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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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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%.

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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,

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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-insitu) 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

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