by applying a fourth-

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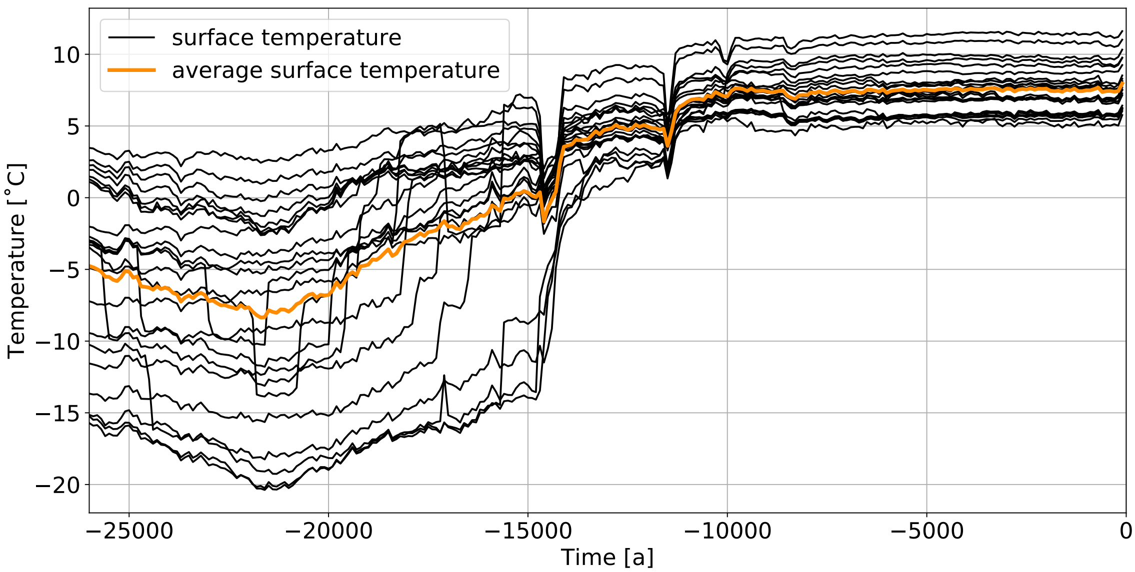

Figure 8. Paleotemperature reconstruction for all reconstruction points inside the CEBS model (denoted in black). Furthermore, we plot the average of all data points in orange.

order polynomial fit, we already implicitly account for this. By applying, in addition, a scaling factor of time, we account for all possibly remaining correction terms.

3.3.3 Transient Boundary Condition

In Fig. 11 we compare the transient simulation with a constant upper boundary condition (solid lines – Fig. 6 branch 1a) and with a time-dependent (paleoclimate correction) boundary condition (dashed lines – Fig. 6 branch 1b). We observe for the first four thermal properties (diffusivity of the Cenozoic, Cretaceous, Triassic, and Upper Crust Avalonia) no significant changes for either the first- or total-order contributions between the two models. All remaining parameters have insignificant first- and total-order contributions. Note that we cannot discuss the difference between the two models for these remaining parameters because the errors in their sensitivities are higher than the sensitivities themselves. Furthermore, it is interesting to note that the scale factor, which we used as a measure of the uncertainty of the upper boundary condition, has one of the lowest sensitivities.

3.4 Transient Processes

So far, we have limited our analysis to short-term transient processes (Fig. 6 branch 1) and their sensitivities of the thermal properties. In this section, we focus on the long-term period (Fig. 6 branch 2). Therefore, we increase the simulation time

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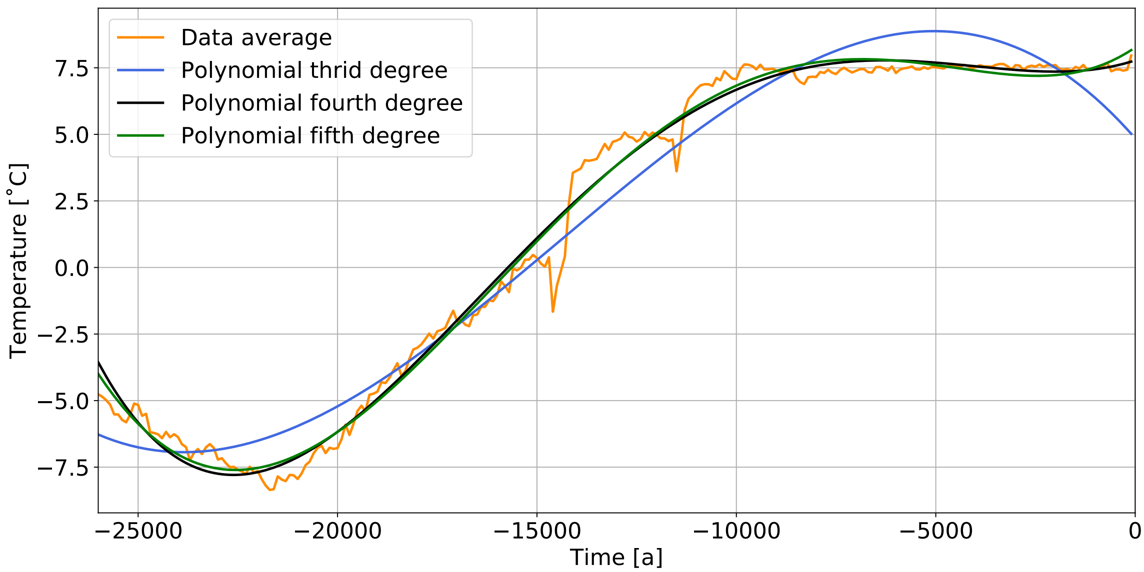

Figure 9. Trend for the paleotemperature upper boundary condition of the CEBS model.

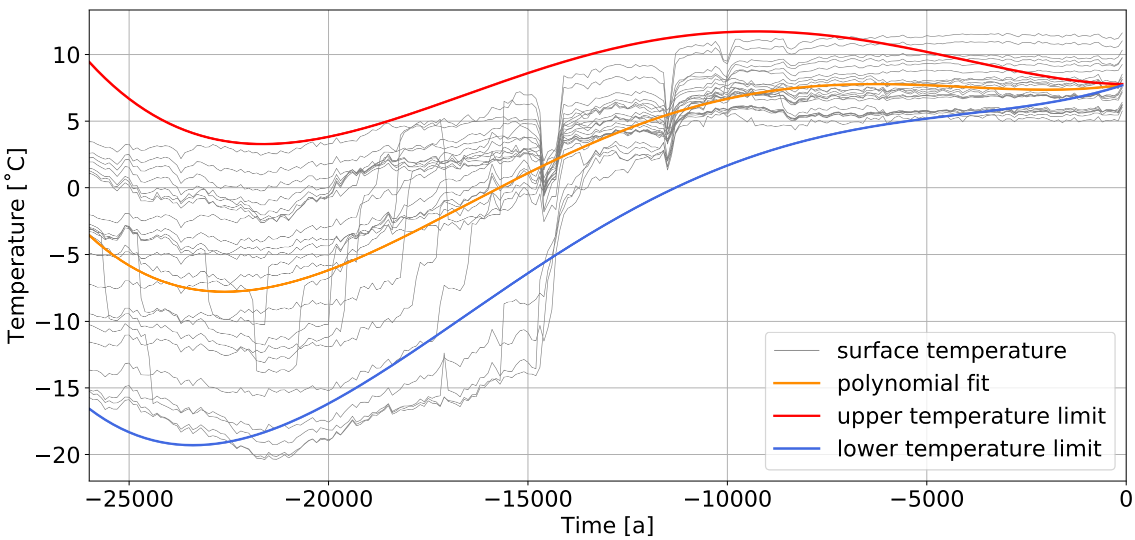

Figure 10. Trend for the paleotemperature upper boundary condition of the CEBS model.

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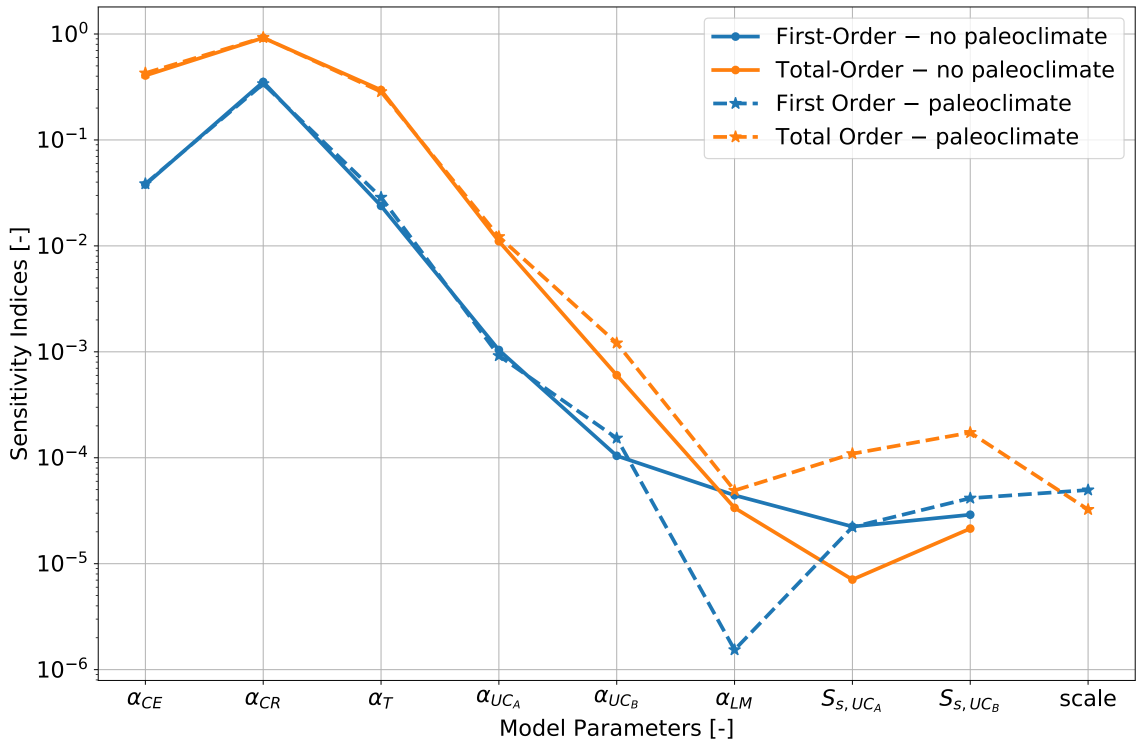

Figure 11. Global sensitivity indices for the analysis including paleotemperature information for the upper boundary condition. The first-order indices are denoted in blue and the total-order indices in orange.

from 26 ka to 255.7 Ma. To maintain affordable computing time, we adopted a different time discretization, where the initial time step of 2 ka increases linearly by a factor of 1.5 upon each successful transient run. We perform four sensitivity analyses considering: i) the entire time period, and the periods between ii) 0 ka and 22.8 ka (Fig. 6 branch 2a), iii) 22.8 ka and 75.8 Ma (Fig. 6 branch 2b), and iv) 75.8 Ma and 255.7 Ma (Fig. 6 branch 2c).

First, we discuss the results considering the whole simulation time. A second discussion point would be on how the sensitivities evolve. By comparing the total-order contributions among all analyses, we can observe that the diffusivities of the Cenozoic, Cretaceous, Triassic, and Upper Crust Avalonia have a similar contribution despite the time window adopted. For the remaining parameters, the long-term total-order contributions are between the short-term and steady-state total-order sensitivities. Except for the diffusivity of the Upper Crust Baltica, all thermal parameters have long-term contributions close to their short-term, but they do differ with respect to the steady-state contributions.

In terms of correlations, we observe a slight decrease in the correlations concerning the short-term analysis. Still, the corre-

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lations are significantly higher than those observed for the steady-state scenario. The highest correlations occur between the diffusivities of the Cenozoic and Cretaceous sediments and between the diffusivities of Cretaceous and Triassic units.

Overall, the main influences can be noticed for the diffusivities of the sedimentary layers. However, the diffusivities of the crustal layers are significantly increased with respect to the short-term analysis. The influence of the diffusivity of the Lithospheric Mantle and the radiogenic heat production remains negligible in all cases. In addition to the consideration of the entire

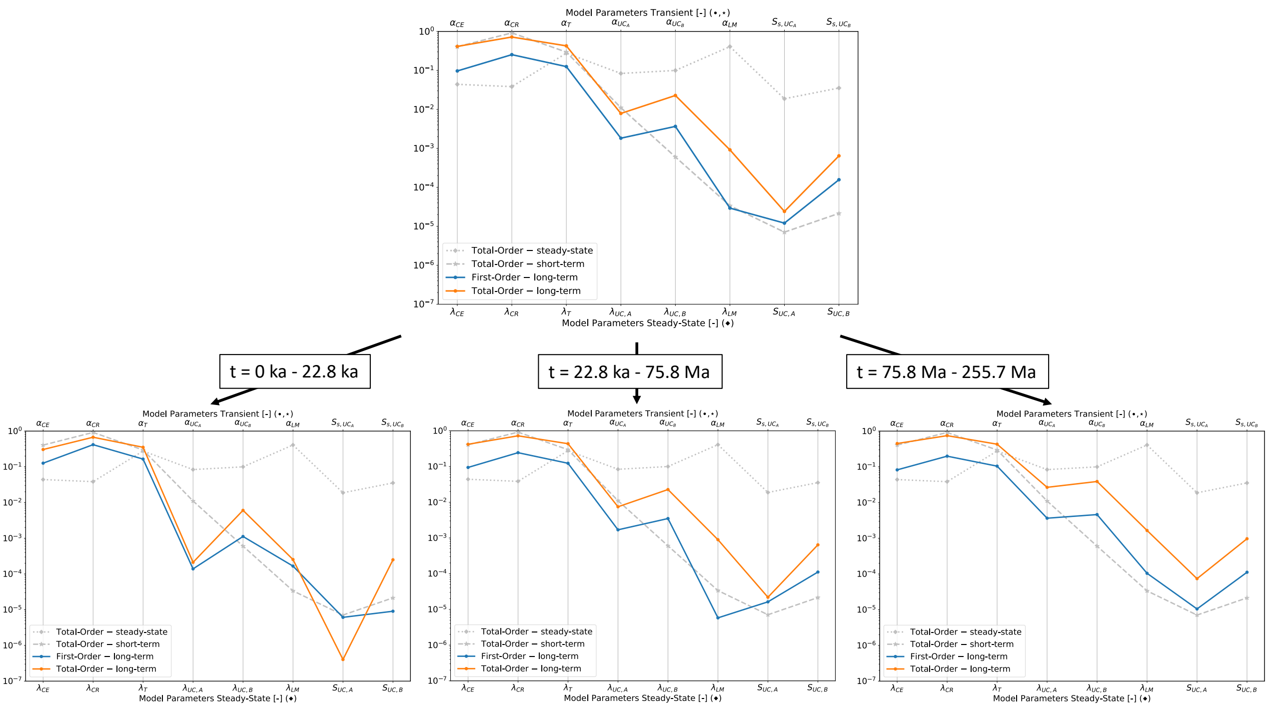

Figure 12. Global sensitivity indices for the analysis considering a simulation time of 255.7 Ma. The first-order indices are denoted in blue and the total-order indices in orange. Additionally, the total-order indices of the short-term (dashed gray line) and steady-state analyses (doted gray line) are plotted.

simulation time frame, it is interesting to investigate how the sensitivities evolve throughout the simulation within specified time windows. Therefore, we subdivided the whole time frame into three different windows. The first period (Fig. 6 branch 2a), from 0 ka to 22.8 ka corresponds to the short-term analysis presented in Section 3.3.1. The results are very similar, where only the crustal diffusivities showing some major changes. The diffusivity of the Upper Crust Avalonia has lower indices, whereas the Upper Crust Baltica has higher sensitivity indices. Furthermore, the correlations are in general smaller. Again the highest correlations occur between the diffusivities of the Cenozoic and Cretaceous sediments, and between the diffusivities of Cretaceous and Triassic.

We observe a significant change from the first to the second period (22.8 to 75.8 Ma, Fig. 6 branch 2b). The influence of the crustal diffusivities and the Lithospheric Mantle significantly increases, this is especially the case for the Upper Crust Avalo-

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nia. Also, the crustal radiogenic heat productions gain in importance. In contrast, no changes can be noticed in the sensitivities indices of the sedimentary diffusivities. Overall the sensitivity indices still follow the trend of the short-term analysis. At the same time, the parameter correlations are also similar to those obtained for the first period. For the second period considered, we can conclude that while the crustal layers gain in importance, the sedimentary layers do not show any systematic variations. Moving to the third and last period (75.8 Ma to 255.7 Ma, Fig. 6 branch 2c), we again observe some significant changes. The thermal properties of the Upper Crust become more important as well as the diffusivity of the Lithospheric Mantle, which has now higher sensitivity indices. In contrast, the crustal diffusivities resemble those of the steady-state analysis. The sensitivity indices of the sedimentary layers remain unchanged. The highest parameter correlation can be found among the diffusivities of the Cenozoic and Cretaceous sediments.

4 Discussion

In the following, we open a discussion on the results obtained for the steady-state model and those found while considering a transient system. Note that all results of the sensitivities analyses presented are highly dependent on the quantity of interest chosen. Therefore, we must call for caution while discussing these results and use comparable quantity of interests throughout the entire paper.

4.1 Steady-State

The sensitivities of the steady-state model are mainly controlled by a combination of the volumetric contributions of the individual layers and their thermal properties. Generally, the thermal conductivity has a significantly higher influence on the total amount of heat than the radiogenic heat production, which does follow our expectations. The only layers for which the radiogenic heat production has some significant influence are the Upper Crust layers. For the sediments, the differences between the relevance of the role of the thermal conductivity and the radiogenic heat production are higher than for the crustal layers. This is caused by the higher radiogenic heat production of the latter rocks.

Lower thermal conductivities yield a higher impact on the model response since a lower thermal conductivity results in a larger amount of heat stored within a layer, i.e. blanketing thermal effect. This is also the reason why the Zechstein layers have a smaller impact although being relatively thicker than the other sedimentary units. In contrast, the Lithospheric Mantle has a relatively prominent influence although it has a high thermal conductivity. This is because this layer counts for most of the total system volume.

Higher heat production values yield a higher influence since they result in a larger amount of generated heat. That is the reason why the influence of the Upper Crust is so significant.

The steady-state analyses have only negligible higher-order contributions, as apparent by the difference between the first- and total-order contributions. This means that we have no significant parameter correlations.

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4.2 Paleoclimate

In the following, we use the steady-state sensitivities as our "base" scenario and discuss the results of the transient case only concerning relative changes with respect to the latter scenario.

4.2.1 Short-Term Transient Processes

Considering a simulation time of 26,000 years (short-term window, Fig. 6 branch 1a), we observe that the model response is most sensitive to the diffusivity of the sedimentary layers. Both the diffusivity of the crustal and mantle layers and their radiogenic heat production do not influence the model response. This can be related to having considered a finite temporal extent. Given the thermal properties typical of crustal and mantle rocks, and their respective thickness, thermal equilibrium cannot be reached within the allotted time of 26,000 years (Fig. 13). Heat transfer occurs mainly in the uppermost layers (closer to the surface boundary conditions), hence their great impact. As demonstrated by the steady-state analyses, the radiogenic heat production in these layers does not have a significant influence. Given the short time window considered, imposed variations in the surface boundary conditions could not diffusive into the crust. Therefore, the model is relatively insensitive to any variations in either the diffusivities or radiogenic heat production for those deeper layers.

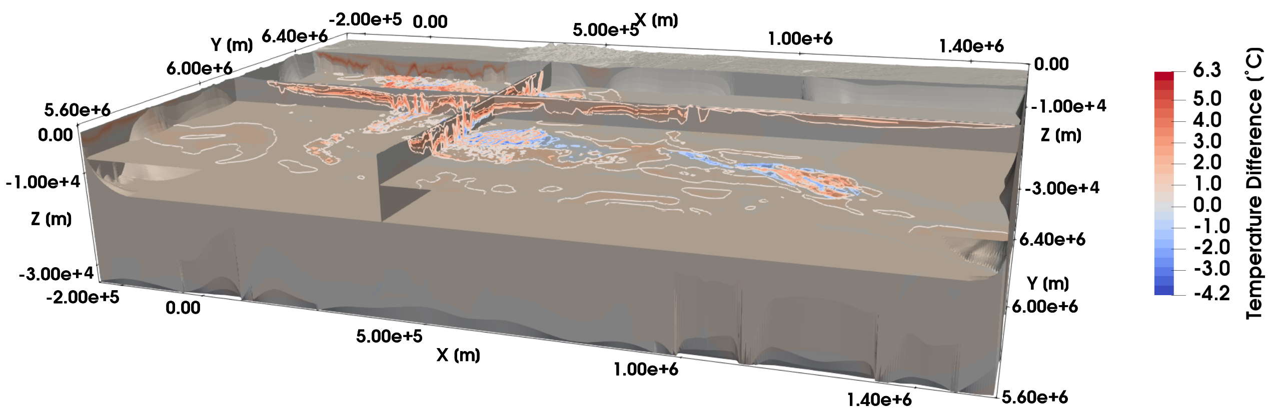

Figure 13. Difference in the temperature distribution for the upper 30 km between the state at time 22.8 ka and the initial condition for the transient simulation considering a simulation time of 255.7 Ma.

4.2.2 Transient Boundary Conditions

We observe no differences in the sensitivities of the thermal model parameters when considering paleoclimate corrections by means of the adopted transient boundary condition. Furthermore, the model is insensitive to the scaling factor for the upper boundary condition, which accounts for possible uncertainties of the boundary condition. Note that this scaling factor allows variations of up to 15 °C. Hence, we already allow every physically plausible temperature along the upper boundary condition. Additionally, we account for increasing uncertainties over time (from present-day backward).

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The reason why the model is insensitive to changes in the upper boundary condition is likely related to the chosen setting. For both the time-dependent and -independent case, we apply a Dirichlet type constraint. A Dirichlet constrain forces the model to have a defined and prescribed value of the unknown variable at the respective boundary. Additionally, we also account for the basal boundary conditions in terms of a prescribed temperature. Consequently, with this set of constraints, we fix the total amount of heat in the model that corresponds to our quantity of interest. Although we carried out the investigations based on relative changes between the different simulations, we observe no variations. This is because we pre-define, through the type of boundary conditions, the total amount of heat in the system.

At the current stage, this is unavoidable since we can neither define a different meaningful quantity of interest nor a different type of boundary condition to imposed as derived from global ESM models. Classically, the quantity of interest is defined as the norm of the misfit between simulated and measured temperature values. However, this is in our case not possible since we are interested in changes over the whole model. This is especially relevant while investigating the sensitivity of parameters for rocks buried at greater depths (higher than a few kilometers) where we lack any temperature measurements against which to compare the obtained results. This would then lead to a bias in the final estimates, with deeper regions being systematically under-represented in terms of their plate-like influence. Additionally, it is worth mentioning that we can only rely on direct measurements for the present time. Hence, the influence of past time steps would be also underestimated accordingly.

A possible solution to this would be to adopt in future studies a different upper boundary condition, moving from a Dirichlet to a more representative Robin-type constraint. This would make improve the global sensitivity analysis also in relation to the physics occurring at the surface interface since it would enable us to consider proper interactions between the atmosphere and the earth's subsurface. The use of a Robin boundary condition, however, would require to have detailed information about the heat in- and out-flux across this interface. This is currently not possible and would require a dedicated effort and closer interactions between the climate and subsurface communities.

4.3 Transient Processes

Although both "short-term" analyses (Fig. 6 branches 1a and 2a) consider a comparable time frame their sensitivities are similar but not identical. Note that in this paper, we use the expression "short-term" for all simulations with a time frame smaller than 26,000 years.

To investigate the reason for this difference, we compare the time-stepping approaches of both simulations. The short-term analysis conducted for the investigation of paleoclimate effects (Fig. 6 branch 1a) uses a constant time step size of 200 a, resulting in 130 time steps for a simulation time of 26 ka. In contrast, the other short-term investigation (Fig. 6 branch 2a) uses an initial time step size of 2 ka that grows linearly by a factor of 1.5. Due to the different time-stepping approaches, the paleoclimate short-term analysis has equally distributed "snapshots" over time. The short-term analysis that makes use of a non-constant time stepping provides more snapshots at later periods. Therefore, the thermal properties that become important later on in the system appear more pronounced than in the paleoclimate short-term analysis.

The logical consequence would be to use only constant time step sizes for the sensitivity analyses to avoid any bias by the time-stepping method. However, this is for long simulation periods unfeasible since it would result in unaffordable computational

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costs. Another possibility is to introduce a weighting scheme to compensate for the bias introduced by the time stepping. Since this paper aims to investigate the influences of transient processes, in general, this is not of primary concern here. Nonetheless, it would be interesting to investigate this phenomenon in future studies.

Focusing on how the sensitivities change over time, we observe that for the short-term period (Fig. 6 branch 2a) mainly the diffusivities of the sedimentary layers have an impact on the model response. For the second period (Fig. 6 branch 2b), the influence of the crustal and mantle diffusivities gain in importance, whereas the impact of varying radiogenic heat productions remain negligible. We consider a conductive heat transfer problem with the radiogenic heat production as the source term. Hence, we take a diffusive dominated process into account. Additionally, we have a cold upper and a warm lower boundary condition, resulting in a temperature gradient that increases with depth. Hence, the heat in the system is transported from the lower to the upper boundary. Therefore, the sedimentary layers, which are located at the uppermost part of the CEBS has a relatively prominent influence on the short-term system dynamics.

At longer time, the "heat-signal" is transported over longer distances within the plate (Fig. 14). Consequently, the crustal and mantle diffusivities grow in relevance. These observations also imply that we can use the sensitivity analyses to investigate specific regions of interest where heat transfer is active and, therefore, how any thermal signal (perturbation to a steady background state) propagates over time.

The radiogenic heat production has the highest impact in the last period analyzed. This is indicative that, during the whole evolution considered, the system could equilibrate by diffusion(Fig. 15). Even for the last period (Fig. 6 branch 2c), the sen-

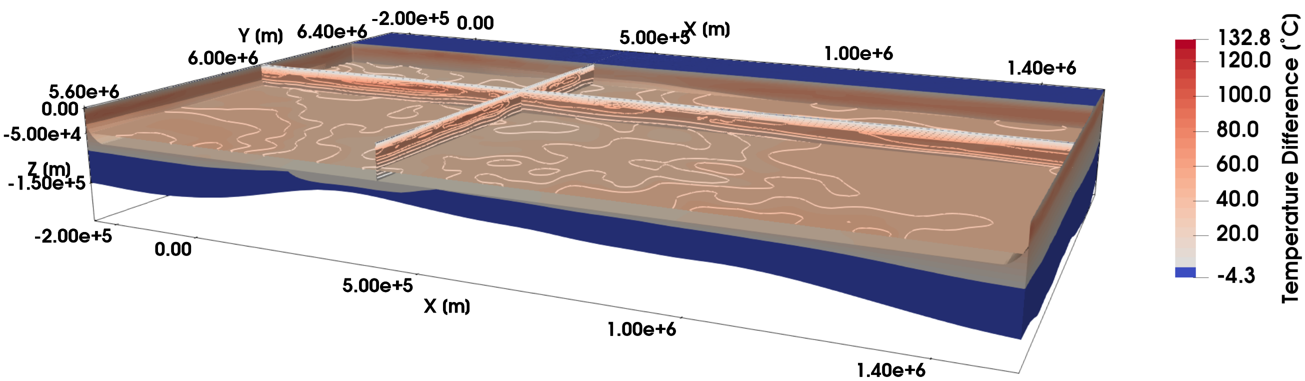

Figure 14. Difference in the temperature distribution between the state at time 10.0 Ma and time 583.9 ka for the transient simulation considering a simulation time of 255.7 Ma.

sitivities of the diffusivity of the Lithospheric Mantle and the crustal radiogenic heat productions are not as high as for the steady-state scenario. This can be partially associated with the fact that we have not yet reached a full equilibrium, that is that we are looking at a dynamic equilibrium in the system evolution. There is ad additional reason for this discrepancy observed. For the transient sensitivity analysis, we can face two options: either we consider the entire simulation period or only a portion of it. If we take into account the entire time frame, we never get a sensitivity distribution close to the steady-state scenario since

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we incorporate early and late time steps and hence get a weighted average over the sensitivities, where the weighting depends on the number of time steps. If, in turn, we consider only a certain time window, i.e. the very last time steps, we will still not get a representation of the steady-state system. This is because a steady-state system does not consider any time-dependency in its formulation. This is in contrast to a transient system, where these effects even if small are taken into account. If we compare the temperature distributions at this final period, we would observe no significant differences. However, the sensitivity analysis investigates the relative changes within a certain system. Therefore, also small in magnitudes changes can lead to a higher than expected sensitivity. Therefore, our analysis also bought us to conclude that in any geological system, we will never reach a final thermal equilibrium, but rather we will always observe variations from such an equilibrium, even if small in magnitudes. It is only by considering these variations that could enable us to obtain equal sensitivity distributions for steady-state and transient simulations.

The analysis considering the entire simulation time is almost identical to the analysis for the second period.

The subdivision into three time periods has the aim to identify short, medium, and long-term transient effects. Since the diffusion of a thermal signal requires several million years to propagate throughout a typical lithospheric plate, the effects of any spatial distribution of internal heat sources can only affect the temperature configuration at a later stage in the evolution of the system. This also enables us to subdivide the whole time evolution into different stages following the dominant physics.

The early period (short-term analysis above) is chosen such that it matches the time frame from the paleoclimate analysis. The third period contains the very last time steps, were visual changes due to the radiogenic heat production occurs. The second period contains all remaining time steps. Consequently, the different periods compromise a different number of time steps. The first consists of eight, the second of 19, and the third of fourth time steps. Since the second period has significantly more time steps than the other two it majorly influences the entire sensitivity distribution (considering the whole simulation time). Furthermore, the parameter correlations are significantly higher for the transient than for the steady-state simulations. In the

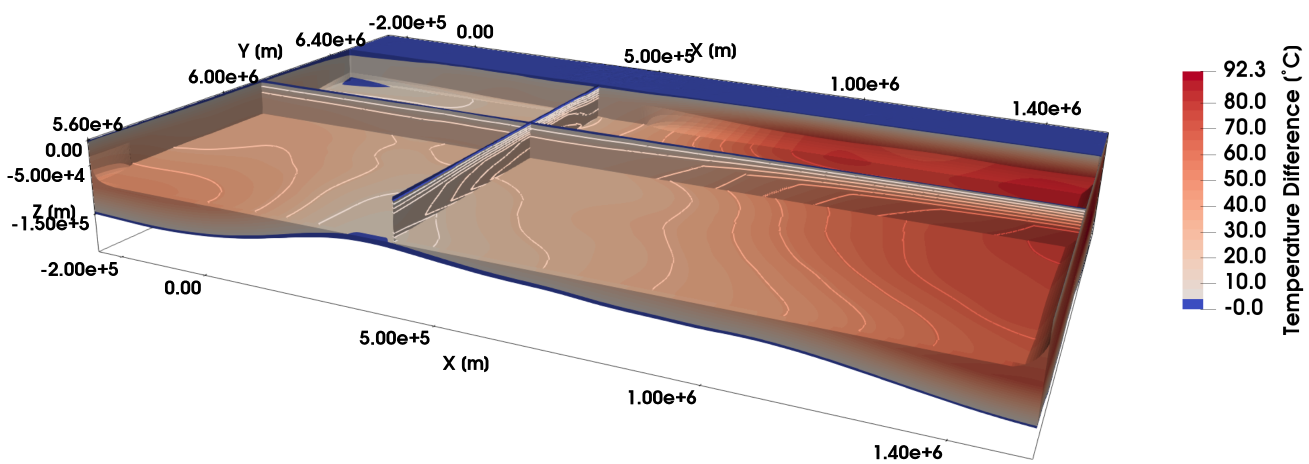

Figure 15. Difference in the temperature distribution between the state at time 255.7 Ma and time 75.8 Ma for the transient simulation considering a simulation time of 255.7 Ma.

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transient case, the highest correlations always occur between the diffusivities of the top geological layers, which is caused by their overall high impact on the model response. The parameter correlations are higher for the transient case since here the temperature diffuses over time towards the bottom of the model. Therefore, the interaction between the layers becomes more important.

5 Conclusions

We presented in this paper a quantitative framework for determining the impact of transient processes, including paleoclimate boundary conditions, on conductive heat transfer problem for basin-scale models.
Transient processes have a significant influence on the sensitivity distribution, generally leading to higher impacts of the sedimentary layers. Furthermore, the sensitivities are influenced by the time-stepping approach and by the simulation time. Hence, it is important to consider this in the analysis and carefully chose an appropriate time-stepping method and simulation time to avoid biased results. It is furthermore advisable to perform separate analyses for portions of the simulation time to investigate how the sensitivities of the thermal properties evolve.
The sensitivity analyses are a good tool to determine which physical processes are currently dominating the model and at which position in the model they are currently most active.
Considering transient Dirichlet boundary conditions for incorporating paleotemperature information is not necessary. We showed that the thermal properties are not impacted by the changes in the upper boundary condition. However, that does not mean that it is in general not necessary to consider an interaction between the atmosphere and the earth's subsurface. For conductive heat transfer problems, we would need to change the type of boundary condition to a Robin boundary condition. This change is physically meaningful since it closer describes the natural processes. However, currently the information about the heat in- and out-flux is not sufficient. Hence, further research in this area is required.
The usage of global sensitivity analyses is essential since local analyses do not return parameter correlations (Sobol, 2001; Wainwright et al., 2014; Degen et al., 2020a). Furthermore, previous studies have shown that local sensitivity analyses tend to overestimate the impact of the individual model parameters (Degen et al., 2020a). Using the finite element method the here presented analyses computationally prohibitive, only the utilization of a surrogate model allows the execution of these analyses. We investigated the changes in the entire model that is the reason why we use the reduced basis method to construct our surrogate model. In contrast to other surrogate models, it is not restricted to the observation space (Miao et al., 2019; Mo et al., 2019). We performed in total 12,000,000 steady-state forward simulations yielding with an average compute time varying between 1 ms and 4.2 ms for a single forward simulation of the various model scenarios. For the transient analyses, we require 560,000 forward simulations with an average duration of 13 ms to 200 ms for the various model realizations. If we would have used the finite element method instead, these investigations would have been infeasible since even on a high-performance infrastructure we obtain simulation times in the order of minutes for the steady-state simulations and hours in case of the transient ones.

Code availability. For the construction of the reduced models, we used the software package DwarfElephant (Degen et al., 2020b, c). The software, which is based on the finite element solver MOOSE (Alger et al., 2019), is freely available on Zenodo (https://zenodo.org/badge/latestdoi/117989215). The sensitivity analyses are performed with the Python library SALib (Herman and Usher, 2017).

Data availability. The global paleoclimate data have been generated with the MPI-ESM model code, which is freely available to the scientific community and can be accessed with a license on the MPI-M model distribution website (http://www.mpimet.mpg.de/en/science/models). The global paleoclimate data set is owned by the Max Planck Institute and can be obtained on request (publications@mpimet.mpg.de). The derived temperature trend used in this study (Section 3.3.2) is freely available together with all information to understand and reproduce the results from the paper. The 3D geological model of the CEBS, is available from https://doi.org/10.1016/j.tecto.2013.04.023. The link to the archive is automatically regenerated upon clicking on "Download all supplementary files". The data for the refined sedimentary sequence with respect to the above described model as adopted in this study is available as DOI and online material via the following link https://doi.org/10.5880/GFZ.4.5.2020.006.

Author contributions. All authors discussed and interpreted the presented work. DD carried out the simulations and all authors read and approved the final manuscript.

Competing interests. The authors declare that they have no conflict of interest.

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