Proceedings World Geothermal Congress 2020
Reykjavik, Iceland, April 26 – May 2, 2020

3D-Temperature Estimation Using Geostatistical Methods

Thorsten Agemar

Leibniz Institute for Applied Geophysics, Stilleweg 2, 30655 Hannover, Germany

thorsten.agemar@leibniz-liag.de

Keywords: temperature, kriging, geostatistics, 3D, information system, GeotIS

ABSTRACT

The temperature field down to a depth of 5000 m below sea level has been estimated for Germany and Upper Austria in a consistent manner with universal kriging in 3D space. Conventional temperature mapping interpolates the temperature between sample locations at certain depths. This way, no consistency between different depth levels is ensured. Information from shallower levels gets lost. Kriging provides the best fit to measured temperatures. Another major advantage of kriging over conventional mapping algorithms is the prediction of the uncertainty associated with the temperature estimate. Any temperature estimate would lose much of its meaning without considering the uncertainty. 3D kriging resolves most of the limitations of conventional mapping techniques, however, like any statistical estimation it does not take into consideration varying thermal conductivities or the thermal convection of fluids. The 3D subsurface temperature model is used as an example to demonstrate what has to be considered when applying the 3D kriging method. Details are also given on current research that focuses on handling various data qualities in the kriging system.

1. INTRODUCTION

The subsurface temperature field is heterogeneous. Although temperature generally increases with depth, there are locations in Germany and Upper Austria where the temperature gradient is higher or lower than the average value of approximately 32 K/km. Particularly, in some parts of the Upper Rhine Graben, the area around Bad Urach at the foothills of the Swabian Alb, or at the Landshut-Neuöttinger fault zone near Landshut in Bavaria, or in some parts of the North German Basin, the temperature increases by more than 5 K per 100 m depth. These areas are affected by so-called positive temperature anomalies. These anomalies are beneficial for geothermal energy utilisation because the targeted temperature can already be reached at shallower depths resulting in lower drilling costs. Thus, mapping subsurface temperature distribution from available measurements is an important step for assessing geothermal resources (Agemar et al. 2018, Agemar et al. 2014). In order to estimate the temperature of a geological body at any depth, it is necessary to determine the temperature at any point in a consistent 3D-temperature model. A 3D interpolation method suitable for developing such a model is universal kriging, a geostatistical approach. Universal kriging makes it possible to accommodate a trend in data which is essential for the estimation of subsurface temperatures. Generally, kriging estimates are weighted linear or non-linear combinations of the available data. It is the only method which allows the inclusion of measured spatial variability in the estimation process. Another major advantage of kriging is the calculation of the uncertainty associated with the predicted values. The subsurface temperature model for Germany presented here is also part of the public geothermal information system GeotIS. Subsurface temperatures are estimated for depths ranging from ground level to 5000 m below sea level. The geostatistical temperature model has been continuously updated, most recently in 2018. This temperature model is calculated with 3D kriging on the basis of various temperature data of the subsurface measurements available in the Geophysics Information System (FIS-GP) and soil temperature values derived from average air temperature data.

2. DATA

All subsurface temperatures were taken from the Geophysics Information System of the LIAG, which has temperature data from approx. 11,000 boreholes. The majority of these data are from Germany but data from some neighboring countries are also available. Soil temperatures were derived from air temperature measurements of the German Meteorological Organisation (DWD) and meteorological organisations abroad of the period 1961-1990 as described in Agemar et al. (2012).

The Geophysics Information System contains a large amount of geophysical data, primarily within Germany, consisting of a main system and various subsystems. The geothermal subsystem (Schulz and Werner, 1989) contains validated subsurface temperature and provides manual and automated correction of raw data (Table 1). Equilibrium temperature logs and reservoir temperatures are considered to be optimal data which require no corrections. Because of the regular monitoring of production wells over many years, reservoir temperatures are available in time series; the fluctuation in these temperatures is mainly less than 1 K. Bottom-hole temperature data (BHT) are also stored in the geothermal subsystem. These BHT values are recorded in almost all industrial boreholes at the deepest point of the well immediately after drilling has stopped. BHTs are frequently measured at different depths during the drilling operation, resulting in two or more BHT-depths per well.

3. METHODS

The temperature field around a borehole is usually disturbed by mud circulation related to the drilling process. A number of methods to extrapolate the undisturbed temperature have therefore been developed based on various assumptions about the cooling effect of the circulating mud and the thermal behavior of the borehole and the surrounding rock. A review of existing correction methods can be found in Hermanrud et al. (1990). The choice of the most appropriate correction method depends on the availability of data such as the circulation period, the elapsed time after the end of drilling, the number of subsequent measurements, and the well radii. Despite such corrections, these results still have errors of up to ±8 to 10 K (Hermanrud et al., 1990; Förster, 2001), and are therefore much less accurate than equlibrium temperature logs.

Table 1: Available subsurface temperature data from Germany and some bordering areas of neighbouring countries. The last two columns show the increase in available data over four years. Also note the division of the top category in two categories in 2018.

<table>
<tr><th>Code</th><th>Type</th><th>Quality category</th><th>Number of wells 2018</th><th>Number of wells 2014</th></tr>
<tr><td>LOG-1</td><td>Equilibrium log</td><td rowspan="3">1</td><td rowspan="3">2613</td><td rowspan="4">3602</td></tr>
<tr><td>RESERVOIR</td><td>Reservoir</td></tr>
<tr><td>MINE</td><td>Mine or tunnel</td></tr>
<tr><td>TEST</td><td>Hydr. testing</td><td>2</td><td>1028</td></tr>
<tr><td>3Z</td><td>BHT, > 2 shut-in times
Cylinder Source Model</td><td rowspan="6">3</td><td rowspan="6">4462</td><td rowspan="6">4367</td></tr>
<tr><td>2L</td><td>BHT, 2 shut-in times
Instantaneous Line Source Model</td></tr>
<tr><td>2H</td><td>BHT, 2 shut-in times
Continuous Line Source Model</td></tr>
<tr><td>LOG-2</td><td>Non-equilibrium log
(moderately disturbed / corrected for NE-Germany)</td></tr>
<tr><td>1E</td><td>BHT with 1 shut-in time & radius
Cylinder Source Model</td></tr>
<tr><td>1ES</td><td>BHT with 1 shut-in time</td></tr>
<tr><td>1ER</td><td>BHT with radius but without shut-in time</td><td rowspan="2">4</td><td rowspan="2">4011</td><td rowspan="2">4057</td></tr>
<tr><td>1EO</td><td>BHT without details</td></tr>
</table>

The best correction results can be obtained for BHTs if a series of two or more shut-in times is available. In this study, depending on the quality and quantity of the available data, the following correction methods have been applied (Schulz et al., 1992; Schulz and Schellschmidt, 1991):

Cylinder source model: If three or more BHT values are available for one depth at different times after mud circulation stops, the thermal stabilization method for a cylindrical borehole can be used (Leblanc et al., 1982; Middleton, 1982). In this approach, it is assumed that the temperature of the mud when circulation stops (t = 0) is constant, and varies by a ΔT from the undisturbed rock temperature:

$$\boldsymbol{T_\infty = BHT(t) - \Delta T\left(e^{\frac{-a^2}{4\kappa t}} - 1\right)} \qquad (1)$$

where T_∞ = undisturbed rock temperature (°C)

BHT = measured bottom hole temperature (°C)

ΔT = initial temperature disturbance (K)

a = borehole radius (m)

κ = thermal diffusivity (m²/s)

t = time after circulation stops, shut-in time (s)

The undisturbed rock temperature is calculated by a fitting method varying ΔT and κ, where κ is the effective thermal diffusivity of the mud and the surrounding rock (Schulz et al., 1992).

Continuous line source model: If only two BHT values are available, a line source approach is derived from the negative heat transfer during the circulation time of the mud (Horner, 1951).

$$T_\infty = BHT(t) - \frac{q}{4\pi\lambda}\ln\left(\frac{t+s}{t}\right) \qquad (2)$$

where q = heat flow rate per length unit (W/m)

λ = thermal conductivity (W/mK)

s = circulation time (s)

Instantaneous line source model: If the circulation time can be ignored, a line source approach with an "explosion" heat sink is used (Lachenbruch and Brewer, 1959):

$$T_\infty = BHT(t) - \frac{Q}{4\pi\lambda t} \qquad (3)$$

where Q = heat per length unit (J/m)

Cylinder source model using estimated parameters: If only one shut-in time is available, the cylinder source model (Eq. 1) is used again. The initial temperature disturbance is estimated on the basis of an empirical relation between undisturbed rock temperature and well radius (Agemar 2020):

$$\Delta T = \frac{(T_\infty - T_0)}{31a} \qquad (4)$$

where T_0 = surface temperature [°C]

a = well radius [m]

Furthermore, non-equilibrium logs, if not discarded at all, have been corrected for the eastern part of the North German Basin. Mud circulation results in higher temperatures in the upper part of the well, whereas the lower part of the well is cooled. Any correction of non-equilibrium logs requires knowledge of depth level of the cross-over point where temperature is neither raised nor lowered. Förster (2001) established an empirical relation of the this cross-over point for the eastern part of the North German Basin:

$$X = 0.39\,TVD + 267 \qquad (5)$$

where X = cross-over point [m]

TVD = true vertical depth [m]

The amount of correction applied has been derived by comparison of surface temperature and extrapolated surface temperature from the upper part of the log.

The methodology applied is largely the same as described in Agemar et al. (2012). However, the distance rules for the quality filter in data selection were tightened and an additional quality category for temperature measurements by pump tests has been introduced. Research in borehole records has shown that temperature measurements from pump tests often do not reflect the undisturbed formation temperature as reliably as certain reservoir temperatures or undisturbed temperature logs, but are generally better than corrected bottom hole temperatures (BHT). The subsurface temperature measurements are divided into 4 quality categories:

- Equilibrium logs and steady state reservoir temperatures (category 1)
- Temperature records from pump tests (category 2)
- Non-equlibrium logs and corrected BHTs with known shut-in times (category 3)
- BHTs corrected on the basis of guessed shut-in time (category 4)

The distance rule states that less reliable measurements up to a certain distance from a higher quality measurement are not used if they are located no more than 500 m lower than the higher quality measurement. Measurements of the second quality category are not used within a radius of 5 km of a measurement of the highest category 1. For category 3 measurements the radius shall be 10 km and for category 4 measurements the radius shall be 20 km. The background of this distance-based filtering is that the significance of a temperature measurement for the prognosis decreases with increasing distance, depending on the spatial variance. The tightening of the distance rules compared to Agemar et al. (2012) was due to a new assessment of the data quality and a stronger weighting of the spatial variance especially in southern Germany. The lowest data quality (category 4) was used for the forecast of the temperature field only at 37 wells with 69 measurements, since in all other areas measurements of higher quality were in the vicinity. 5534 BHTs had to be discarded due to missing shut-in time.

After data acquisition, validation, correction and selection, geostatistics were applied for the prediction of subsurface temperature at unsampled locations. The geostatistical approach generally assumes spatial continuity and does not consider varying geological settings. Rocks and minerals have a broad range of thermal conductivities: for example, the thermal conductivity of halite is 2–3 times higher than most other minerals. Thus, a geostatistical prediction may not reflect the true temperature field where salt domes or salt pillows occur. In such a setting, local numerical models may provide more meaningful results. On the other hand, numerical models require detailed knowledge of subsurface thermal conductivity and heat flow density, information which is only partly available. Furthermore, convective heat transfer in porous, fractured or karstified rocks is extremely difficult to model because knowledge of subsurface fluid pathways and hydraulic potentials is incomplete. Numerical models of subsurface temperature are therefore limited in space and accuracy.

The geostatistical estimation process is based on a model of the spatial variability of subsurface temperature. Here, a spherical model function has been fitted to the measured variability (semi-variogram model). It relates spatial kriging variance to distance between sample pairs and describes the spatial dependence of a random field. The intercept is commonly called the nugget effect. It is attributed to small-scale random variability. Regarding subsurface temperature data, heat conduction should mitigate any discontinuity. Here, the nugget effect is probably due to measurement errors. A high nugget effect acts as a smoothing term during kriging estimation as it makes weights more similar. With growing separation, the kriging variance value also increases until it reaches a plateau. The separation distance beyond which the variogram value remains constant is commonly called the range, which defines the scope of the kriging estimation. The plateau level is called the sill. It refers to the variogram value reached at the range distance. Estimates of unsampled areas are produced from weighted combinations of the neighboring samples with respect to both distance and redundancy. The individual weights are assigned on the basis of minimizing the kriging variance. This ensures the most precise estimates possible from the available data. Since the estimates are only as good as the model fits to the observed variogram values, it is important that the variogram is accurate over the whole estimation area. If this second-order stationarity assumption is inappropriate, it might help to subdivide the data set into smaller regions within which samples appear to be more homogeneous.

Universal kriging can calculate a trend automatically and produces good local estimates even when the estimate is extrapolated from neighboring sample values. Some data sets exhibit a non-normal distribution of sample values. The kriging variance and mean are related to probability through the assumptions of a Gaussian distribution. If the available data do not satisfy the criteria of statistical normality, applying a data transformation before geostatistical operations can solve this problem.

Kriging not only yields values for unsampled locations but also the uncertainty associated with these values, a result that other prediction methods are unable to provide.

The gridded soil temperature derived from air temperatures serve as the upper limit in the estimation process and cover Germany and adjacent areas of neighbouring countries. The sample coverage of the subsurface is less optimal. The distribution of samples reflects the geographical as well as the stratigraphic interests of oil and gas exploration. Most wells with temperature data are in the North German Basin. The remaining wells are concentrated in the Thuringia Basin, the Upper Rhine Graben and the Molasse Basin in southern Germany. Subsurface temperature data for other regions are quite scarce. Besides the variable geographical distribution, there is also a decline in data density with depth (Fig. 1). Another problem is the co-existence of log data and scattered point data in the same data set. Log data is distributed along the well path and would be weighted too high compared to wells or mines with few samples. Furthermore, this data distribution could erroneously lead to a temperature field with locally negative gradients. In order to overcome this problem, virtual profiles were created by vertical interpolation between samples at various depths of the same well or between one sample and surface temperature. This has been accomplished by applying a linear temperature/depth relation, ignoring the effect of varying thermal conductivity. However, even with this approach, very few grid nodes of the kriging estimate show small negative geothermal gradients. Tiny gradient anomalies are considered as artefacts due to a locally too low vertical range parameter. These anomalies were removed by smoothing since the subsurface temperature field is predominantly controlled by heat conduction and most negative gradients are very unlikely to exist in reality.

The complete data set shows a distribution with a small tail for higher temperatures for single depths. Thus, the data set does not fully satisfy the basic assumption of statistical normality. The data produces an slightly asymmetric histogram. This problem has been resolved by applying multi-Gaussian kriging. Each sample value is mapped from its original cumulative frequency to the standard S-shaped curve corresponding to a normal distribution. The normal score values have a mean value of 0 and a standard variance of 1.

Table 2: Grid specifications and kriging parameters applied.

Grid resolution (orthogonal)	lateral: 2000 m	
	vertical: 100 m	
Coordinate system	Gauss Krueger	
	central meridian at 9°E	
Map dimensions	660 km x 880 km	
	Easting: 3267000 – 3927000	
	Northing: 5225000 – 6105000	
Kriging parameters:	North:	South:
Model fit	spherical	spherical
Range lateral	75 km	75 km
Range vertical	2 km	2 km
Sill	1.0 (normal score)	1.0 (normal score)
Nugget	0.2	0.2

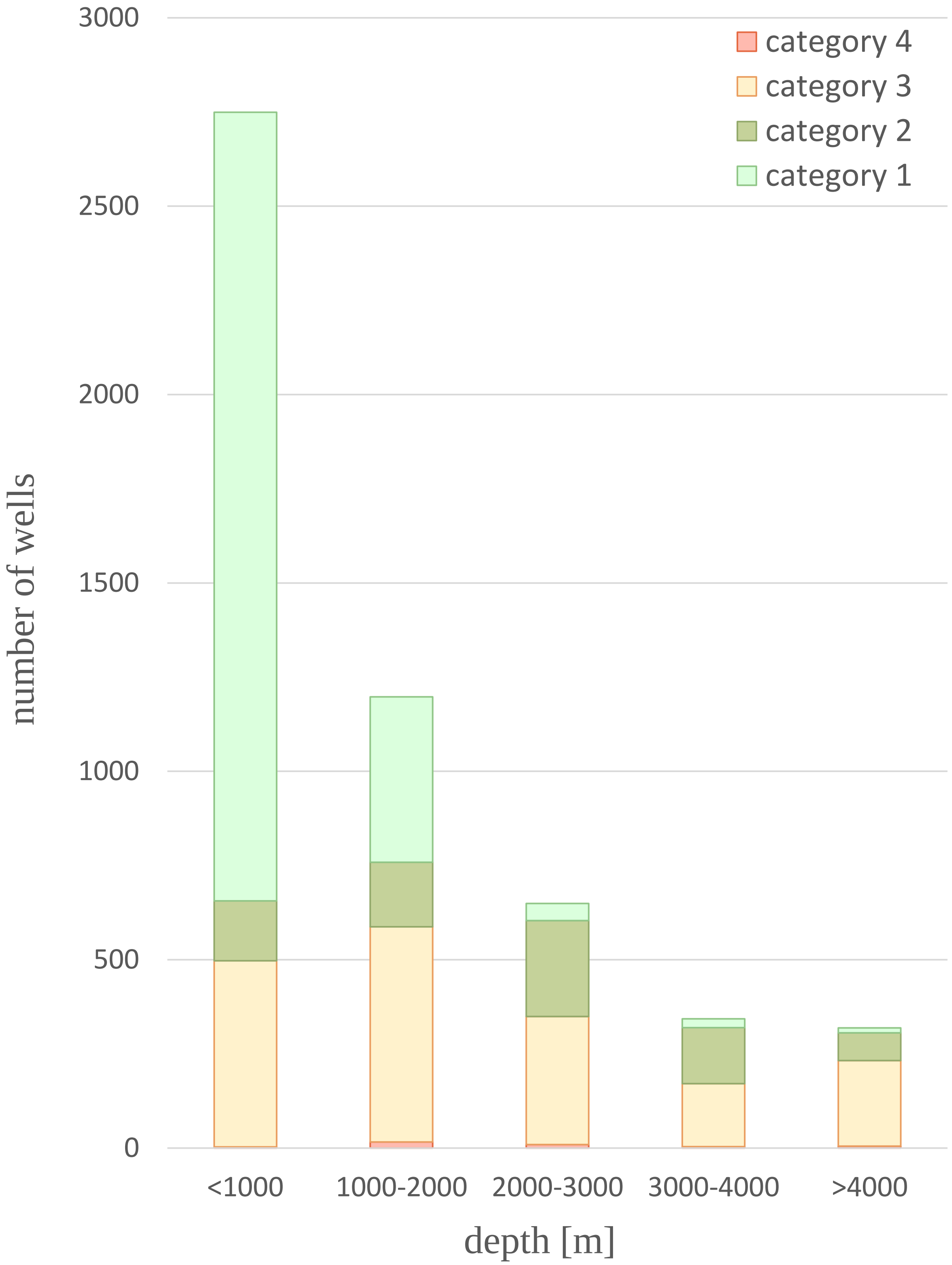

Figure 1: Input data selected for the 3D subsurface temperature model. Each column represents a different depth range. Deep wells make up a only a small fraction of total wells with temperature data. Top quality temperature records become rare with increasing depth. Medium quality temperature records prevail in depths larger than 2000 m.

The values at unsampled locations are drawn from an inverse normal score transformation of the estimates developed in Gaussian data space. This approach has basically two benefits. First, it simplifies the development of a useful variogram relationship, and second, it damps peak values and thus improves the kriging estimate in areas of low data density. Confidence envelopes can be determined by adding the estimated standard deviation to the estimate for the upper limit, and subtracting for the lower limit.

Unfortunately, GOCAD/SKUA does not allow the transformation of upper and lower limits back to original values. The confidence interval must be approximated by analysing the relation between depth and lateral variance for each model (north and south). The probability that the true value is either less than (or greater than) the predicted value is 50%. The probability that the true value falls within one standard error either side of the estimated value is 68%; and the risk that it is less than the lower limit is 16%. Because of the non-linear transform of subsurface temperature data to normal score before kriging, the confidence interval is now also non-linear and not exactly symmetrical about the estimate on the original scale. Hence, the combined statement of predicted value and confidence envelope must be treated with care – the estimate may have less than 68% confidence.

The geostatistical analyses and the kriging estimation of subsurface temperatures were performed using Paradigm's GOCAD/SKUA software package. The 3D grid of the kriging estimates is orthogonal and the vertical axis is set to zero at sea level, not at ground level.

3D-model specifications and kriging parameters derived from the variogram analysis are summarized in Table 2. The sill of the northern part is generally lower than for the southern part. If spatial variability is analysed for various depth levels one can show that the sill is low close to the surface and reaches maximum values between 2.000 and 4.500 below sea level. This has implications for the estimation of the correct kriging variance but not for the temperature estimates. The kriging variance depends on depth and regional spatial variability.

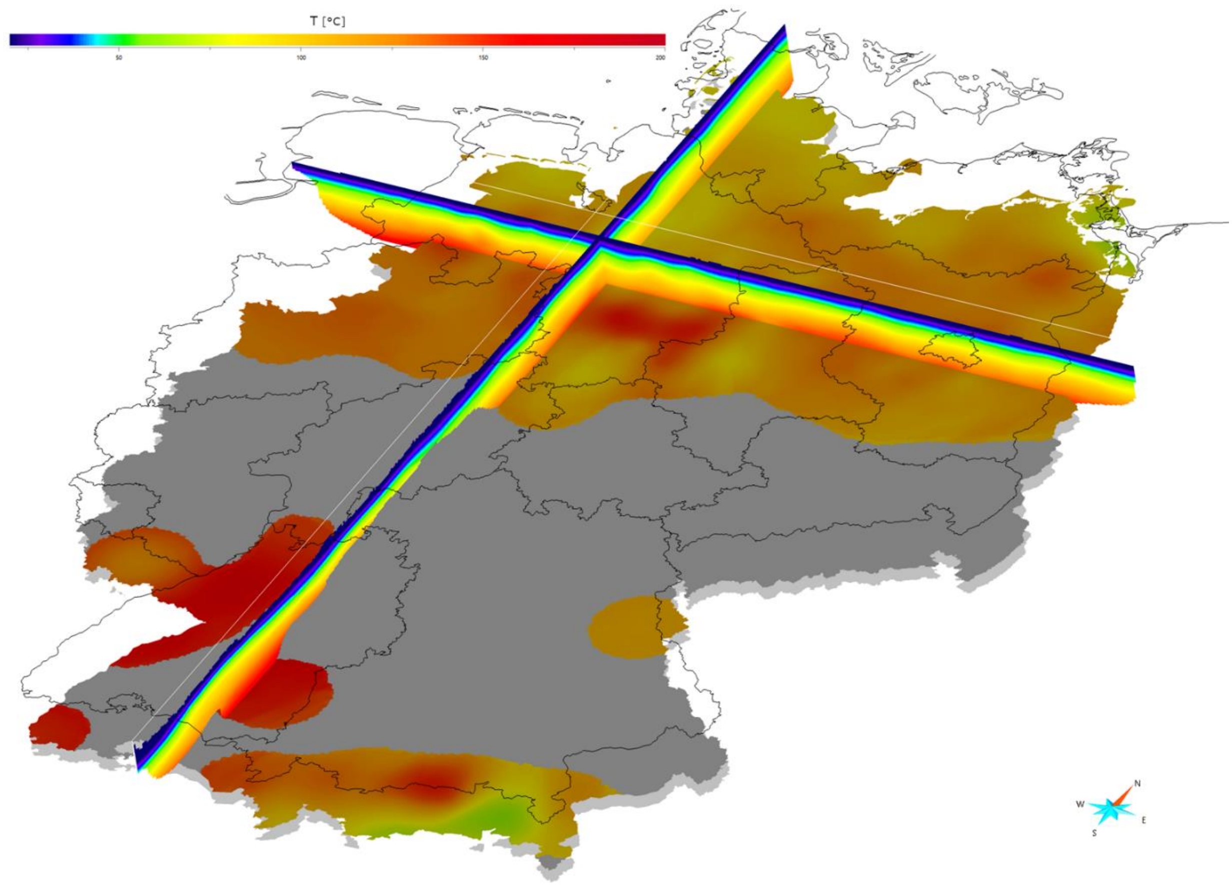

Figure 2: 3D subsurface temperature model of Germany as implemented in the geothermal information system GeotIS.

4. RESULTS

Figure 2 shows the 3D subsurface temperature model. The reduced data density at deeper levels results in expanded gaps in the temperature model predominately in the Central German Uplands and in southern Germany. The mapped 3D temperature model ends where the normalized kriging variance reaches 1.0 and, hence, the kriging estimate becomes less reliable than a simple prediction on the basis of the average geothermal gradient.

At 1000 m below sea level, temperatures range from 30 °C to 122 °C with a mean value of 48 °C. At 2500 m below sea level, temperatures range from 61 °C to 161 °C with a mean value of 94 °C. At this depth level, many areas show temperatures above 100 °C. Areas with temperatures above 150 °C are found in the northern part of the Upper Rhine Graben. These unusually high temperatures are probably limited to areas of upwelling groundwater along fracture zones (Clauser and Villinger, 1990; Pribnow and Clauser, 2000; Pribnow and Schellschmidt, 2000). This could also explain the high spatial variability of subsurface temperature in the Upper Rhine Graben.

Low geothermal gradients are encountered near the Alps in the southernmost part of the Molasse Basin and in the area of the Wasserburg Trough approximately 40 km east of Munich. In the area of Lake Chiemsee, the geothermal gradient decreases to 25 K/km.

Further north, within the Central German Uplands, there are only a few wells with temperature records below 3 km depth. It is therefore difficult to assess the subsurface temperature field. The deepest temperature measurements stem from wells of the Deep Continental Crust Drilling (KTB) in the Oberpfalz (Upper Palatinate) with a maximum depth of 9101 m. The wells of the Central German Uplands are located far apart from each other in different geological settings. Relatively high subsurface temperatures are found, for instance, at Urach due to high geothermal gradients especially in the first 400 meters. This anomaly can be explained with heat insulating formations close to the surface. The average geothermal gradient for the mapped area is 32 K/km in the depth range from 0 to 2000 m bsl. However, the geothermal gradient exhibits a wide range with locally more than 100 K/km.

Elevated temperatures are also found above the top of salt bodies due to high thermal conductivity of rock salt. The calculation of temperature fields around salt structures is discussed in the literature (Petersen and Lerche, 1995, and references therein). Local upwelling of thermal waters may also result in positive temperature anomalies or even hot springs. Another mechanism for high subsurface temperatures relates to crustal thinning below graben structures that raise regional heat flow density.

5. CONCLUSIONS

The kriging estimate of the subsurface temperature represents the best fit to the available data. The most important prerequisites for the 3D subsurface temperature model are the amount and accuracy of temperature measurements. Kriging, like any other geostatistical estimation, cannot compensate for missing or false data. The rejection of less accurate data in the vicinity of more accurate data improves the quality of the estimation. In comparison to the former 3D temperature model (Agemar et al. 2012) the stricter quality rules, the improved BHT correction (Agemar 2020), and the acquisition of new data led to a better predictability of subsurface temperatures. The filtering cascade with four instead of three quality categories is simple to apply. However, round about 60 % of subsurface temperature data were not used because of low quality. A more sophisticated approach could be to increase sample weighting according to measurement accuracy. In this study, the constant nugget effect refers to a combination of small-scale variability and measurement error of the filtered data set.

This subsurface temperature distribution is an integral part of the public geothermal information system for Germany (GeotIS) and can be accessed via the Internet with standard browsers. Users can display temperature estimates on geologic horizons as well as on horizontal or vertical cross sections. The use can also retrieve temperature estimates and kriging related standard deviation by moving the mouse pointer over the area of interest.

ACKNOWLEDGEMENTS

Part of this work has been funded by the German Federal Ministry for Economic Affairs and Energy (BMWI) within the framework of the Geofaces project (Grant no. 0324025A).

REFERENCES

Agemar, T.: Improving Bottom-Hole Temperature Corrections on the Basis of Statistical Correlations. *Proceedings of the World Geothermal Congress 2020*, April 26 – May 2, Reykjavik, Iceland

Agemar, T., Schellschmidt, R., and Schulz, R.: Subsurface temperature distribution in Germany. *Geothermics* **44**, (2012), 44, 65–77.

Agemar, T., Weber, J., and Schulz, R.: Deep Geothermal Energy Production in Germany. *Energies*, **7**, (2014), 4397–4416. doi.org/10.3390/en7074397

Agemar, T., Weber, J., and Moeck, I.S.: Assessment and Public Reporting of Geothermal Resources in Germany: Review and Outlook. *Energies*, **11**, (2018), 332; doi:10.3390/en11020332

Agemar, T., Weber, J., and Schulz, R.: Deep Geothermal Energy Production in Germany. *Energies*, **7**, (2014), 4397–4416.

Clauser, C., and Villinger, H.: Analysis of conductive and convective heat transfer in a sedimentary basin, demonstrated for the Rheingraben. *Geophysical Journal International*, **100 (3)**, (1990), 393–414.

Förster, A.: Analysis of borehole temperature data in the Northeast German Basin; continuous logs versus bottom-hole temperatures. *Petroleum Geoscience*, **7**, (2001), 241–254.

Hermanrud, C., Cao, S., and Lerche, I.: Estimates of virgin rock temperature derived from BHT measurements: Bias and error. *Geophysics*, **55(7)**, (1990), 924-931.

Horner, D.R.: Pressure build-up in wells. Third World Petroleum Congress, The Hague, (1951), Netherlands.

Lachenbruch, A.H., and Brewer, M.C.: Dissipation of the temperature effect of drilling a well in Arctic Alaska. *Geological Survey Bulletin*, **1083 (C)**, (1959), 73–109.

Leblanc, Y., Lam, H.-L., Pascoe, L.J., and Jones, F.W.: A comparison of two methods of estimating static formation temperature from well logs. *Geophys. Prosp.* **30**, (1982), 348-357.

Middleton, M.F.: Bottom-hole temperature stabilization with continued circulation of drilling mud. *Geophysics*, **47**, (1982), 1716-1723.

Petersen, K., and Lerche, I.: Quantification of thermal anomalies in sediments around salt structures. *Geothermics* **24** (2), (1995) 253–268.

Pribnow, D.F.C., and Clauser, C.: Heat and fluid flow at the soultz hot dry rock system in the Rhine Graben. In: Iglesias, E., Blackwell, D., Hunt, T., Lund, J., Tamanyu, S. (Eds.), *Proceedings of the World Geothermal Congress 2000*. Kyushu – Tohoku, Japan, May 28 – June 10, (2000), IGA, Auckland, pp. 427–432.

Pribnow, D.F.C., and Schellschmidt, R.: Thermal tracking of upper crustal fluid flow in the Rhine Graben. *Geophysical Research Letters*, **27**, (2000), 1957–1961.

Schulz, R., and Schellschmidt, R.: Das Temperaturfeld im südlichen Oberrheingraben. Geologisches Jahrbuch, **48(E)**, (1991), 153-165.

Schulz, R., Haenel, R., and Kockel, F.: Federal Republic of Germany - West federal states. - In: Hurtig, E., Cermak, V., Haenel, R., Zui, V. (Eds.): Geothermal Atlas of Europe, Gotha, Germany, (1992), 34-37.

Schulz, R., and Werner, K.H.: Geothermal Resources and Reserves: Updating of Temperature Data Base. - In: Louwrier, K.,Staroste, E., Garnish, J.D., Karkoulias, V. (Eds.): European Geothermal Update. In: *Proceedings of the 4th International Seminar on Results of EC Geothermal Energy Research and Demonstration*, Kluwer Academic Publishers, Dordrecht, (1989), 490-499.