Influence of geological structure and geophysical parameters on the geothermal field below the city of Berlin, Germany

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ABSTRACT

The goal of this study is to analyze the influence of the geological structure of model units on conductive and fluid-driven heat transport in the subsurface of the city of Berlin, Germany, as calculated by 3D numerical simulations.

The results show that the structural configuration (i.e. thickness distribution) of the Rupelian clay aquitard has the strongest impact on the shallow and deep geothermal field. In the purely conductive environment, a general increase of the thermal blanketing effect exerted by increased thicknesses of the lowly conductive Rupelian, could be identified. In a coupled hydrothermal environment, a reduction of forced convective cooling induced by a relatively continuous appearance of the Rupelian led to generally warmer predicted temperatures of the models compared to previous studies (up to ± 23 K at -1000 m.a.s.l.). The structural refinement also reduces the influence of the hydraulic boundary condition (BC) and associated gradients to ± 11 K at -1000 m.a.s.l.. Modifications of the upper temperature BC relate to temperature differences up to only ± 2 K at -1000 m.a.s.l. since the implementation of the latter according to measured data has only little impact on the fluid flow system.

1. INTRODUCTION

1.1. Previous Work

The present-day temperature configuration of the subsurface is controlled by different coupled physical processes. These are mainly diffusion of heat by conduction and advective forces such as gravity driven flow, overpressure flow or flow induced by buoyant forces within the fluid.

The study area focusing on Berlin, capital city of Germany, is characterized by a comparatively flat topography (Figure 1a) and no recent seismic activity. However, latest 3D numerical investigations showed that a regional hydro-thermal regime is likely present (Frick et al., 2015; Frick et al., submitted; Noack et al., 2013; Sippel et al., 2013). More precisely, these studies outlined that the thermal field of the sedimentary succession is mainly influenced by conduction of heat from deeper crustal domains which is additionally overprinted by a regional component of pressure driven groundwater flow induced by gradients of the hydraulic head. These observations only account for the first-order aspects of the present-day thermal configuration and show local and systematic misfits to measured temperatures. The predicted temperatures are generally too low which has been suggested to be caused by (1) a lack in the accuracy of the utilized surface thermal and hydraulic conditions or (2) an insufficiently detailed representation of the Cenozoic aquifer-aquitard complex (Sippel et al., 2013). The first of those assumptions was already targeted by Frick et al. (2015), implementing (a) measured groundwater levels as hydraulic boundary condition (BC) and (b) measured temperatures as upper thermal BC in their models. The results showed that the implementation of these parameters results in a general increase in predicted temperatures of up to (a) 13.8 K and (b) 5.1 K. The authors suggest reduced forced convective cooling due to a lowering of the hydraulic gradients of the BC as main cause for these temperature differences. Moreover, higher temperatures assigned for the upper thermal BC were proposed to be convectively carried downwards into the deeper model domain (Frick et al., 2015).

This study is part of ongoing research aiming to investigate and quantify the relevance of the aforementioned parameters and their respective influence on the present-day thermal configuration below the city of Berlin. The objective is to systematically analyze the influence of the structural configuration and surface thermal and hydraulic conditions on both, fluid and heat flow. For this goal, a new structural model (Frick et al., submitted) of the study area is tested for its sensitivity to different heat transport mechanisms and surface thermal and hydraulic conditions in comparison to earlier published...
In detail, (1) Model A by Sippel et al. (2013) and (2) Model D by Frick et al. (2015) will be utilized for the analysis described above. Both of these models differ only in the structural model to one of the models in this study which enables isolating the effect of the latter on the thermal and hydraulic field through direct comparison ((1) to M1 and (2) to M2, Section 3).

This approach aims to outline the importance of the highest possible resolution of the shallow model domain geology (i.e. > -250 m.a.s.l.) since associated modifications of the thermal and hydraulic field likely lead to significant differences of predicted temperatures in the deeper model domain (i.e. < -1000 m.a.s.l.).

1.2. Structural Model and Geological Setting

The study presented here utilizes a newly constructed structural model presented in Frick et al. (submitted) which comprises 20 (coupled) to 23 (conductive) model units (more details in Figure 1a, Section 2). Horizontally, the model displays a resolution of 100x100 m. Vertically, a total of 18 units representing the sedimentary basin infill and 5 units for the underlying basement (Permocarboniferous Volcanics, Pre-Permian, Upper Crust, Lower Crust, Lithospheric Mantle) are resolved. In comparison to earlier representations of the Berlin subsurface (Sippel et al., 2013), the Cenozoic is differentiated into two more units leading to a total of eight (Figure 1a). To reduce the number of finite elements, the structural model was cut at -6000 m.a.s.l. for the coupled model scenario (see Section 2) considering all sedimentary units plus an impervious basement (Sippel et al., 2013).

The complete sedimentary succession is of Permian to Cenozoic age and is mainly made up of clastics, carbonates and rock salt (Sippel et al., 2013). The latter is of special interest since it makes up a big proportion...
of the sedimentary fill in form of the Permian Zechstein deposits. This stratigraphic unit highly controlled and modified the geometry of the post-Zechstein succession due to its mobilization from Mid-Triassic times onwards (initial thickness 2,500 m, Scheck et al. (2003)). Consequently, this unit displays a complex topological configuration, locally reaching thicknesses of more than 3,400 m (Figure 1b). The remainder of the Mesozoic sediments are predominantly made up of consolidated clastics and carbonates and also contain the two major units of geothermal interest. These are namely the Permian Sedimentary Rotliegend and the Triassic Middle Buntsandstein, both displaying sufficiently high porosities and permeabilities for geothermal exploration (Huenges and Ledru, 2011). In contrast, Cenozoic sediments are mainly composed of unconsolidated clastics which contain the main shallow aquifer system providing the city of Berlin with fresh water. An important stratum in this succession is the Oligocene Rupelian clay, which separates the overlying saline aquifers (Limberg and Thierbach, 2002). Hence, its structural configuration and the representation in coupled thermal and hydraulic models is of crucial importance for understanding possible scenarios where the sustainability of these systems might be impeded.

Earlier studies already outlined that this unit is discontinuous in the Northeast German Basin as well as the model area (mainly due to erosion during glacial times) leading to possible connections between the two aforementioned aquifers at depth (Figure 1c, Noack et al., 2013; Sippel et al., 2013). In this respect, the structural model utilized here and presented in Frick et al. (submitted) implemented a large database including well logs, geological cross-sections and deep seismics to build a more precise representation of the shallow fresh water and saline aquifer complex. This structural configuration includes a higher differentiation of geological units and significantly modified thickness distributions of Cenozoic model units. The most important modification concerns the Rupelian clay aquitard, which was assumed to be largely discontinuous in the model area (Sippel et al., 2013), but only shows few areas with 0 m thickness in the new model (Figure 1c, Frick et al., submitted). Another important structural modification results from the implementation of deep seismics located in Tempelhof (Figure 1c, Moeck et al., 2015). A general drop in the elevation the top Zechstein along with a steeper dip angle of towards S (dip/dip direction: 20/190) at this location results in a thickness reduction of the unit of up to 230m (Minimum 0 m thickness, Figure 1b, Frick et al., submitted).

2. MODELING METHOD

2.1. Conductive Simulation (M1)

The first model run in this study considers conductive heat flow as only heat transport mechanism. For this purpose, the finite element numerical solver tool GMS (Bayer et al., 1997) was utilized. The governing equation under the assumption of steady state ($\frac{dT}{dt} = 0$) is described by:

$$ S = \nabla \cdot (\lambda^{(b)} \nabla T) \quad [1] $$

with $S = $ radiogenic heat production, $\nabla = $ Nabla operator, $\lambda^{(b)} = $ bulk thermal conductivity, $T = $ temperature. From equation [1] follows that predicted subsurface temperatures depend only on the radiogenic heat production, solid thermal conductivity and porosity of model units as well as the BC chosen. For this purpose, each geological unit of the structural model (Figure 1a) is assigned a constant value for $\lambda^{(b)}$ and $S$ (Table 1, Sippel et al., 2013).

2.2. Coupled Simulation (M2)

The coupled fluid and heat flow simulations were carried out with the commercial software FEFLOW® (Diersch, 2009). This software allows to solve for (un)saturated groundwater flow in porous media taking into account conductive, advective and buoyant (fluid density related) heat transport processes within a finite element based computational framework. A detailed description of the mathematical and numerical background can be found in Diersch (2009).

Within this framework, model units were assigned unique values for thermal conductivity, heat capacity, radiogenic heat production, porosity and hydraulic conductivity in accordance with published data (Sippel et al., 2013). In order to guarantee a good horizontal to vertical shape ratio for the coupled model, the original 20 model units have been further subdivided into a total of 56 computational layers whereas each model unit consists of at least two.

### Table 1: Properties of the Cenozoic geological units as used for the thermal calculations. Properties of all units (Cretaceous and older not shown) as detailed in (Sippel et al., 2013). $\lambda^{(b)} =$ bulk thermal conductivity, $S =$ radiogenic heat production, $c^{(s)} =$ heat capacity of solid, $\Phi =$ porosity, $K =$ hydraulic conductivity.

<table>
<thead>
<tr>
<th>Geological unit</th>
<th>$\lambda^{(b)}$ [W/m$\cdot$K]</th>
<th>$c^{(s)}$ [J/kg$\cdot$K]</th>
<th>$S$ [J/kg$\cdot$K$\cdot$K]</th>
<th>$\Phi$ [-]</th>
<th>$K$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neogene</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Holocene to Weichselian</td>
<td>3.5</td>
<td>0.9</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Eemian to Saalian</td>
<td>3.5</td>
<td>0.9</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Holstein</td>
<td>3.5</td>
<td>0.9</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Elsterian</td>
<td>3.5</td>
<td>0.9</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Miocene</td>
<td>3.5</td>
<td>1.0</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Pliocene</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cottbus</td>
<td>3.5</td>
<td>1.3</td>
<td>2.16</td>
<td>0.311</td>
<td>9.62E-08</td>
</tr>
<tr>
<td>Rupelian</td>
<td>1.88</td>
<td>1.3</td>
<td>2.36</td>
<td>0.194</td>
<td>impermeable</td>
</tr>
<tr>
<td>Pre-Rupelian</td>
<td>3.1</td>
<td>1.3</td>
<td>2.26</td>
<td>0.255</td>
<td>9.62E-08</td>
</tr>
</tbody>
</table>
Since the coupling of fluid and heat flow presents a highly non-linear problem, the model has been run in transient state for both, fluid and heat transport until reaching quasi steady-state. The latter is assumed to be achieved after a maximum of $10^8$ days ($250$ kyrs) final simulation time, with an initial and maximum time step length of $10^{-3}$ days and $5 \times 10^3$ days.

2.3. Boundary and Initial conditions

To solve the mathematical problems presented in the preceding, thermal as well as hydraulic BC were implemented. The models utilized closed lateral boundaries for fluid and heat flow. The upper temperature BC was assigned as (1) $8\,^\circ$C for the conductive model (Sippel et al., 2013) and as (2) observed temperature distributions at the uppermost four stratigraphic interfaces for the coupled model (Topography, Holstein, Saale, Elster, Frick et al., submitted; SenStadtUm, 2014). The lower thermal BC is assigned in two different ways as well: (1) $1300\,^\circ$C at Lithosphere-Asthenoosphere-Boundary (LAB), representing the depth where the mantle adiabat cuts the geotherm corresponding to i.e. the solidus of mantle peridotite (Model 1 (M1), Noack et al., 2013; Sippel et al., 2013), (2) temperature distribution predicted at -6000 m.a.s.l. by Model A of Sippel et al. (2013) (Model 2 (M2)). The hydraulic BC was implemented as a constant pressure head ($M2$, 0 Pa, Dirichlet) at groundwater level derived from measured hydraulic heads (Frick et al., 2015; Frick et al., submitted; SenStadtUm, 2013).

The purely conductive simulation has been run in steady state due to the assumptions described in Section 2.1. In contrast, the coupled model was run in steady state for both, heat and fluid transport, separately, in order to derive the pressure and temperature initial conditions.

3. MODEL RESULTS AND DISCUSSION

The first model scenario investigated the influence of the new structural configuration described above (Frick et al., submitted), on the purely conductive thermal field. Predicted temperatures at -1000 m.a.s.l. range from 35.5$^\circ$C to 49.5$^\circ$C (mean = 43.0 $^\circ$C, Figure 2a) with local temperature maximal in the very E. W and NNW. The temperature distribution at this depth correlates strongly with the thickness distribution of the Permian Zechstein (Figure 2b), where highest predicted temperatures are located at thickness maxima and vice versa. This observation is connected to the thermal properties and geometries of model units. Due to the high thermal conductivity of the Permian Zechstein salt ($\lambda = 4.5 \frac{\text{W}}{\text{mK}}$) heat is carried upwards most effectively where the model unit is thickest (chimney effect). In combination with the overlying lowly thermally conductive sediments ($\lambda_{\text{average}} = 2.74 \frac{\text{W}}{\text{mK}}$) the increased upward heat flow is impeded (thermal blanketing) leading to positive thermal anomalies. At -5000 m.a.s.l. predicted temperatures show minimum values of 104.0 $^\circ$C and maxima are as high as 127.7 $^\circ$C (Figure 2b). The distribution of highest and lowest temperatures here is the direct opposite to those at -1000 m.a.s.l. due to a position largely below the base of the Zechstein at this depth level. Hence, negative thermal anomalies caused by the chimney effect are located where thickness maxima of the Zechstein are located and vice versa.

To single out the absolute effect of the modified structural configuration on the thermal field, the results of the preceding are compared to the purely conductive model (Model A) of Sippel et al. (2013) which only differs in this parameter. Differences in the thermal field are most clearly pronounced in the upper model domain, where temperature differences range from +1.6 K to -1.4 K at -1000 m.a.s.l. (Figure 2c). These differences correlate well with the modified thickness distribution of the Rupelian clay (Figure 2c), which displays low thermal conductivities ($1.88 \frac{\text{W}}{\text{mK}}$, Table 1). The thickness differences of this unit between the different structural model realizations correlate linearly to the changes in predicted temperatures: predicted temperatures increase by 0.1 K per 10 m increase in thickness and vice versa (Figure 2c). This correlation becomes less pronounced at higher depths where modifications of the thickness distribution of the Permian Zechstein are more influential. A reduction of the total thickness of the latter in the S of the model area leads (Section 1.2, ~230 m, Frick et al., submitted) to up to 3.1 K higher temperatures at -3500 m.a.s.l. due to a reduction of the heat withdrawn through the highly thermally conductive Zechstein. The differences in predicted temperatures at this location are also a derivative of the superposition of the decreased thickness of the Zechstein and increased thickness of the Rupelian. In conclusion the conductive model shows, that changes of the geometry of model units can lead to an increase of thermal blanketing enacted by lowly thermally conductive sediments (e.g. Rupelian) and a reduction of the chimney effect of thermally highly conductive sediments (e.g. Zechstein). In combination this might lead to temperature differences up to 3.1 K.

The second model run in this study implemented convection as an additional heat transport process along with a more precise temperature BC (after measured data, see Section 2.3, Frick et al., submitted; SenStadtUm, 2014) and measured groundwater levels as hydraulic BC (see Section 2.3, Frick et al., 2015; Frick et al., submitted; SenStadtUm, 2013) to be comparable to Model D of Frick et al. (2015). The latter implemented approximately the same BC thus differing only in the structural configuration of model units. This approach enables isolating the effect of modifications of the structural configuration on the subsurface thermal and hydraulic field.

Model 2 of this study predicts temperatures at -1000 m.a.s.l. ranging from 36.5 $^\circ$C to 50.1 $^\circ$C (mean = 43.4 $^\circ$C, Figure 2d). Major maxima and minima are in agreement with the results of M1 and also to temperatures predicted by Model D of Frick et al.
Temperature differences between M2 and M1 are up to ±3.5 °C at -1000 m.a.s.l. (Figure 2c, e). These differences are mainly located in areas where the Rupelian is discontinuous (hydrogeological windows, Figure 1c, Figure 2e). Additionally, areas where the hydraulic boundary condition displays high gradients show coldest temperatures (up to -3.1 K at -1000 m.a.s.l., Figure 2d) and vice versa (up to +3.5 K at -1000 m.a.s.l., Figure 2e). Elevated temperatures at -1000 m.a.s.l. below the city center of

**Figure 2:** Model results for Models 1 and 2. (a) Predicted temperatures for Model 1 (M1) at -1000 m.a.s.l., (b) at -3500 m.a.s.l., (c) Differences between predicted temperatures of M1 and Sippel et al. (2013) Model A at -1000 m.a.s.l., stippled contour lines indicate thickness differences between the different structural models for the Oligocene Rupelian (positive = higher in new structural model, negative = lower), (d) Predicted temperatures at -1000 m.a.s.l. for Model 2, yellow cross = Gt Velten 2/90, blue cross = Gt Berlin-Wartenberg 2/86, (e) Difference between the temperature of M2 and M1 at -1000 m.a.s.l., (f) Differences between predicted temperatures of M2 and Frick et al. (2015) Model D at -1000 m.a.s.l., (e, f) shaded grey areas represent 0 m thickness of Rupelian (darker = new -, brighter = old structural model), hashed blue areas represent high hydraulic potential (derived from measured groundwater levels, SenStadtUm, 2013).
Berlin relate closely to the implemented upper thermal BC which displays higher temperatures at those locations as well (surface sealing, Limberg and Thierbach, 2002). These results indicate, that while forced convective cooling is likely the major driving mechanism for convective heat transport, it is much less influential and pronounced than previously assumed (Frick et al., 2015; Sippel et al., 2013). In comparison to Model D by Frick et al. (2015) which basically only differs in the structural model configuration, this observation is outlined most clearly. Here, M2 predicts temperatures up to 12.0 K warmer and 0.7 K colder at -1000 m.a.s.l. (Figure 2f). Highest differences are generally located in regions where the previous structural model showed discontinuities of the Rupelian aquitard which do not appear in the new geometrical representation of the latter. These differences reach their maximum values where the regions described above are additionally close to or directly below areas of high hydraulic potential (Figure 2e). Lowest to no changes in predicted temperatures are visible where Rupelian discontinuities prevail or where a low hydraulic potential is evident. In comparison with the first coupled model presented by (Sippel et al., 2013), where forced convective cooling of the deeper (> 1 km) subsurface was identified to account for up to -22.5 K, the implementation of new data led to a drastic reduction of the influence of this process which can mainly be attributed to the structural modifications of the new model (Frick et al., submitted).

The validity of these models is difficult to determine, since a wide database of e.g. measured temperatures is not existent at this point of time. At the two available deep wells (1) Gt Berlin-Wartenberg 2/86 and (2) Gt Velten 2/90, predicted and modeled temperatures of M2 (as most refined model of this study) show a good fit. Especially in the shallow model domain (<1000 MD = measured depth [m]) modelled temperatures are largely within ±2 K compared to the measured values (Figure 3). At higher depths, predicted temperatures are generally too cold, which is most pronounced at Gt Velten 2/90, where borehole bottom temperatures are up to 6.5 K colder than the measured values (Figure 3). This misfit is likely a derivative of a lack in accuracy of the physical parameterization of the Pre-Cenozoic succession due to only sparsely distributed information on the latter as has been discussed in Frick et al. (submitted). Additionally, Frick et al. (submitted) presented a new approach for physical property assignment which might offer some future possibilities for more accurate differentiations of model units in terms of e.g. hydraulic conductivities. Additionally, the hydraulic BC might lead to an overestimated infiltration of cold surface waters even despite the fact that it was implemented according to measured groundwater levels.

Consequently, ongoing studies focus on the implementation of surface water bodies, groundwater recharge rates and groundwater wells for a more precise representation of the surface and shallow subsurface hydraulic conditions. These parameters could also be used for model validation, aiming at a consistent model of the present-day thermal and hydraulic configuration of the Berlin subsurface. Solute transport should also be considered in future studies as salinization problems are common in the NEGB (e.g. Kaiser et al., 2013; Magri et al., 2008).

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**Figure 3**: Modeled versus measured temperatures for M2 at observation wells (1) Gt Berlin-Wartenberg 2/86 and (2) Gt Velten 2/90. Location in Figure 2d. Vertical black lines indicate ±2 K bins. Depth coverage of (1): +56 m.a.s.l. to -1693 m.a.s.l., (2) +33 m.a.s.l. to -1628 m.a.s.l., sampling interval = 1 m. MD = measured depth [m].
4. CONCLUSIONS

The models run in this study show clearly that the geometrical configuration of model units asserts major influence on the geothermal field. Especially the structural configuration of the shallow Rupelian aquitard significantly affects both, the purely conductive and coupled thermal and hydraulic fields. The results also indicate that the overall magnitude of forced convective cooling of the subsurface is drastically lower than in earlier studies in the Berlin area. These findings underline the importance of the implementation of highly resolved structural data into 3D models as soon as they become available since associated modifications of the thermal and hydraulic field might drastically change temperature predictions at depths of interest for geothermal exploration. Additionally, a higher model unit differentiation might assist to identify possible scenarios of shallow aquifer salinization.

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