Supporting Information for "Uncertainty Quantification for Basin-Scale Conductive Models"

Denise Degen[1], Karen Veroy[2,3], Florian Wellmann[1]

[1]Computational Geoscience and Reservoir Engineering (CGRE), RWTH Aachen University, Wüllnerstraße 2, 52072 Aachen, Germany

[2]Centre for Analysis, Scientific Computing and Applications, Department of Mathematics & Computer Science, Eindhoven University of Technology (TU/e), Groene Loper 5, Eindhoven, The Netherlands

[3]Faculty of Civil Engineering, RWTH Aachen University, Schinkelstraße 2, Aachen, Germany

Contents of this file

1. Text S1 to S2
2. Figures S1 to S8

Additional Supporting Information (Files uploaded separately)

1. Caption for large Tables S1: Thermal properties of the Brandenburg model before and after the uncertainty quantification. The prior thermal properties are from (Noack, 2012; 2013). We denote all parameters that are not involved in the uncertainty quantification, due to too low sensitivities, with n/a. Additionally, the affine decomposition for the model reduction is provided.

Introduction

This supporting material provides additional information regarding the methodology of uncertainty quantification (Text S1). Furthermore, we provide the decomposition of the weak formulation (Text S2) required for the construction of the reduced order model, as referenced in the main manuscript. Additionally, we present supporting Figures S1 to S8 as referenced in the main manuscript.

Text S1: Uncertainty Quantification

Bayes Theorem is the basis of the Markov Chain Monte Carlo (MCMC) method (Iglesias & Stuart, 2014):

$$P(u|y) \propto P(y|u)\ P(u). \tag{1}$$

The prior $P(u)$ describes our knowledge about the unknown variable without taking the data into account. The posterior $P(u|y)$, is the knowledge we have about our unknown variable u given the data y. Furthermore, $P(y|u)$ is the likelihood, which describes the likelihood of the parameters given the observation data. Often, we do not have a very accurate or detailed knowledge of our unknowns, which means that determining the priors is challenging. Without using an uncertainty quantification method such as MCMC, we would simply sample from our prior and determine the uncertainties from that. This would result in relatively large uncertainties. On the other hand, MCMC incorporates the data to reduce the uncertainties through the given data. MCMC is a method to draw samples from a probability distribution. This is based on the generation of a Markov Chain. A Markov Chain develops based only on the knowledge of the present and previous events (Iglesias & Stuart, 2014).

Text S2: Weak Form and Affine Decomposition

We derive the weak formulation, where $u(\mu) \in X$ satisfies (Hesthaven et al., 2016; Prud'homme et al., 2002; Quarteroni et al., 2015):

$$a(u(\mu), v; \mu) = f(v; \mu), \qquad \forall v \in X. \tag{2}$$

In particular, the bilinear form a has the following decomposition:

$$a(w, v; \lambda) = -\sum_{q=0}^{n} \lambda_q \int_{\Omega} \nabla w \; \nabla v \; d\Omega, \qquad \forall v, w \in X, \; \forall \lambda \in \mathcal{D}, \tag{3}$$

where w is the trial function, v the test function, the index "q" denotes the number of the training parameter (for more information see Table S1), X the function space $(H_0^1(\Omega) \subset X \subset H_1(\Omega))$, Ω the spatial domain in $\mathbb{R}^3$, and D the parameter domain in $\mathbb{R}^p$ with p being the number of parameters. In our example p is equal to 14. The linear form f is decomposed in the following way:

$$\begin{gathered} f(v; \lambda, s) = -\sum_{q=0}^{n} \lambda_q \; s \int_{\Gamma} \nabla v \; g(x,y,z) \; d\Gamma + \quad s \int_{\Gamma} \nabla v \; S \; d\Gamma, \qquad \forall v \in X, \; \forall \lambda \in \mathcal{D}, \\ \text{with } g(x,y,z) = T_{\text{top}} \frac{h(x,y,z) - z_{\text{bottom}}(x,y)}{d(x,y)}. \end{gathered} \tag{4}$$

Here, Γ is the boundary in $\mathbb{R}^3$, s the scaling parameter for the lower boundary condition, $g(x, y, z)$ the lifting function, T_{top} the temperature at the top of the model, $h(x, y, z)$ the location in the model, $z_{\text{bottom}}(x, y)$ the depth of the bottom surface, and $d(x, y)$ the distance between the bottom and top surface.

References

Hesthaven, J. S., Rozza, G., Stamm, B., et al. (2016). *Certified reduced basis methods for parametrized partial differential equations.* SpringerBriefs in Mathematics, Springer.

Iglesias, M., & Stuart, A. M. (2014). Inverse Problems and Uncertainty Quantification. *SIAM News*, 2–3.

Prud'homme, C., Rovas, D. V., Veroy, K., Machiels, L., Maday, Y., Patera, A. T., & Turinici, G. (2002). Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods. *Journal of Fluids Engineering*, *124*(1), 70–80.

Quarteroni, A., Manzoni, A., & Negri, F. (2015). *Reduced Basis Methods for Partial Differential Equations: An Introduction.* Springer International Publishing.

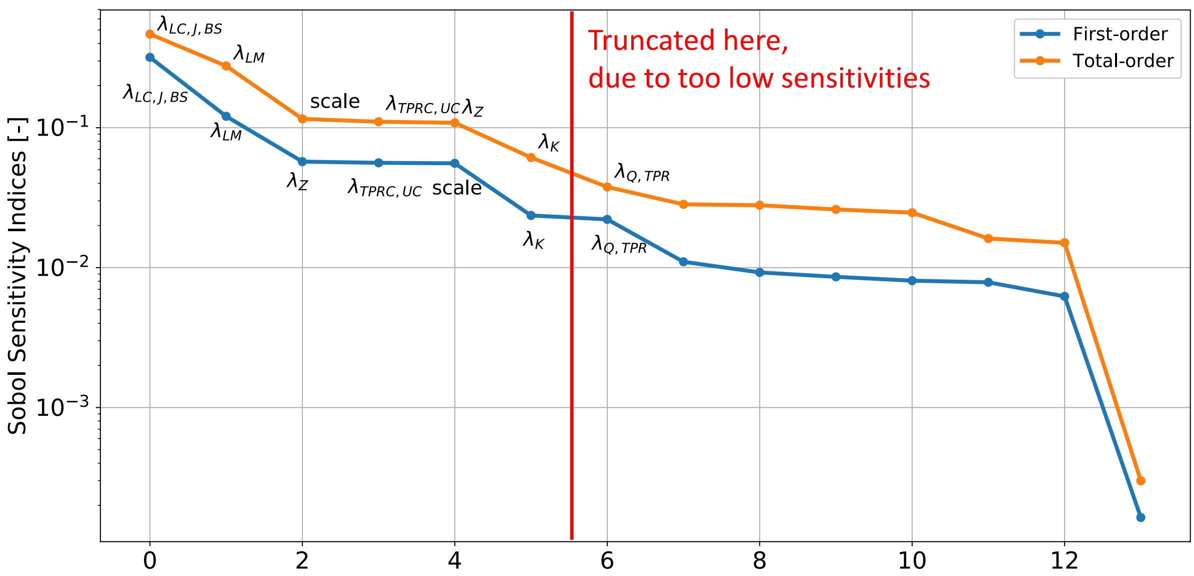

Figure S1. Global Sensitivity analysis for the Brandenburg model. We show the first- (blue) and total-order contributions (orange).

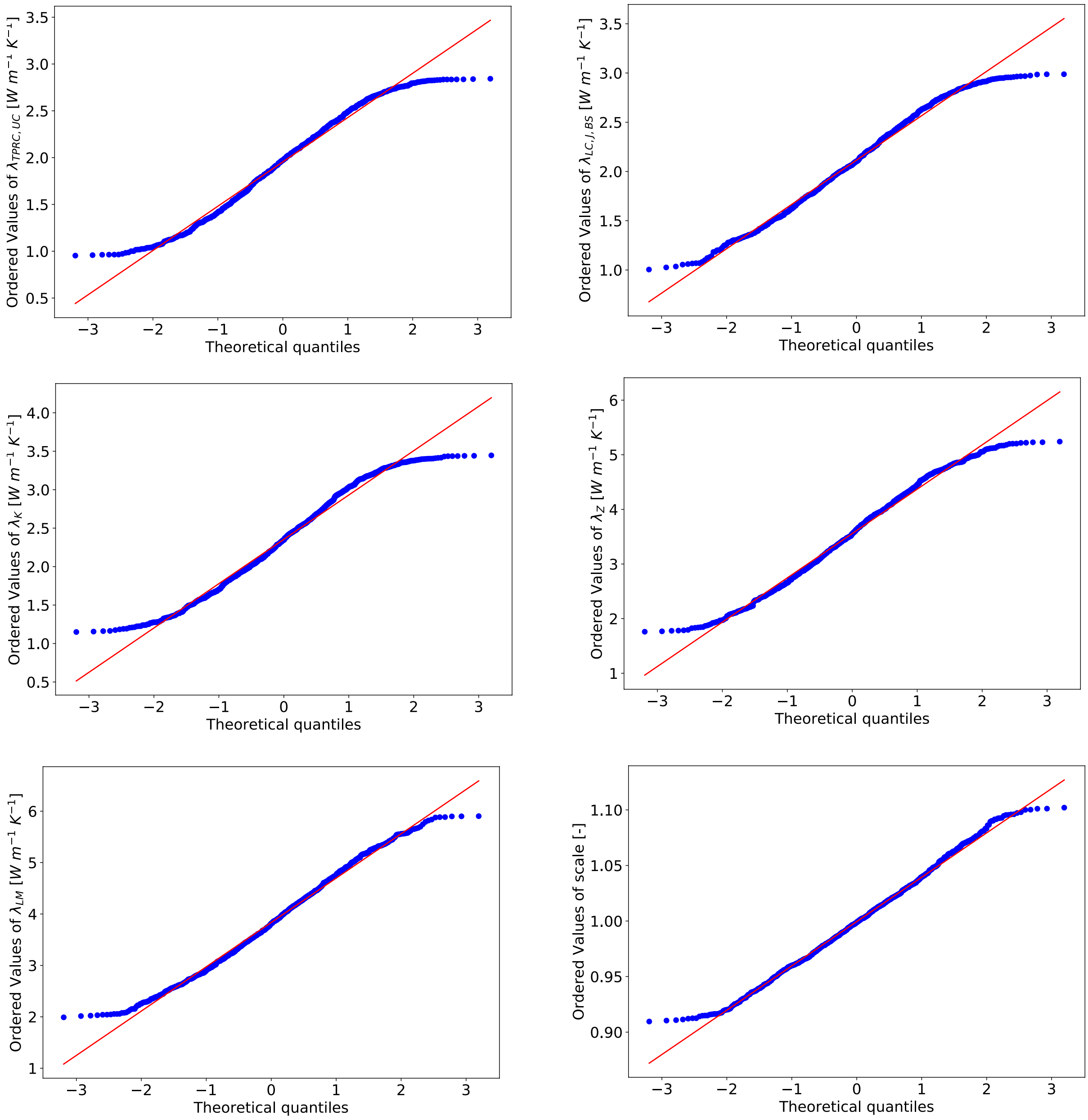

Figure S2. Quantile-Quantile plots for all thermal conductivities considered in the uncertainty quantification of the Brandenburg model.

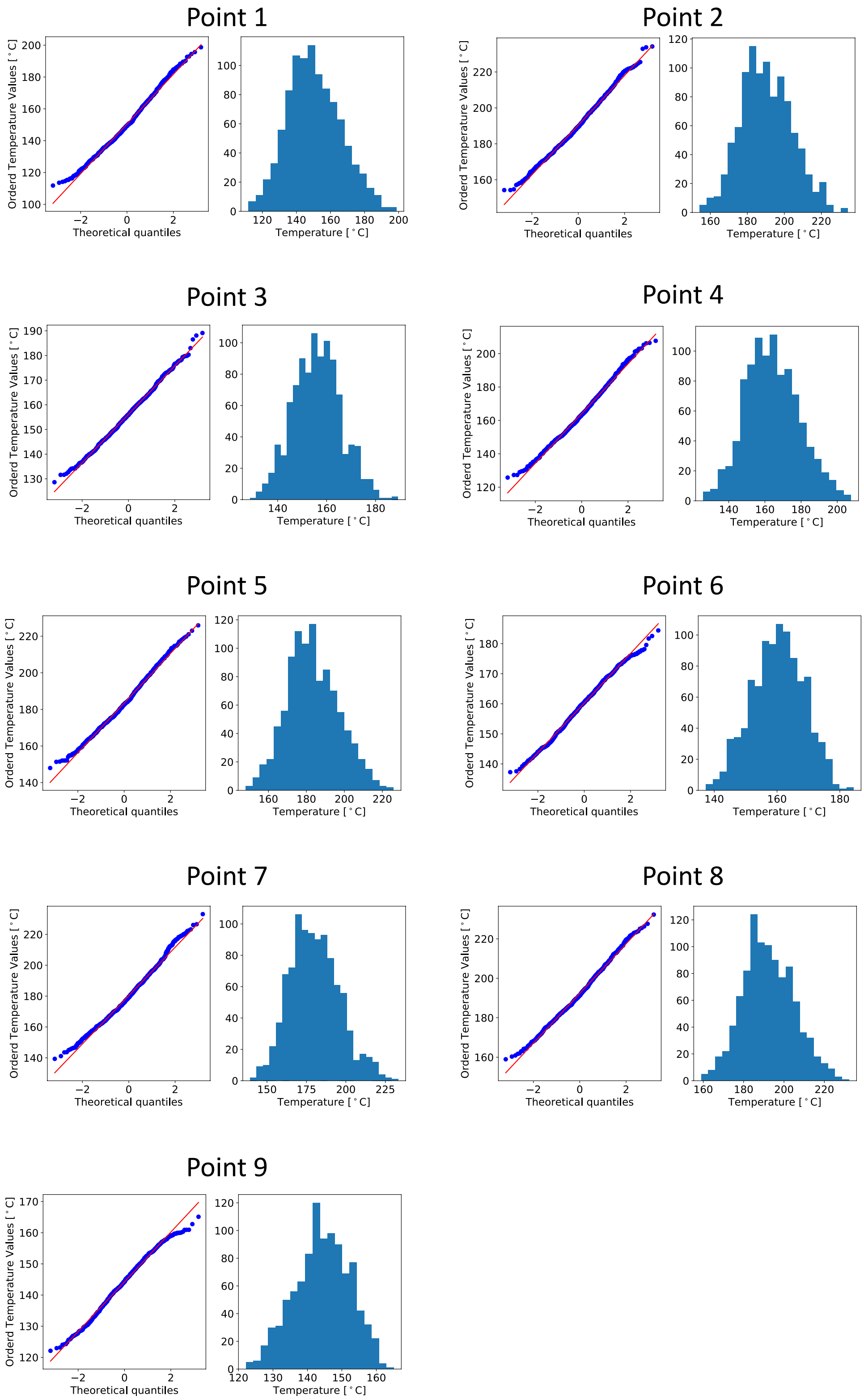

Figure S3. Quantile-Quantile plots and histograms of the temperatures for all parameters from the MCMC analysis for the Brandenburg model at nine points.

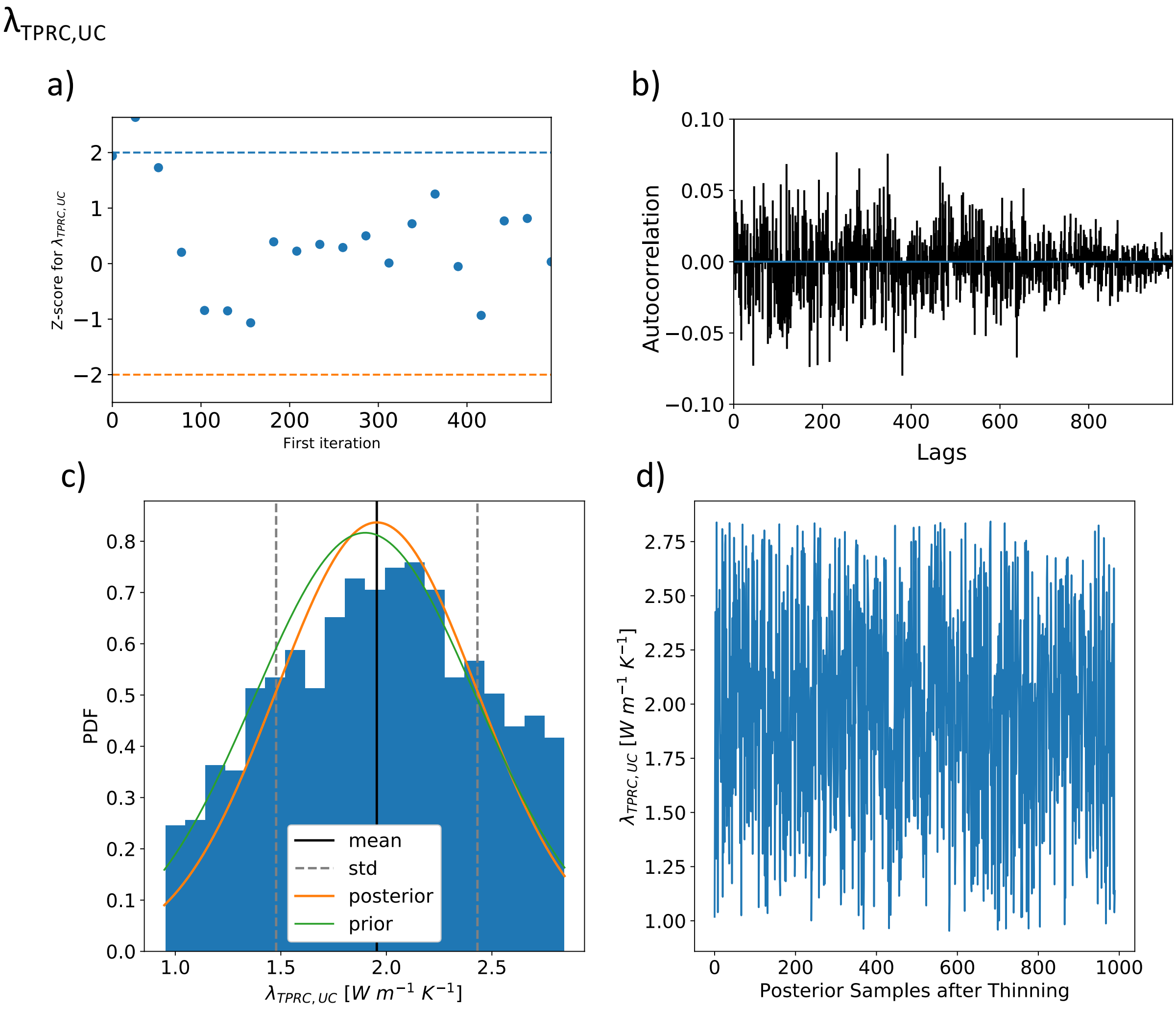

Figure S4. Posterior Analysis of the Tertiary-pre-Rupelian-clay (TPRC) and the Upper Crust (UC). Shown are the a) Geweke Plot b) autocorrelation, c) posterior parameter distributions, and d) the trace.

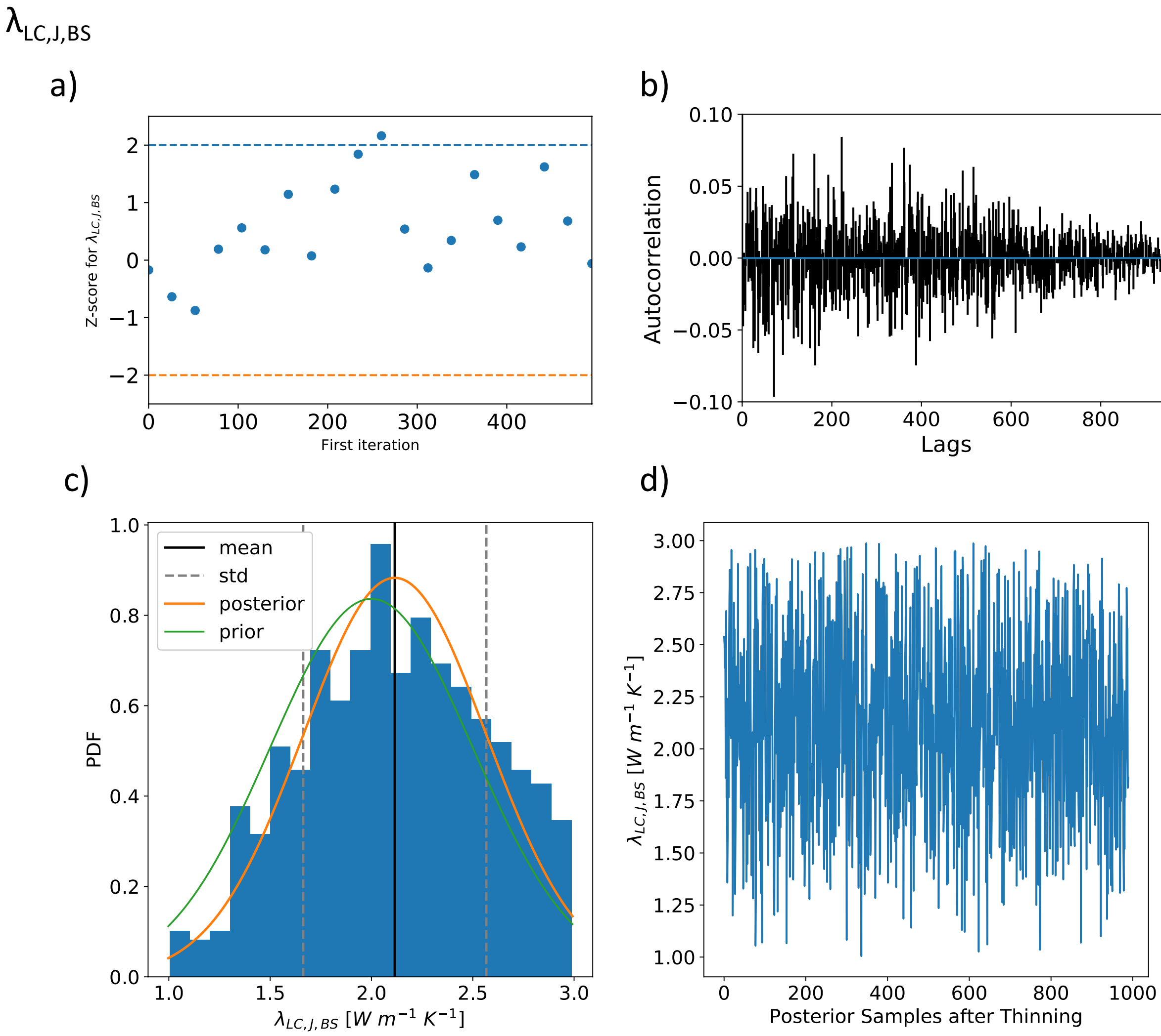

Figure S5. Posterior Analysis of the Lower Crust (LC), the Jurassic (J), and the Buntsandstein (BS). Shown are the a) Geweke Plot b) autocorrelation, c) posterior parameter distributions, and d) the trace.

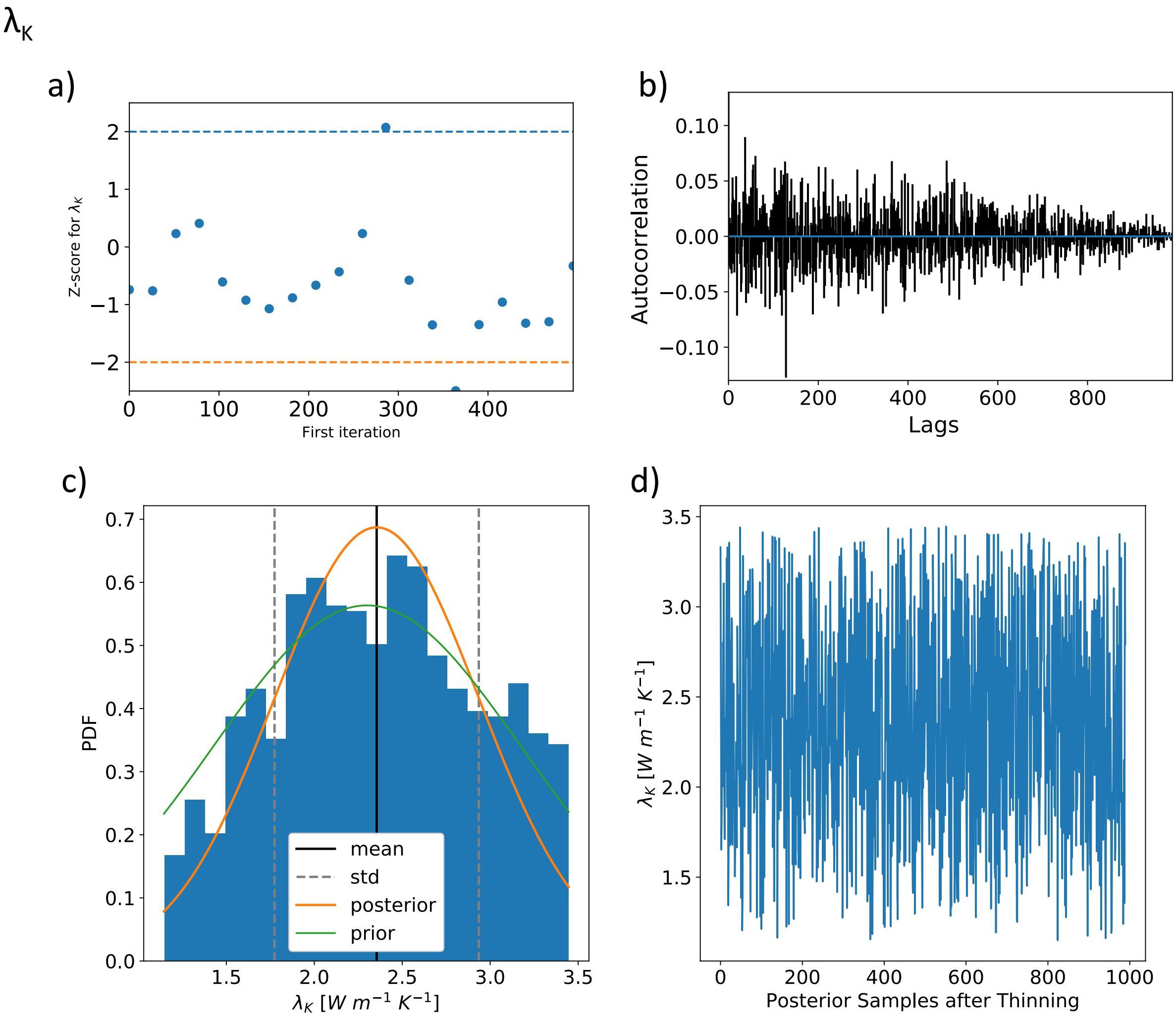

Figure S6. Posterior Analysis of the Keuper (K). Shown are the a) Geweke Plot b) autocorrelation, c) posterior parameter distributions, and d) the trace.

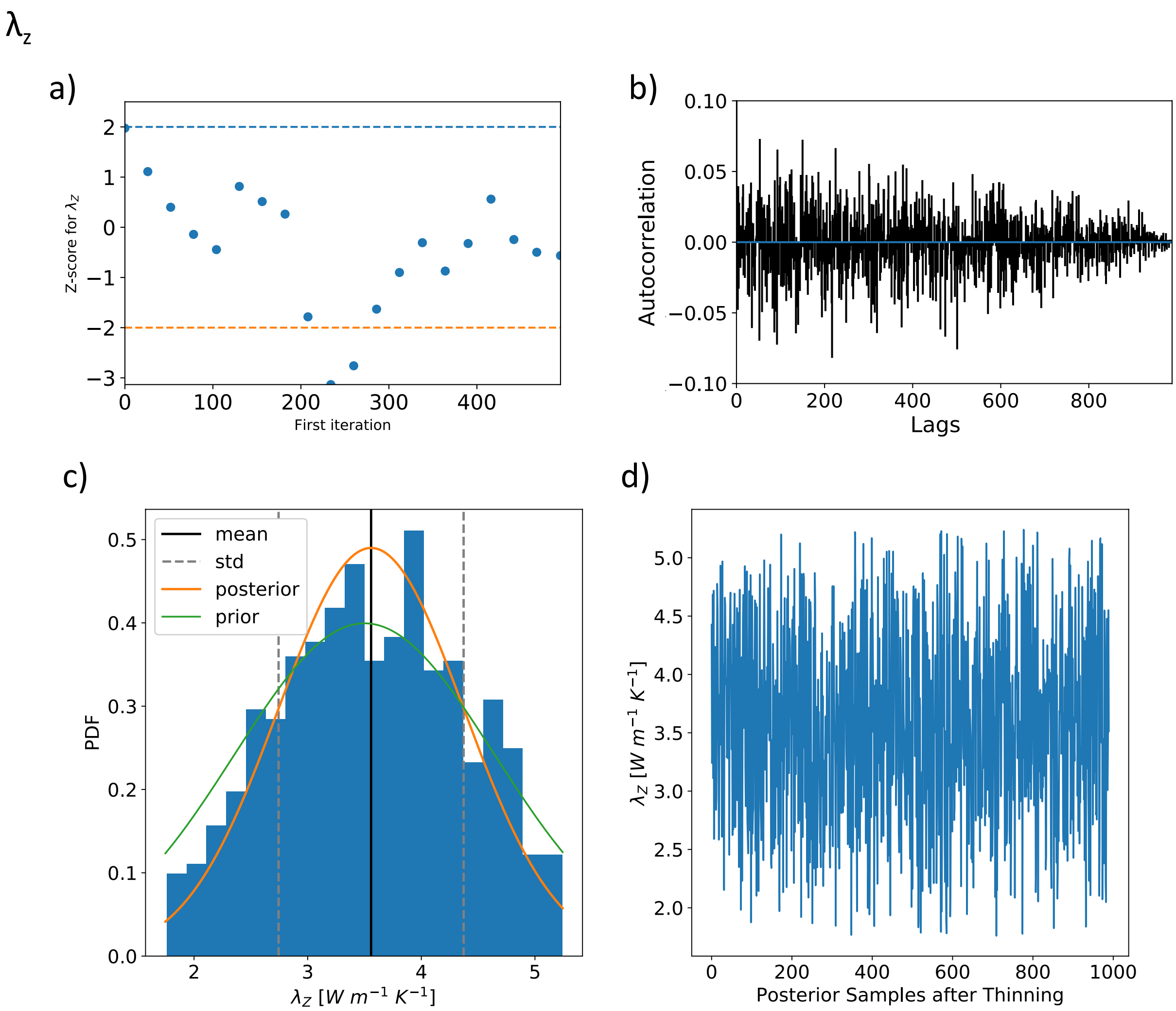

Figure S7. Posterior Analysis of the Zechstein (Z). Shown are the a) Geweke Plot b) autocorrelation, c) posterior parameter distributions, and d) the trace.

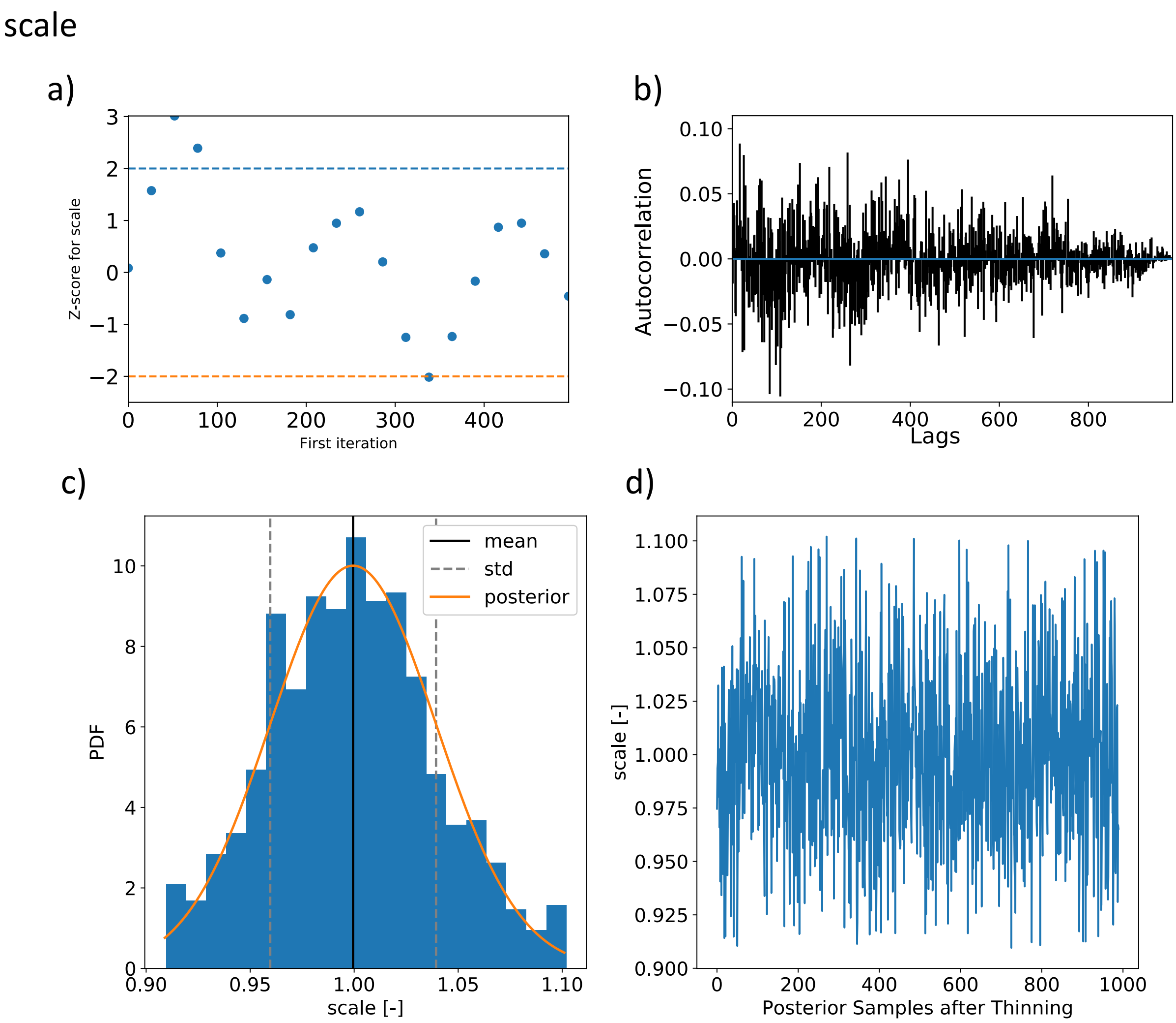

Figure S8. Posterior Analysis of the scaling parameter for the lower boundary condition. Shown are the a) Geweke Plot b) autocorrelation, c) posterior parameter distributions, and d) the trace.