

# Supporting Information for “Crustal-Scale Thermal Models: Revisiting the Influence of Deep Boundary Conditions”

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## Additional Supporting Information (Files uploaded separately)

1. Caption for large Tables S1: Thermal Properties of all models for and after the automated model calibration. The initial thermal properties are from Noack, Scheck-Wenderoth, and Cacace (2012); Noack, Scheck-Wenderoth, Cacace, and Schneider (2013). We denote all parameters that are not involved in the model calibration, due to too low

sensitivities or that are not applicable for the specific model version, with n/a. Additionally, the IDs of the training parameters  $\mu$  are provided. We denote the radiogenic heat production with  $S$ , the initial thermal conductivity with  $\lambda_{\text{init}}$ , and the calibrated thermal conductivity with  $\lambda_{\text{cal}}$ .

## Introduction

This supporting material provides additional information regarding the results of the model calibration for the thermal conductivities (Text S1 and Table S1). Figure S1 shows the convergence for the maximum relative error for all three versions of the Berlin-Brandenburg model.

## Text S1: Model Calibration – Thermal Conductivities

Table S1 presents the changes in the thermal conductivity between the initial and the best-calibrated values for all models. Regarding the Berlin-Brandenburg LAB model, we observe an increase from  $2.0 \text{ W m}^{-1} \text{ K}^{-1}$  to  $2.45 \text{ W m}^{-1} \text{ K}^{-1}$  for the Lower Cretaceous-/Jurassic/Buntsandstein layers. For the Berlin-Brandenburg combined model, we see a more pronounced increase, resulting in a value of  $2.53 \text{ W m}^{-1} \text{ K}^{-1}$ . Furthermore, a substantial increase in thermal conductivity is observed for the Lithospheric Mantle, resulting in conductivities of  $5.93 \text{ W m}^{-1} \text{ K}^{-1}$  for the BB-LAB and combined model. Additionally, the scaling parameter for the lower boundary condition shows an increase to 1.10 for BB-combined model. Also, we obtain decreased thermal conductivities for the Zechstein layer of  $3.45 \text{ W m}^{-1} \text{ K}^{-1}$  (BB-LAB model), and an increased value of  $3.73 \text{ W m}^{-1} \text{ K}^{-1}$  (BB-combined model). The calibration of the Berlin-Brandenburg LAB model leads to an increased thermal conductivity of  $1.99 \text{ W m}^{-1} \text{ K}^{-1}$  for the Quaternary/Tertiary layer, and

the calibration of the Berlin-Brandenburg combined model to an increased thermal conductivity of the Tertiary-pre-Rupelian-clay/Upper Cretaceous layer to  $1.93 \text{ W m}^{-1} \text{ K}^{-1}$ . The parameter distribution for the BB-6km model shows an increased thermal conductivity of  $2.78 \text{ W m}^{-1} \text{ K}^{-1}$  for the Basement layer. The scaling factor for the mean temperature is 21.54 after the calibration resulting in a mean temperature of  $180^\circ\text{C}$ .

For the discussion of the thermal conductivities of the calibration results, we talk about the results from the Berlin-Brandenburg LAB and combined model because of the uninformative nature of the Berlin-Brandenburg 6 km model. We observe similar trends for both the original and the refined model. Although, the parameter distribution of the BB-combined model after the calibration is closer to the initial parameter distribution than the one from the BB-LAB model. This demonstrates the need for model calibration. It is incredibly challenging and time-consuming to construct a model that accounts for all structural effects. Taking the lack of data into account, it becomes a somehow impossible task. Therefore, we follow a different approach in this work. We compensate, for the model errors, by replacing the physical by effective thermal conductivities. In that way, we obtain a representative model. Also, keep in mind that the major shortcoming of the BB-6km model could only be revealed using a global sensitivity analysis. However, this requires so many forward simulations that it is not realizable, even with state-of-the-art finite element solvers, on a basin-scale without using surrogate models.

Considering the geological setting, the significant increase in thermal conductivity for the Lower Cretaceous/Jurassic/Buntsandstein layers (BB-LAB model and BB-combined model) is most likely caused by unresolved salt structures. Further investigations are required to analyze whether all layers (Lower Cretaceous/Jurassic/Buntsandstein) or only

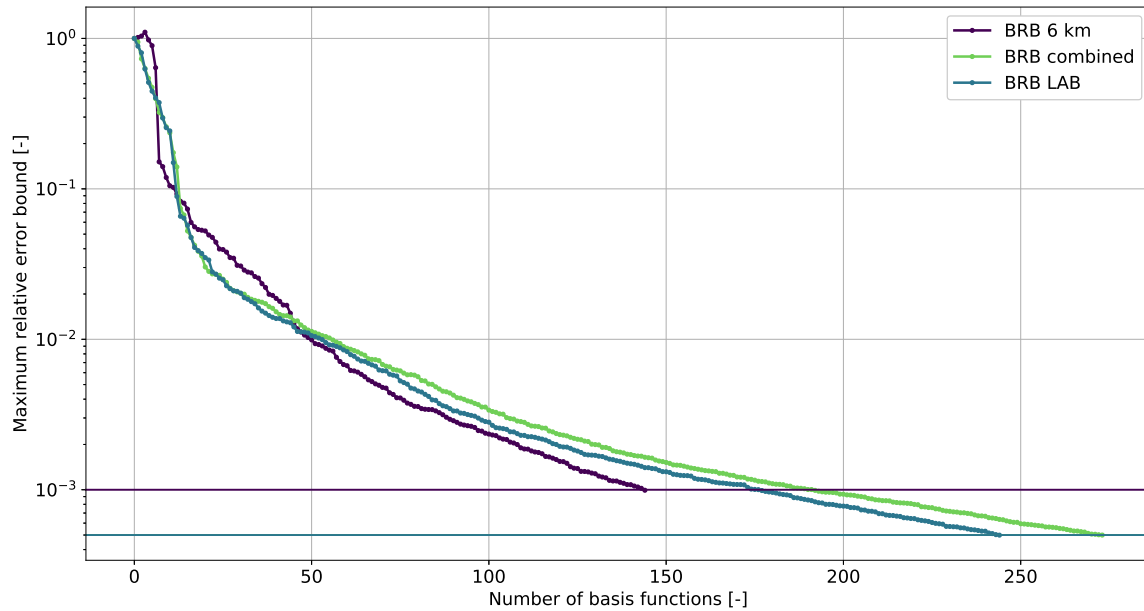
one layer contain unaccounted structures. The increase in thermal conductivity for the Zechstein layer is also most likely caused by unaccounted salt structures. Note that the increase in thermal conductivity for the Zechstein layer is significantly lower for the Berlin-Brandenburg combined model than for the Berlin-Brandenburg LAB model leading to the conclusion that the geological refinement captured successfully missing salt structures. The Keuper layer has after the calibration nearly the same value as the Muschelkalk layer leading to the assumption that we underestimated the sediment thickness of the Muschelkalk.

Combining the increase in thermal conductivity of the Lithospheric Mantle and the variation of the lower boundary conditions leads to the conclusion that a wrong geometrical parameterization of the LAB causes this increase. The correlation between both parameters confirms this. The fact that fixing the boundary condition to 1300 °C leads to an even higher increase in thermal conductivity further emphasizes this. For further studies, one could either allow a larger variation at the lower boundary condition or use a boundary condition that is either derived by data assimilation or considers tomography-derived temperatures.

Regarding the BB-6km model, we already stated that it is completely boundary dominated. Therefore, we focus the discussion on the Berlin-Brandenburg LAB and combined model. From the sensitivity analysis, we know that the main influence from the upper layers is arising from the Tertiary-pre-Rupelian-clay. Again, the increase is less dominant for the BB-combined model than for the BB-LAB model. This leads us to the conclusion that structural effects mainly cause this mismatch. The refined model version resolves this much better.

## References

- Noack, V., Scheck-Wenderoth, M., & Cacace, M. (2012). Sensitivity of 3D thermal models to the choice of boundary conditions and thermal properties: a case study for the area of brandenburg (NE German Basin). *Environmental Earth Sciences*, 67(6), 1695–1711.
- Noack, V., Scheck-Wenderoth, M., Cacace, M., & Schneider, M. (2013). Influence of fluid flow on the regional thermal field: results from 3d numerical modelling for the area of brandenburg (north german basin). *Environmental earth sciences*, 70(8), 3523–3544.



**Figure S1.** Convergence of the maximum relative error bound for the Brandenburg 6 km model (denoted in purple), the Brandenburg combined model (denoted in green), and the Brandenburg LAB model (denoted in blue). We are using an error tolerance of  $1 \cdot 10^{-3}$  for the Brandenburg 6 km model, and an error tolerance of  $5 \cdot 10^{-4}$  for the Brandenburg combined and LAB model.