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Abstract

We present a 3D numerical crustal temperature model with inverse optimisation methodology and analyse the present-day conductive thermal field of the Danish onshore subsurface. The model is based on a comprehensive analysis and interpretation of borehole and well-log data for thermal and petrophysical rock properties and their regional variability and spatial distribution across the country. New values of terrestrial surface heat flow derived from 21 deep well locations are 65–76 mW·m⁻² (mean: 72±3) for the Danish Basin, 77–86 (81±5) for the Danish part of the North German Basin, and 61–63 (62±1) for the Sorgenfrei-Tornquist-Zone/Skagerrak-Kattegat Platform, respectively. The observed heat flow variations are consistent with the position of the Danish area in the transition zone between the old Precambrian Baltic Shield (low heat flow) and central European accreted terrains and deep basin systems (significantly higher heat flow).

For the temperature modelling, conductivities and heat flow are constrained and validated (rms: 1.2°C, ame: 0.7°C) by borehole temperature data covering a depth range of up to 5 km (137 values from 46 wells). Significant modelled temperature variations are caused by (i) complex geological structures (thickness variations, salt structures) and (ii) the variation of rock thermal conductivity between and within geological formations as well as lateral variation in background heat flow. Modelled temperature for major geothermal reservoirs indicate substantial potential for low enthalpy heating purposes. Reservoir temperatures above 130°C, of interest for the production of electricity, are observed for some local areas, however, likely, too deep for non-stimulated sufficient reservoir quality.

Keywords: Deep basin temperature field, heat-flow density, borehole analysis, 3D calibrated thermal modelling, core-log integration, uncertainty analysis, geothermal energy

Highlights

- This paper presents a 3D numerical temperature and heat-flow study of Danish onshore areas including deep sedimentary basins.
- We present 21 new heat-flow values with significant variation according to regional structural and tectonic background.
- Most of Denmark provides suitable conditions for low enthalpy geothermal utilization; local potential for electricity production.
- A spatial variable thermal parameterization excels the homogeneous approach in terms of temperature prediction accuracy.

Acknowledgements

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1.0 Introduction

General knowledge of heat flow and thermal structure of sedimentary basins is of critical importance for the understanding of basin formation and their tectonic evolution. Most basin generating mechanisms include important thermal components and may leave significantly different thermal signatures to be interpreted together with crustal and lithospheric structure for a proper understanding of basin formation and evolution (Allen and Allen, 2013). Furthermore, information about the internal thermal structure of basins is essential for the treatment of many practical and economic aspects. Examples include the assessment of geothermal resources, hydrocarbon maturity, and energy storage potential. Particularly, the recent year's awareness, that waste amounts of geothermal energy resources are present in sedimentary basins and may play an important role in future sustainable energy supply (e.g. Lund and Boyd 2015; Antics et al. 2016), has resulted in the need for accurate thermal information and thermal models.

This study presents a 3D numerical crustal temperature and heat-flow model for onshore Denmark. For the first time on a countrywide scale, a comprehensive analysis of well-log data provides well-constrained input for a fully parameterized and calibrated numerical subsurface temperature model. Early subsurface temperature models for the Danish area (e.g. Balling et al. 1981; 2002) were based on a dense grid of 1D analytical temperature-depth profiles. Now, 3D numerical models have been developed (Balling et al. 2016; Fuchs and Balling, 2016b; Poulsen et al. 2017), with emphasis on the parameter inverse calibration methodology and its application. Inverse parameter calibration procedures are widely used in groundwater modelling (e.g. Hill & Tiedeman 2007), but, so far, with little application for subsurface thermal modelling. Valuable exceptions include Wang and Beck, (1986), Gemmer and Nielsen (2001) and Vosteen et al. (2004). Such parameter estimation, or optimization procedures, were demonstrated to be of great importance, in particular in applying borehole-temperature data for constraining the thermal rock properties (Fuchs and Balling, 2016b; Poulsen et al., 2017) and are applied in the present study.

Our model builds on lab-constrained well-log derived rock thermal parameters (thermal conductivity [TC], specific heat capacity [SHC], and radiogenic heat production [RHP]), a procedure by Fuchs et al. 2016), new heat-flow determinations for 21 deep-well sites as well as on a new digital structural geological model. This fully updated structural model, based on a reinterpretation of all available reflection seismic lines across the country (Vosgerau et al. 2016), provides information on depth levels and thicknesses of 15 sedimentary units used as 'model input layers' for the sedimentary succession. With a model base at 15 km depth, also the upper parts of the crystalline crust are included.

As outlined in the following section, the Danish subsurface is characterised by thick sequences of sedimentary rocks forming deep basins separated by basement highs. So far, onshore, hydrocarbons have not been found in commercial amounts; however, the basins contain reservoir units with vast amounts of geothermal resources (e.g. Balling et al. 2002; Nielsen et al. 2004; Mathiesen et al. 2009). At present, three geothermal district heating plants are in operation in Denmark (positions in Fig. 1) and several more at planning stage. Current production is from Lower Jurassic and Triassic sandstone reservoirs at depths of 1.2–2.6 km and temperatures of 44–75°C and with plant thermal capacities between 7 and 14 MW (Røgen et al. 2015). Resource assessments and modelling studies indicate that geothermal energy has the potential for supplying the Danish district heating network with sustainable energy for centuries (Mathiesen et al. 2009; Mahler and Magtengaard 2010; Poulsen et al. 2017).

Figure 1. Left: Map of study area with structural elements and deep wells (colour code – red dots: with accurate equilibrium temperature logs; orange: with formation test temperatures; dark blue: with corrected bottom-hole temperatures (BHT; equilibrium estimates); light blue: wells with uncorrected BHTs (only minimum temperature estimates); small black circles: with no temperature information). Good quality temperature data from 46 wells are available, petrophysical logs from 39 wells (with yellow circle) provide information on rock thermal properties and new heat flow values are presented for 21 deep well sites (red diamond signature). Right: Depth to top Pre-Zechstein emphasizing deep basins and other structural elements shown in the structural map.

In the present study, in addition to providing general information on subsurface thermal structure, emphasis is on presenting detailed temperature information for potential geothermal reservoirs. Furthermore, we discuss crustal temperatures and deep heat flow in relation to the

special structural position of the Danish area in a tectonic transition between old Baltic Shield and central European accreted terrains and deep basin systems (*cf.* Gee and Stephenson, 2006; McCann et al. 2006; Balling, 2013).

2.0 Study area and geological setting

Information about the deep geological setting in Denmark originates largely from hydrocarbon exploration activities with seismic profiles and wells covering most of the country, however with an uneven distribution (Vosgerau et al., 2016). The interpretation of these data (Section 3.2) provides information on the regional structural setting and spatial distribution of sedimentary units. A comprehensive compilation of maps for geological formations and depth level is available in the geothermal webGIS portal from GEUS (<http://data.geus.dk/geoterm/>).

The Danish onshore subsurface is divided into five major structural units (largely from north to south): the Skagerrak–Kattegat Platform (SKP), the Sorgenfrei–Tornquist Zone (STZ), the Danish Basin (DB), the Ringkøbing–Fyn High (RFH) and the North German Basin (NGB) (Fig. 1). The sedimentary basins contain Palaeozoic, Mesozoic and Cenozoic sedimentary sequences of up to 5–10 km in total thickness. In contrast, sedimentary thicknesses of 1–2 km, and less, are found in areas with shallow basement highs (the RFH and SKP). The RFH consists of shallow basement blocks, where the thin Mesozoic sedimentary cover mainly comprises erosional remnants of Triassic sediments and Upper Cretaceous Chalk with a low geothermal potential. In contrast, the two basins host very large geothermal resources and several potential reservoirs. The basins are classic low-enthalpy sedimentary basins formed by crustal thinning followed by long-term thermal subsidence (Frederiksen et al. 2001) and infilling by a variety of sediments (e.g. Michelsen et al. 2003; Michelsen & Nielsen 1991). These structural differences exert a decisive influence on the geothermal prospectivity of the Danish subsurface, as they essentially determine the distribution, thicknesses, facies types and burial depths of the potential reservoirs (e.g. Nielsen 2003; Nielsen et al. 2004; Erlström et al., 2018).

The geographical coverage and quality of the data vary considerably. The seismic data combined with information from deep wells have been used for largescale mapping of depth, thickness and lateral extent of lithostratigraphic units in general, and with special emphasis on units known to contain geothermal reservoir sandstones, as well as for identification and mapping of major faults and salt domes (Vosgerau et al., 2016). The deepest mapped seismic reflector is the Top Pre-Zechstein horizon (Fig. 1B). The lack of data coverage and seismic data with high resolution hampers the interpretation and mapping of the deepest horizons and consequently, mapping uncertainties are generally larger for the deepest horizons than for the shallower horizons and the associated reservoir units.

Regional maps were interpreted in two-way travel time (TWT) and were converted to depth insuring that the difference between measured depths in wells and those extracted from the depth-converted maps are as small as possible. The mapped and depth-converted surfaces applied in the present model are estimated to have uncertainty between 5 and 10%, generally increasing with depth, and may be up to 15% in areas with poor seismic data coverage.

Figure 2. Schematic lithostratigraphic units across main structural elements from south/southwest to north/northeast (North German Basin, NGB; Ringkøbing-Fyn High, RFH; Danish Basin; Sorgenfrei-Tornquist Zone, STZ; Skagerrak-Kattegat Platform, SKP, see also Fig. 1). The main potential geothermal reservoirs are shown in yellow and orange with indicated total thickness ranges. The Gassum and the Bunter-Sandstone-Skagerrak reservoirs have a large regional distribution, and other reservoirs a more limited distribution. Lithological units, implemented into the numerical geothermal model are indicated with their associated numbers (right column), maintained throughout this paper (e.g. Table 1).

The derived subsurface 3D structural model with main lithological units (Fig. 2) includes information on potential geothermal reservoirs with burial depth and spatial distribution. Well data contain information about the reservoir quality (e.g. distribution of sandstone layers, facies type, heterogeneity, porosity, and permeability) as well as information on temperature and geochemistry of the formation water, where such data were measured (e.g., Poulsen et al., 2013; Olivarius et al., 2015b; Kristensen et al., 2016; Weibel et al., 2017).

Four main lithostratigraphic units with regional geothermal potential have been identified (Nielsen et al. 2004; Mathiesen et al. 2009, 2010). Within these four main units, five important geothermal reservoirs have been defined on the basis of their stratigraphical and spatial extent and include the Lower to Upper Triassic Bunter Sandstone and Skagerrak reservoirs (unit no. 14 in Fig. 2), the Upper Triassic – Lower Jurassic Gassum reservoir (unit no. 10), the Middle Jurassic Haldager Sand reservoir (unit no. 8) and the Upper Jurassic – Lower Cretaceous Frederikshavn reservoir (unit no. 6). Other reservoirs may locally also contain potential aquifers (e.g. the Lower/Upper Cretaceous Arnager Greensand). Each reservoir generally comprises several sandstone layers with reservoir properties. Most interest is currently devoted to reservoirs with burial depth within the range of 800–3,000 m and with a cumulative thickness of reservoir sand of good reservoir quality of more than c. 15 m (Vosgerau et al., 2016).

So far, the focus has been on the combined Bunter Sandstone-Skagerrak reservoir and the Gassum reservoir, with current geothermal production (Røgen et al. 2015) for which temperature maps are presented. The Bunter Sandstone Formation includes the Bunter Sandstone reservoir and is present south of the RFH, on parts of this high and in the DB with thicknesses of up to 300 m. It grades into the Skagerrak Formation towards the north-eastern basin margin (Bertelsen, 1978; 1980; Michelsen and Clausen, 2002). The Bunter Sandstone Formation is dominated by fine-grained sandstones, mainly deposited in an arid continental environment dominated by fluvial channels, aeolian dunes and marginal marine facies. The Skagerrak Formation with the Skagerrak reservoir is less well known, but its distribution along the northern and north-eastern basin margin, and the coarse-grained, often poorly sorted sandstones interbedded with claystones, suggests deposition in alluvial fans and lakes.

The Gassum Formation, which includes the Gassum reservoir, is present in almost the entire Danish area and shows a remarkable lateral continuity (Fig. 3). It has typical thicknesses of 50–150 m in the central and distal parts of the basin and locally up to more than 300 m, though with reduced thicknesses on the SKP and absent on the RFH (Fig. 3) (Michelsen et al. 2003; Nielsen, 2003). The formation consists of well-sorted fine- to medium-grained, locally coarse-grained sandstones interbedded with heteroliths, claystones and thin coals. The laterally

continuous shore-facies sandstones were deposited by repeated shoreline progradation. Fluvial and estuarine sandstones dominate the lower–middle part of the Gassum reservoir in the STZ.

Figure 3. Depths of the top and thickness of the Gassum Formation containing a geothermal reservoir of primary interest. The maps are generated from deep-borehole observations and seismic interpretations.

3.0 Background data and data analysis

3.1 Temperature data

In this study, temperature data were used for the heat-flow analysis as well as for calibration and validation of the numerical temperature model. The quality of measured temperature data is therefore mandatory for the reliability of the derived information on heat flow and the predicted temperatures. A significant amount of borehole temperatures was measured in the study area over the past decades. For the present study, high-precision continuous temperature logs (in thermal equilibrium unaffected from drilling perturbations) from five deep wells (50 values sampled; Aarhus University in-house data files; data on request) and from 16 shallow wells (Møller et al., 2019) are used. In addition, numerically corrected bottom-hole temperature (BHT) values from 41 deep wells (87 values; data and correction procedure described in Poulsen et al., 2012; 2013) were applied. Uncorrected BHT's were not included.

In our modelling, the final temperature data were attributed with an uncertainty of one standard deviation (SD) for the BHT values and of 0.1°C for temperature logs. These data are randomly subdivided into a calibration (55% of data; $n = 76$) and a validation set (45% of data, $n = 61$). An additional weight factor reflects the associated quality (log data = 1, cylindrical-source-method-inversion corrected BHT = 0.75) when implemented in the calibration. **Figure 4** shows the temperature-depth distribution of the used temperature data. Mean temperature gradients between 21 and $37^{\circ}\text{C}\cdot\text{km}^{-1}$ (25% and 75% quantiles $Q_{25\%}$ – $Q_{75\%}$): 29 – $31^{\circ}\text{C}\cdot\text{km}^{-1}$) can be observed covering borehole depths between 50 and 5,300 mbsl (meter below sea level).

Figure 4. Corrected BHT's and equilibrium temperature-logs available for wells in the study area. Grey dashed lines are $25^{\circ}\text{C}\cdot\text{km}^{-1}$ (light) and $35^{\circ}\text{C}\cdot\text{km}^{-1}$ (dark) geothermal gradients.

3.2 Petrophysical properties

The modelling of subsurface heat transfer processes requires information on several rock properties: thermal conductivity λ (TC) [$\text{W}(\text{m}\cdot\text{K})^{-1}$], the volumetric heat capacity ρc (RHOC) [$\text{J}(\text{m}^3\cdot\text{K})^{-1}$], or the thermal diffusivity κ (TD) [$10^{-6} \text{ m}^2\cdot\text{s}^{-1}$], which are interrelated by $\lambda = \rho c \kappa$. The source term is given by the radiogenic heat production H (RHP) [$\mu\text{W}\cdot\text{m}^{-3}$]. For a comprehensive description of these parameters in the various geological formation and across the country (**Fig. 1A and Fig. 2**), a combination of well-log interpretation and drill-core analysis was applied.

Geological borehole and well-log data from 109 deep wells were analyzed and offered a broad spectrum of varying ages and data quality. After the preselection in terms of quality (e.g. log

processing, borehole conditions) and detailed quantity of available data, we were left with 39 deep wells from across the country and drilled through the various lithological units. For each of these boreholes, a minimum number of three out of the following well-logs were available: gamma ray, density log, neutron log, sonic velocity log, borehole caliper, and self-potential. Using the well-log based approach of Fuchs et al. (2015), TC, TD and SHC were calculated for the sedimentary succession of each borehole (top to bottom). Profiles of the RHP were calculated, typically with uncertainties of less than 10%, either from spectral gamma logs (Th, U, K contents) and density after Rybach (1986) or using empirical equations from Bucker and Rybach (1996). The integrative analysis from sonic and density logs and of the volume fraction of shale (from gamma or self-potential) was used to estimate porosity profiles.

For the various thermal model parameters, statistical values, like the arithmetic mean (am), standard deviation (sd), minimum (min) and maximum (max) values, 25% and 75% quantiles ($Q_{0.25}$, $Q_{0.75}$), and the 95% confidence interval ($CI_{0.95}$), were calculated for each sedimentary unit at each borehole location. A summary of these data is presented in Table 1 for the overall study area and all model units.

For details on data handling, quality control, and the interpretation workflow, we refer to the comprehensive workflow description from Fuchs (2018). In that “pre-study”, 23 wells in the DB, included in the present work, were analyzed in detail in terms of thermal and other petrophysical properties and its basin-internal formation-specific variability. We applied exactly the same approach to the additional 16 wells in the NGB, the STZ and the SKP (Fig. 1A).

Table 1. Formation thermal properties derived for the geological units (numbers as in Fig. 2). Data from well-log analysis. n indicate number of wells applied for each unit.

Model unit	Geological unit	Rock TC					RHP					SHC
		W·(m·K) ⁻¹					μW·m ⁻³					J·(kgK) ⁻¹
		n	mean	SD	min	max	n	mean	SD	min	max	mean
1	Quaternary/Tertiary	2	2.11	0.68	1.40	3.43	2	0.4	0.32	0.16	1.30	2,269
2	Chalk Fm. top	20	2.21	0.37	1.45	3.39	15	0.12	0.04	0.11	0.31	2,142
3	Chalk Fm. middle	20	2.58	0.22	2.04	3.26	18	0.13	0.06	0.07	0.41	1,787
4	Chalk Fm. bottom	20	2.94	0.27	2.16	3.77	15	0.17	0.07	0.06	0.55	1,528
5	Rødby Fm. & Vedsted Fm.	26	2.21	0.43	1.34	3.55	30	0.92	0.21	0.39	1.62	1,834
6	Frederikshavn Fm.	17	2.28	0.27	1.61	2.99	17	0.86	0.14	0.55	1.29	1,639
7	Børglum/Flyvbjerg	14	1.81	0.30	1.59	2.77	17	1.08	0.15	0.64	1.39	1,772
8	Haldager Sand	15	2.54	0.31	1.84	3.34	15	0.71	0.24	0.34	1.29	1,622
9	Fjerritslev Fm.	20	2.03	0.31	1.50	3.24	23	1.07	0.17	0.62	1.55	1,726
10	Gassum Fm.	28	2.40	0.44	1.97	3.53	28	0.94	0.27	0.38	1.61	1,594
11	Vinding - Tønder Fm.	16	2.50	0.51	1.52	4.71	18	1.00	0.25	0.25	1.80	1,557
12	Falster Fm.	12	2.63	0.36	1.62	4.03	11	0.97	0.18	0.45	1.39	1,399
13	Ørslev-Fm.	10	2.70	0.55	1.63	4.30	10	1.06	0.29	0.29	1.51	1,308
14	Bunter Sandstone Fm. - Skagerrak	12	2.62	0.30	1.94	3.90	11	0.77	0.23	0.41	1.51	1,304
15	Bunter Shale	11	2.41	0.26	1.65	4.06	11	1.11	0.16	0.48	1.73	1,249
16	Zechstein	7	3.71	0.65	1.81	5.10	9	0.16	0.28	0.10	1.79	1,001
17	Pre-Zechstein sediments	8	2.33	0.43	1.42	3.78	7	0.54	0.43	0.29	1.16	1,078
18	Crystalline Basement	2	2.98	0.21	2.57	3.33	9	1.80	0.2	1.5	2.3	834

For an independent validation of log-derived TC profiles, laboratory core data from different sources were used. Mineralogical data (point-counting) and associated plug porosities were implemented in a mixing-model approach to derive bulk conductivities of the rock samples (cf. Drury & Jessop, 1983; Ray et al., 2015; Fuchs et al., 2018). We applied the geometric mean model (cf. Fuchs et al., 2013) and mineral/pore-fluid conductivity-end-member values (Horai, 1971; Brigaud et al., 1990), as it was repeatedly reported to be the most accurate mixing model for sedimentary rocks (cf. Brigaud et al., 1990; Fuchs & Förster, 2010). Furthermore, laboratory measured TC data are taken from Balling et al. (1992) (mean values from densely spaced measurements along 5–20 m deep core sections) and from Miele (2018) (single core sample measurements). Those values reflect the laboratory ambient pT conditions and need to be corrected for *in-situ* pressure and temperature conditions (cf. Förster et al., 2019) when compared with log data. We applied the approach of Emirov et al. (2018) as an approximate correction for the combined pT effect.

Figure 5. Comparison of log- and lab-derived thermal conductivities. Except for the mineralogical data (providing bulk conductivity), the vertical conductivity components are compared (core measurements perpendicular to bedding – in direction of core axis – versus conductivities derived from logs that include sonic data emphasizing vertical component information). Black solid line is 1:1 line, black dashed lines are $\pm 10\%$ difference. Grey whiskers are the associated uncertainty of determination or $\pm$ one standard deviation for core mean values. Coloured dashed lines are regression trend lines of data.

The overall fit of such data, compared to log-derived values, averaged to 0.5-m intervals (cf. Figure 5) is good (the majority is within 10% uncertainty), considering the different scale of

lab (mostly point; cm-to-m scale) and log data (profile, m-to-km scale). However, log data apparently tend to slightly underestimate the higher lab TC values and vice versa, slightly overestimate the smaller lab values, which we interpret as prediction tendency towards the mean of the individual rock types. This is partly due to the difficulties by the log-derived procedure to resolve details of low vertical component TC in clay-/mudstone with significant thermal conductivity anisotropy. Steps were taken to address this issue by including all available sonic logs, which primarily resolves the vertical component of P-wave velocity and thus emphasizes vertical component TC and, furthermore, by the possibility of TC adjustments by the calibration procedure (section 4.5).

3.3 Heat-flow density determination

Based on the temperature data and well-log derived TC profiles, interval heat-flow densities q_i were calculated for different borehole locations and depth intervals applying the method of Fourier:

$$q_i = \lambda_i \cdot \text{grad}T. \quad (1)$$

Therein, $\text{grad}T$ is the temperature gradient of a certain depth interval (in $^{\circ}\text{C}\cdot\text{km}^{-1}$), and λ is the mean TC of that interval (in $\text{W}(\text{m}\cdot\text{K})^{-1}$). Initial heat-flow calculations were conducted for more than 47 depth intervals in 25 boreholes. However, for the heat flow reported in Table 2, only those values are included that fulfil three strict quality criteria. First, temperature measurements for depth larger than 1.5 km are considered only, which excludes the shallow sedimentary succession, which is still effected by the paleoclimate impact of the last glaciation (*cf.* Balling, 1979, 2013, Majorovicz et al., 2008, Fuchs et al., 2015).

Second, a minimum interval length of 1.5 km was considered to reduce the impact of the BHT uncertainties on the temperature-gradient calculation. The only exception to these strict rules is the Ørslev-1 well, which is an important observation point in the very southeastern part of Denmark and used to link across the Baltic Sea. Here, a smaller interval length of only 0.5 km is applied. Finally, a minimum distance of 3 km to significant salt structures was taken into account to avoid major disturbances according to heat refraction and ‘chimney effect’ (e.g. Jensen, 1990; Norden et al., 2008, Noack et al., 2010, also discussion below).

Temperature gradients were computed either between individual temperatures measured at different borehole depths, or between measurements at depth and the present-day mean surface-temperature. This surface temperature is here set to 8°C for onshore and 4°C for offshore localities. The interval length for the determination of the interval heat flow is c. 2.5 km on average (minimum: 1.5 km, maximum: 5.3 km). Thermal-conductivity interval mean values were calculated with the thickness-weighted harmonic mean.

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346
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Table 2. Heat-flow data for 21 deep boreholes in Denmark derived from temperature data (numerically corrected BHT, temperature logs) and well-log analysis. See text for explanation.

Well	UTM			Interval			Interval length	Temperature			Temperature gradient		Interval TC			Heat-flow density					
	Easting	Northing		top	bottom	top		bottom	ΔT	<i>mean</i>	<i>1σ</i>	<i>unc.</i>	<i>q_i</i>	<i>unc.</i>	<i>q_s</i>	<i>q_{15km}</i>	<i>q_{Moho}</i>				
	X	Y																			
	<i>m bsl</i>	<i>m bsl</i>																<i>m</i>	°C	°C	°C·km ⁻¹
Terrestrial heat-flow density																					
Danish Basin																					
															71.2	71.7	51.4	33.3			
Aars-1A	531115	6294871	DB	1645.0	3145.0	1500.0	46.5	± 0.1	105.1	± 0.1	39.0	± 0.1	†	1.90	± 0.37	0.17	74.0	6.7	75.0	56.0	35.0
Farsø-1	522231	6293253	DB	1649.0	2899.0	1250.0	50.5	± 0.1	103.2	± 0.1	42.2	± 0.1	†	1.78	± 0.47	0.16	75.0	6.8	76.3	56.4	35.8
Hyllebjerg-1	521267	6296957	DB	-28.0	2846.0	2874.0	8*	n.a.	104.0	± 3.7	33.4	± 1.2	‡	2.14	± 0.75	0.19	71.4	6.9	71.7	53.0	29.2
Jelling-1	523599	6177266	DB	-97.6	1932.4	2030.0	8*	n.a.	68.0	± 4.1	29.6	± 1.8	‡	2.21	± 0.73	0.20	65.3	7.1	65.5	40.7	22.4
Linde-1	465571	6254591	DB	-24.2	1722.8	1747.0	8*	n.a.	60.0	± 2.7	29.8	± 1.3	‡	2.23	± 0.61	0.20	66.5	6.7	66.9	46.4	28.9
Mejrup-1	480036	6248279	DB	-50.0	2452.0	2502.0	8*	n.a.	79.0	± 1.3	28.4	± 0.5	‡	2.33	± 0.72	0.21	66.2	6.1	66.3	42.9	26.2
Mors-1	492978	6306403	DB	-18.0	5196.0	5214.0	8*	n.a.	135.0	± 1.7	24.4	± 0.3	‡	2.82	± 0.62	0.25	68.6	6.2	69.9	50.6	27.7
Nøvling-1	488201	6225062	DB	-62.2	3463.8	3526.0	8*	n.a.	103.0	± 2.2	26.9	± 0.6	‡	2.63	± 0.73	0.24	70.9	6.6	71.8	52.0	33.8
Oddesund-1	473537	6268654	DB	-11.0	3525.0	3536.0	8*	n.a.	101.0	± 2.2	26.3	± 0.6	‡	2.74	± 0.97	0.25	72.0	6.7	72.4	52.6	35.8
Rødding-1	488042	6278244	DB	-31.4	2148.6	2180.0	8*	n.a.	75.0	± 3.3	30.7	± 1.4	‡	2.43	± 0.65	0.22	74.8	7.5	74.6	54.9	33.2
Rønde-1	588795	6240966	DB	-42.1	5250.9	5293.0	8*	n.a.	141.0	± 1.9	25.1	± 0.3	‡	2.95	± 0.58	0.27	74.1	6.7	74.9	58.3	48.8
Skive-1	500188	6276032	DB	-28.0	2280.0	2308.0	8*	n.a.	79.0	± 2.4	30.8	± 0.9	‡	2.37	± 0.69	0.21	72.8	6.9	72.7	52.9	31.8
Stenlille-1	665212	6158574	DB	-41.6	1622.4	1664.0	8*	n.a.	59.0	± 3.6	30.6	± 1.9	‡	2.38	± 0.74	0.21	72.9	7.9	72.6	50.0	30.6
Voldum-1	578228	6249673	DB	-34.7	2047.3	2082.0	8*	n.a.	77.0	± 5.6	33.1	± 2.4	‡	2.19	± 0.83	0.20	72.6	8.4	72.6	53.3	46.5
North German Basin																					
Løgumkloster-2																					
Ørslev-1	691889	6074743	NGB	-22.0	2768.1	2790.1	8*	n.a.	89.0	± 2.5	29.0	± 0.8	‡	2.98	± 0.88	0.27	86.6	8.2	87.3	65.4	43.0
Søllested-1	647758	6075246	NGB	-11.0	2661.0	2672.0	8*	n.a.	86.0	± 4.3	29.2	± 1.5	‡	2.64	± 1.19	0.24	77.4	7.7	77.8	55.0	34.1
Sorgenfrei-Tornquist-Zone/Skagerrak-Kattegat Platform																					
																	60.3	62.0	42.4	28.7	
Hans-1	686086	6250777	STZ	-22.9	2953.6	2976.5	4*	n.a.	78.0	± 2.6	24.9	± 0.8	‡	2.46	± 0.65	0.22	61.2	5.9	62.6	40.5	23.9
Felicia-1	458660	6366522	STZ	-40.0	5180.0	5220.0	4*	n.a.	137.0	± 2.5	25.5	± 0.5	‡	2.33	± 0.58	0.21	59.4	5.5	61.4	44.4	33.5
Heat flow in intermediate depth (paleoclimatically perturbed (Sønderborg-1 and local anomaly (Sæby-1))																					
																	55.7				
Sønderborg-1	553832	6087324	DB	920.0	1160.0	240.0	39.2	± 0	47.7	± 0	35.6	± 0.1	†	1.65	± 0.4	0.17	58.8	5.3			
Sæby-1	583972	6358623	SKP	-64.3	1781.7	1846.0	8*	n.a.	46.0	± 2.0	20.6	± 0.9	‡	2.56	± 0.54	0.23	52.7	5.3			

348
349
350

Note: * Assumed mean surface temperature, † temperature log, ‡ BHT corrected by cylindrical-source-method-inversion (CMI). Abbreviations: 1σ = TC variability along the heat-flow interval, unc. = uncertainty of the log-derived mean calculation.

This approach is of advantage with the use of BHT data, which are afflicted with significant uncertainties compared to temperature log data. The longer the selected intervals are, the smaller becomes the impact of the BHT uncertainty on the computed interval temperature gradient. For the example of a 1 km depth interval with a given background gradient of $30\text{ }^{\circ}\text{C}\cdot\text{km}^{-1}$, a $\pm 5^{\circ}\text{C}$ uncertainty results in a gradient range of 25 to $35^{\circ}\text{C}\cdot\text{km}^{-1}$. The same uncertainty for a 4 km long interval results in an average gradient range of 28.75 to $31.25\text{ }^{\circ}\text{C}\cdot\text{km}^{-1}$ and thus, subsequently, affects the heat-flow computation far less.

Second, a minimum interval length of 1.5 km was considered to reduce the impact of the BHT uncertainties on the temperature-gradient calculation. The only exception to these strict rules is the Ørslev-1 well, which is an important observation point in the very southeastern part of Denmark and used to link across the Baltic Sea. Here, a smaller interval length of only 0.5 km is applied. Finally, a minimum distance of 3 km to significant salt structures was taken into account to avoid major disturbances according to heat refraction and ‘chimney effect’ (e.g. Jensen, 1990; Norden et al., 2008, Noack et al., 2010, also discussion below).

Temperature gradients were computed either between individual temperatures measured at different borehole depths, or between measurements at depth and the present-day mean surface-temperature. This surface temperature is here set to 8°C for onshore and 4°C for offshore localities. The interval length for the determination of the interval heat flow is c. 2.5 km on average (minimum: 1.5 km, maximum: 5.3 km). Thermal-conductivity interval mean values were calculated with the thickness-weighted harmonic mean. This approach is of advantage with the use of BHT data, which are afflicted with significant uncertainties compared to temperature log data. The longer the selected intervals are, the smaller becomes the impact of the BHT uncertainty on the computed interval temperature gradient. For the example of a 1 km depth interval with a given background gradient of $30\text{ }^{\circ}\text{C}\cdot\text{km}^{-1}$, a $\pm 5^{\circ}\text{C}$ uncertainty results in a gradient range of 25 to $35^{\circ}\text{C}\cdot\text{km}^{-1}$. The same uncertainty for a 4 km long interval results in an average gradient range of 28.75 to $31.25\text{ }^{\circ}\text{C}\cdot\text{km}^{-1}$ and thus, subsequently, affects the heat-flow computation far less.

The heat-flow values at the surface (q_s), the model base ($q_{15\text{km}}$) and the crust-mantle boundary (q_{Moho}) were calculated (Table 2) considering the RHP of the overlying (for q_s) and underlying rocks (for $q_{15\text{km}}$ and q_{Moho}). For q_{Moho} calculations, data for the Moho depth from Artemieva & Thybo (2013) were implemented. In this computation, the RHP was considered from the middle of the interval to the surface for q_s and to the model base, or crust-mantle boundary, for $q_{15\text{km}}$ and q_{Moho} , respectively. Where no borehole-specific RHP was available from the well-log analysis, mean values computed for all wells in the study area were implemented (cf. Table 1).

For the DB ($n = 14$), the mean heat flow ($\text{mean} \pm 1\sigma$) is $71.7 \pm 3.4 \text{ mW} \cdot \text{m}^{-2}$ for q_s (range: 65–76), $51.4 \pm 5.0 \text{ mW} \cdot \text{m}^{-2}$ for q_{15km} (range: 40–58), and $33.3 \pm 7.2 \text{ mW} \cdot \text{m}^{-2}$ for q_{Moho} (range: 22–48). For the STZ/SKP further north ($n = 2$), the mean heat flow is significantly lower (independent student t -test, $p < 0.001$). It amounts to $62.0 \pm 0.8 \text{ mW} \cdot \text{m}^{-2}$ for q_s , $42.4 \pm 3.5 \text{ mW} \cdot \text{m}^{-2}$ for q_{15km} , and $28.7 \pm 9.4 \text{ mW} \cdot \text{m}^{-2}$ for q_{Moho} . Heat flow in the Danish part of the NGB ($n = 3$) instead shows significantly higher values compared to the DB (independent student t -test, $p < 0.001$). The mean heat flow there is $80.9 \pm 5.5 \text{ mW} \cdot \text{m}^{-2}$, $58.6 \pm 5.8 \text{ mW} \cdot \text{m}^{-2}$, and $36.5 \pm 5.7 \text{ mW} \cdot \text{m}^{-2}$, respectively. The q_{15km} -mean values were chosen as lower boundary condition in our numerical model, whereas the individual q_s -values serve as validation data for the numerically modelled heat flow (cf. section 6.4). Additional, two heat-flow values from intermediate depth are reported to indicate the palaeoclimatic impact of the last glaciation (Sønderborg-1) and a local anomalously low value (Sæby-1).

4.0 Model set up, workflow and governing equations

4.1 Modelling approach

A conductive transient thermal model was developed based on the input of structural information from a detailed 3D geological model (Section 4.2), petrophysical rock properties determined for these structural units (Section 4.4) and reliable boundary conditions (Section 4.3). From the analysis of the available temperature logs, we assume conduction as the main heat-driving process. The 3D heat equation for the energy transport, with heat conduction as the only heat driving process, is written as:

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + H, \quad (1)$$

where ρ is the rock density [$\text{kg} \cdot \text{m}^{-3}$], c is the SHC [$\text{J}(\text{kg} \cdot \text{K})^{-1}$], $\frac{\partial T}{\partial t}$ is the temperature change with time, λ is the rock TC [$\text{W}(\text{m} \cdot \text{K})^{-1}$], H is the RHP [$\text{W} \cdot \text{m}^{-3}$], and $\frac{\partial T}{\partial x}$, $\frac{\partial T}{\partial y}$, $\frac{\partial T}{\partial z}$ are the temperature gradients in x, y, and z directions, respectively. Considering transient conditions at the upper boundary ($\frac{\partial T}{\partial t} \neq 0$), the temperature solution depends on rock TC, volumetric heat capacity (RHOC), RHP, and the given boundary conditions. The commercial finite-element based software *FEFLOW 7*® (Diersch, 2014) was used for the 3D heat transport simulation.

As an important element for deriving the final model solution, initial rock TC, RHP and the lower boundary condition were calibrated by implementing temperature observations (constraining method) using the *FEFLOW* Parameter estimation program (*FePest*®). *FePest* is based on a non-linear estimation technique of the Gauss-Levenberg-Marquardt algorithm (GLMA), where any given parameter is incrementally adjusted, within given limits, until an objective function, implementing the sum of weighted squared deviations between measured

temperatures (calibration data set) and the associated modelled temperatures, is minimized. Further details on this inverse parameter optimization procedure are given e.g. in Doherty (2002, 2015); applications in geothermal modelling are demonstrated in Fuchs & Balling, 2016a and in Poulsen et al., 2017.

4.2 *Structure and mesh generation*

The new structural geological 3D model comprises 15 sedimentary lithostratigraphic units (cf. Section 2) and two layers reflect the crystalline rocks of the upper and lower crust down to the lower model boundary at 15 km depth. As the Danish crust is characterized by varying tectonic features (DB, RFH, STZ/SKP), care must be taken to the structural configuration of the non-sedimentary crust. We applied regional crustal structure from Artemieva and Thybo (2013) and from Maystrenko and Scheck-Wenderoth (2013). From the latter one, we used the top crystalline crust interface, as it showed, on average, slightly smaller deviations compared to borehole observations in the study area.

Faults are implemented as structural offset only and are not parameterized independently as geological features due to lack of detailed knowledge. The upper crystalline crust is subdivided into four numerical layers, to keep the relation between lateral and vertical extent of the meshed elements within reasonable numerical limits. At the lithostratigraphic interfaces, a 0.1m thin buffer layer is included as extra numerical *FEFLOW* layer. This procedure limits a common model bias to the thin buffer layers, as the temperature calculation at the nodes is based on the rock thermal properties, averaged from all neighbour model elements. Where geological units are not present (hiatus) a minimum thickness of 0.1 m (with parameters adopted from the original geological unit in question), is automatically assigned to assure continuum conditions. The *FEFLOW* internal Grid-builder routine was applied to generate a numerical mesh consisting of 3,719,715 three-dimensional prismatic mesh elements and 1,913,692 nodes. The vertical resolution varies according to the variable thickness of the structural units. The horizontal resolution varies within the model area, with an average distance between nodes generally between c. 0.5 km for onshore areas and c. 1.5 km for offshore areas. The average horizontal element size is 0.16 km². At salt structures (+2 km buffer), the grid is further refined to an average node distance of c. 0.25 km.

4.3 *Thermal boundary conditions*

For the upper model boundary (i.e. model topography), we applied a transient temperature condition (Dirichlet boundary condition) with temperatures ranging between +8 and -5°C for the last 130.000 years (Balling, 2013), accounting for the paleoclimate impact of the last

glaciation upon the shallow subsurface thermal structure. The applied relatively high increase of surface temperature (-5 to 8°C) from ‘Late Glacial Maximum’ (LGM) to post-glacial times is consistent with similar values indicated by interpretation of deep borehole observations in northern Poland (Majorowicz et al., 2008) in areas of equivalent positions along the southern rim of the Scandinavian ice sheet.

For the lower model boundary, a Neumann boundary condition (basal heat flow at the constant depth of 15 km) was applied. The heat-flow boundary values vary spatially between the major tectonically units as derived from borehole heat-flow analysis (Section 3.3). Initial model-boundary heat-flow values (15 km depth) are 42 mW·m⁻² for the STZ/SKP, 51 mW·m⁻² for the DB, and 59 mW·m⁻² for the NGB. The lateral boundaries are ‘no-flow boundaries’. During calibration, these lower boundary values are adjusted, but by very small amounts (Section 4.5)

4.4 Parameterization

The thermal parameterization was based on the calculation of formation-specific parameters and statistics from the detailed petrophysical analysis of borehole data as described in section 3.2 (cf. Table 1).

The Chalk group is generally far thicker (average ca. 900 m, range: 140–1,855 m) than any other Mesozoic and Cenozoic unit (averages: 100–600 m). A strong increase of TC with depth (related to decrease of porosity) is known from laboratory core measurements (Balling et al., 1981) and seen in our log analysis as well (cf. Table 1). Therefore, we numerically three-parted the Chalk group and parameterized these sublayers separately (upper, middle and lower, cf. Table 1) to avoid depth dependent over-/underestimations of parameters which would significantly affect the variation of temperature gradients with depth. For the other, less thick units of more complex composition, spatial variability was taken care of by the calibration procedure (section below).

For Precambrian crystalline basement, with biotitic gneiss, basement breccia and quartzite observed in deep boreholes on the RFH (Mesoproterozoic zircon ages; Olivarius et al., 2015a), we applied TC values based on measurements from crystalline rocks from the island of Bornholm (Kristiansen et al., 1982; Møller et al., 2019), which is adjacent to our model area, as well as literature values (e.g. Kukkonen et al., 2011; Fuchs et al., 2018). A summarizing statistic is compiled in Table 1, giving an overview for all lithological units, with data from all boreholes in the entire model area.

The spatial variability of TC within the individual sedimentary units was implemented as parameter set into the modelling software. The *FEFLOW* internal regionalization was conducted by using an ordinary kriging procedure (Krige, 1951). The radiogenic heat

production and volumetric heat capacity are applied homogeneously (average value over all observations) for each modelled geological unit.

4.5 Model calibration

Quality weighted temperature observations (cf. section 4.1) were implemented into *FePest* (Doherty, 2002) to calibrate the model by adjusting TC (spatially, 176 pilot points across all units) and radiogenic heat production (homogeneously) of the modelled layers as well as the three-parted basal heat flow (cf. section 4.3). In this process, TC is allowed to vary within one standard deviation ($\pm 0.5\sigma$) as calculated for each formation at each borehole location (hard boundary). Radiogenic heat production is allowed to vary in the same range formation-wise and heat flow (lower boundary) by $\pm 5 \text{ mW}\cdot\text{m}^{-2}$ (hard boundary).

During the calibration, the heat-flow boundary condition at 15 km depth is reduced by $2 \text{ mW}\cdot\text{m}^{-2}$ for NGB (to $57 \text{ mW}\cdot\text{m}^{-2}$) and by $1 \text{ mW}\cdot\text{m}^{-2}$ for DB (to $50 \text{ mW}\cdot\text{m}^{-2}$) and the STZ/SKP (to $41 \text{ mW}\cdot\text{m}^{-2}$), which is within the error of determination for the regional heat-flow values. The calibrated (optimized) formation TC values show somewhat larger, but still small differences compared to the initial input data, averaging to $-1\% \pm 21\%$ (median $\pm 1\sigma$, relative) and $10\% \pm 16\%$ (absolute) (cf. Table 3). Examples for the spatial distribution of calibrated formation thermal conductivities are shown in Figure 6.

Table 3. Calibrated versus initial thermal conductivity data.

Model unit	Geological unit	Calibrated TC		Change to input	
		mean	SD	$\Delta_{\text{abs.}}$	$\Delta_{\text{rel.}}$
		$\text{W}\cdot(\text{m}\cdot\text{K})^{-1}$		$\text{W}\cdot(\text{m}\cdot\text{K})^{-1}$	%
1	Quaternary/Tertiary	2.63	0.89	0.52	25%
2	Chalk Fm. top	2.15	0.51	-0.06	-3%
3	Chalk Fm. middle	2.50	0.51	-0.08	-3%
4	Chalk Fm. bottom	2.84	0.60	-0.10	-3%
5	Rødby / Vedsted Fm.	2.01	0.80	-0.20	-9%
6	Frederikshavn Fm.	2.48	0.73	0.20	9%
7	Børglum/Flyvbjerg	2.04	0.72	0.24	13%
8	Haldager Sand	2.93	1.15	0.38	15%
9	Fjerritslev Fm.	1.56	0.40	-0.47	-23%
10	Gassum Fm.	2.77	0.76	0.37	15%
11	Vinding - Tønder Fm.	2.87	0.98	0.37	15%
12	Falster Fm.	2.81	0.65	0.19	7%
13	Ørslev-Fm.	2.98	0.61	0.28	10%
14	Bunter Sandstone Fm. - Skagerrak	2.71	0.58	0.09	3%
15	Bunter Shale	2.59	0.49	0.18	7%
16	Zechstein	4.36	1.02	0.65	18%
17	Pre-Zechstein sediments	2.48	0.54	0.15	7%
18	Crystalline Basement	2.95	0.15	-0.03	-1%
	absolute mean:			0.25	10%
	absolute sd:			0.17	7%
	median:			0.20	9%

By applying a relatively large number of pilot points, any significant lateral and vertical variation in TC for each lithological unit is accounted for. Variations are likely to result mainly

from differences in composition and lithological facies as well as from depth-dependent porosity. Furthermore, the shortcomings of resolving details of low vertical component TC in clay-/mudstones, as discussed above, seems also accounted for. This is illustrated by the reduction of the TC mean values of the Fjerritslev Fm and the Rødby/Vedsted Fm (from 2.03 to 1.56 $\text{W}(\text{m}\cdot\text{K})^{-1}$ and 2.21 to 2.01 $\text{W}(\text{m}\cdot\text{K})^{-1}$, respectively. These formations include major intervals of clay-/mudstones from which examples of low vertical component TC values have been measured on cored sections (Balling et al., 1981; 1992), some of which are included in the lab data in Fig. 5. Consistent with the indication in Fig 5 of a slight underestimation of the higher conductivity units (mainly quartz-rich sandstones), the mean TC values of the Gassum Fm and the Haldager Sand Fm are adjusted upwards (by 0.38 and 0.37 $\text{W}(\text{m}\cdot\text{K})^{-1}$, respectively cf. Table 3).

Figure 6. Examples of variation of calibrated thermal conductivity across the model area. These maps are based on borehole petrophysical-log and temperature observations and a spatial ordinary kriging. The pattern between boreholes with constraining observations is statistically driven and does not necessarily reflect true lithological or thermal facies changes. The difference between the generally low-conductivity clay-/mudstone dominated Fjerritslev Fm and the sandstone dominated Gassum-, Bunter Sandstone – Skagerrak Fms, of generally higher conductivity, is clearly outlined.

5.0 Thermal modelling results

5.1 Model fit to temperature observations

Temperature observations (Section 3.1) were used to quantify the uncertainties of the modelled temperatures with independent subsets for calibration and validation phase. An excellent agreement between measured and modelled temperatures is obtained for the calibrated transient model. The two-step comparison with both the calibration and the validation temperature dataset consistently results in average errors (rms, absolute arithmetic mean) of approx. 1°C (Fig. 7), which lies in the uncertainty range of most temperature measurements. For more than 85% of the compared temperature data, deviations are less than 1°C; another 10%, show

deviations less than 3°C (Fig. 7). The scatter is generally very small and the quality of fit is independent of the observation depth (no trend with increasing depth is present).

Figure 7. Comparison between modelled and observed borehole temperatures. A: all data; B: equilibrium temperature logs (symbols: modelled values; profiles: borehole measurement); C: Histograms of depth distributions of data and frequency of fit between measured and modelled temperatures.

5.2 Modelled versus measured interval heat flow

Modelled heat flow for the borehole depth intervals of observed values, range between c. 60 and 80 mW·m⁻², with lowest values between 60 and 65 mW·m⁻² in the STZ/SKP and highest values above 75 mW·m⁻² in the NGB (Fig. 8). The overall modelled mean value is 62.5 ± 3.5 mW·m⁻² for the STZ/SKP, 69.6 ± 2.0 mW·m⁻² for the DB, and 79.0 ± 1.0 mW·m⁻² for the NGB, respectively. Modelled and measured q_i values show a good agreement for all three regions with differences for the regional group mean values of less than 2 mW·m⁻². For the DB, this difference is statistically insignificant (n = 14, independent student t-test, p > 0.12).

Figure 8. Comparison between modelled and observed interval heat-flow density. Solid line is 1:1 line; dashed lines are $\pm 5\%$.

5.3 Modelled subsurface temperatures

The modelled subsurface temperature field is generally characterized by significant lateral and vertical spatial variations across Denmark, reflecting the structural geological differences with large variations in formation depth, thermal property distribution, and background heat flow. Modelled temperatures are illustrated for constant depth levels between 1 and 5 km (depth levels of best model constraints) (Fig. 9) as well as for the top of major geothermal sandstone formations (Fig. 10). Additional information in terms of temperature maps for selected depths and lithological units are available as electronic supplement.

At a depth of 1 km (Fig. 9), the temperatures range between 26 and 51°C, yielding temperature gradients between 18 and 43 °C·km⁻¹ with an average of 27 °C·km⁻¹. Temperatures larger than 45°C are observed at the northern margin of the NGB and in the Brande Through (trough within the RFH, southern Jutland). Large areas in the DB show temperature between 30 and 40°C with local positive temperature anomalies usually associated with Zechstein salt structures. Slightly lower temperatures, below 30°C are found offshore between Jutland and Zealand, in the northernmost part of Jutland and in minor areas above the deeper parts of the basin.

For the 2-km depth level, observed temperatures ranges between 49 and 80°C, corresponding to average temperature gradients of 20 to 36 °C·km⁻¹ (mean: 27 °C·km⁻¹). Highest temperatures (>70°C) occur in the central parts of the DB and are again related to the salt structures; lowest temperatures (<55°C) are observed towards the northeast (STZ/SKP).

Figure 9: Modelled temperature distribution for selected constant depth levels as indicated. (Depth below sea level – max. 171 m below ground level; average 34 m).

The temperatures at the 3-km depth level are in the range of 73 to 110°C, indicating average temperature gradients between 22 and 34 °C·km⁻¹ (mean: 27 °C·km⁻¹). The increased

temperature level at salt structures, clearly present for the 1 km and 2 km level, is now unevenly distributed. The highest temperatures ($>105^{\circ}\text{C}$) are still located to the central parts of the DB. However, this central area does show a heterogeneous patchy temperature field (lateral variation by up to 30°C), rather than a homogeneous high level. Low temperatures are again observed towards the northeast (STZ/SKP) and now, also in the western part of the RFH.

At the deeper 5-km depth level, temperatures are ranging between 116 and 159°C . Values $>150^{\circ}\text{C}$ occur only in the central parts of the DB (area between Randers and Holstebro). The influence of salt structures with local positive temperatures anomalies observed for shallow depth of around and less than 2 km, is now reversed to local negative anomalies with temperature reductions by typically around 10 to 15°C . Temperatures below 130°C are mainly observed in the areas of the STZ/SKP and for the Ringkøbing High (western part of the RFH).

For the major geothermal sandstone formations (Gassum Fm and Bunter Sandstone-Skagerrak Fm), we found the highest top formation temperatures in the deeper parts of the DB. The lowest values are observed close to and above the major structural highs (RFH and SKP). Low temperatures are also found locally, where reservoirs are significantly elevated above salt domes. Temperatures larger than 120°C at the top Gassum Fm., technically suitable for the generation of electricity, are observed only locally (around the cities of Viborg, Suldrup and Nykøbing Mors) in the central part of the DB. For the Bunter Sandstone-Skagerrak Fm, larger parts of the DB show this high temperature level. However, reservoir quality is likely to be low at these greater depths. In addition, other formations contain reservoir units of interest as potential geothermal reservoirs or for seasonal heat storage purposes (cf. model studies in Major et al, 2018). This, in particular, applies to the Haldager Sand Fm and the Frederikshavn Fm (cf. Fig. 2). These formations show temperatures up to 70°C , locally up to a maximum of slightly more than 100°C (cf. electronic supplement). Similar to the Gassum and Bunter Sandstone-Skagerrak Fms, highest temperatures are found in the deep sedimentary burial of the north-western part of the DB (cf. electronic supplemental material). Temperatures towards the northern margin of the DB (STZ) are generally 10 to 20°C higher than towards the RFH. For the STZ and further north onshore, current minimum temperatures of around 45°C preferred for district heating are found only for the Gassum Fm and the deeper reservoir units. Further south, in large parts of the DB, all Jurassic reservoir formations show suitable temperatures for district heating. Around and above the shallow crystalline basement in the RFH, generally, too low temperatures are observed and, in addition, some larger areas are without suitable reservoir units (cf. Fig 10). Temperatures for the top Gassum Fm. define the maximum temperatures of the overlaying Fjerritslev Fm. (cf. electronic supplement) which, in the Toarcian marine shales,

contains potential source rocks for hydrocarbons (Petersen et al. 2008), and are thus of interest for deriving levels of thermal maturation.

Figure 10. Temperature distribution modelled at the top of major geothermal reservoirs. Left: Gassum Formation, right: Bunter Sandstone-Skagerrak Formation.

For the deep thermal field, below the thick sedimentary sequences, temperature variations are less pronounced. Maps are not shown here, as constraining borehole data are limited to the upper 5 km (cf. Fig. 4 and Table 2). However, the model may still yield highly valuable information on the general temperature level and trends of variations (Supplementary material show temperature maps down to top Pre-Zechstein sediments and top crystalline crust). At 10 km depth, model temperature varies between 230 and 284°C (mean: $254 \pm 14^\circ\text{C}$; $22\text{--}28^\circ\text{C}\cdot\text{km}^{-1}$) and at the model base (15 km), between 336 and 419°C (mean: $379 \pm 20^\circ\text{C}$; $22\text{--}27^\circ\text{C}\cdot\text{km}^{-1}$). The temperature pattern at 10 km is still, to some extent, influenced by the overlaying salt structures and thick sediments of the DB, whereas at the model base, temperatures do not correlate anymore with the occurrences and thickness of the Zechstein salt.

Based on the temperature estimates at the model base, the temperature field may be extrapolated to the crust-mantle boundary (Moho) by analytically calculated geotherms (cf. Chapman, 1986; Chapman & Furlong, 1992; Förster et al., 2019). Our model thermal conductivities and radiogenic heat productions for upper (cf. Table 1) and lower crustal rocks (supplemented by

values from Förster et al., 2019) and actual heat-flow estimates (Table 2) were applied. From these calculations, 1D geotherms computed at borehole locations yield temperatures between 690 and 800°C at the Moho (28 to 35 km depth; Thybo & Nielsen, 2012; Artemieva & Thybo, 2013). The higher values are found towards the transition zone between the RFH and NGB, and lower values towards the STZ and around the area of the ‘Silkeborg Gravity High’ reflecting a thick lower crustal basic intrusion (Thybo and Nielsen, 2012).

6.0 Discussion

The results of the presented temperature modelling study and present-day thermal field analysis are based on the comprehensive well-log analysis of 39 deep wells from onshore Denmark. This includes the determination of representative formation values of TC, TD, RHP, density and porosity. These parameters are important as the transient model considers the shallow paleoclimate impact as well as should serve as foundation for subsequent local-scale transient process models (e.g. for models on local geothermal heat extraction or heat storage, e.g. Major et al. 2018). Furthermore, our thermal model includes a new geological structural input model, with layer boundaries originating from a recent, fully updated reinterpretation of reflection seismic lines, constrained by well data in our study area.

6.1 *Quality of the temperature model*

Considering a priori the spatial variation of TC within the geological formations and of the heat-flow at the lower model boundary, a transient surface boundary condition as well as implementing a well-constrained temperature data set into the calibration step, yield very small temperature prediction uncertainties when compared to borehole data. Calibrating TC values (and to some extent RHP) within a reasonable range of 1σ , by iteratively minimizing the misfit between measured and predicted temperatures, significantly reduced the uncertainties of the temperature predictions. The difference between a priori and calibrated TC data set is on average around 10% [ca. $0.25 \text{ W(m}\cdot\text{K)}^{-1}$], which is small and emphasizes the quality of the initial well-log based TC input data (cf. Table 3).

The comparison of modelled and measured borehole temperatures reveals an RMS mostly around or smaller than 1°C (Fig. 7), whether the boreholes are implemented as pilot points into the calibration procedure or not. The small prediction differences are clearly within the range of uncertainties of most temperature data. The CMI-corrected BHT values are reported (Poulsen et al., 2012, 2013) with a 1σ uncertainty typically in the range of $2\text{--}4^\circ\text{C}$ (cf. Table 2). Only the high-quality equilibrium temperature logs will reach the uncertainty level of about 1°C and better. The generally good quality of modelled temperatures is also reflected in the relatively

small differences between modelled and observed interval heat flow, which is generally within the uncertainty of determinations (cf. Fig. 8).

Our thermal model is thus highly consistent with the input data. However, limitations and uncertainties are present stemming from the structural model and the depth positioning and thickness of the various geological layers, which is highly dependent on the coverage and quality of local seismic profiles. In particular, uncertainties are expected where complex structural conditions are present, e.g. around salt structures in the DB and towards the tectonically more complex STZ/SKP, where, in addition, less good-quality well- and seismic data are available.

Overall, the small deviations to measured borehole temperatures demonstrate the strength of a numerically calibrated geothermal model parameterized by a detailed spatial analysis of thermal rock properties and therefrom derived heat-flow values. However, the implemented borehole data cover depth down to a maximum of 5.3 km. Below these depth, and in areas with little, or no data, as discussed above, uncertainties are expected to be higher and generally increasing with depth and distance to areas of constraining observational data.

6.2 Previous studies

The most recent thermal modelling study in the study area was carried out by Poulsen et al. (2017), who also summarized a comparison to earlier studies (Balling et al., 1981, 2002). Poulsen et al. (2017) presented the first regional 3D numerical model with emphasis on outlining the inverse calibration methodology on a geothermal application. Therein, constant matrix conductivities were applied for various lithological units, generalised porosity-depth functions and a constant lower boundary heat flow ($65 \text{ mW}\cdot\text{m}^{-2}$ at 5 km depth). The present work is based on a nation-wide detailed log-based and core-validated parameterization of the formation thermal properties and is constrained by data from additional boreholes, including shallow accurate borehole temperatures from Møller et al., (2019) as well as new heat-flow determinations for deep wells. This improved set of input data, including the spatially variable TC and heat flow, is reflected in the better fit between modelled and measured temperatures (rms of 1.2°C) compared to already good results from Poulsen et al. (2017). Poulsen and co-workers used a constant value for background heat flow and generally constant matrix TC values for each lithological unit. Their variation in temperature is thereby dominated by the inter-formation variation in conductivity, depth, and thickness. Furthermore, the new structural model, based on reinterpreted and fully updated seismic horizons, provides improvements on layer interfaces, depths and thicknesses of lithological units, important for model interpolation and extrapolation with respect to observations at well locations.

The above improvements become apparent, when simplifying our parameter analysis into homogeneous formation properties. The magnitude of potential uncertainties (potential errors) introduced by considering homogenous formation TC values (constant mean TC for each lithological unit) is illustrated on the example of the top Gassum Formation temperatures in **Fig. 11**. Differences of modelled temperatures with homogeneous versus spatial variable parameterization of up to 15–20°C are shown (mean: $6 \pm 3^\circ\text{C}$). Although with a significant scatter, we see a general positive correlation between modelled temperature differences and depth of the formation. For temperatures above 100°C at the top of the Gassum Fm., differences average to $\pm 10^\circ\text{C}$. Such differences (potential uncertainties/errors) are of significance in geothermal exploration.

Figure 11: Impact of parameterization. Differences of predicted temperatures between homogeneous and spatial variable TC parameterization of the lithological units, illustrated for the top of the Gassum geothermal reservoir. Right – grey dots: single depth-related differences; dotted black line: regression line.

The general advantage of considering the facies-dependent regional variability of formation TC in geothermal models was outlined earlier (Fuchs & Balling, 2016a,b; Vogt et al., 2010, Mottaghy et al., 2011), but the direct impact on reservoir temperature prognosis is new. These model observations are consistent with a long line of laboratory studies showing natural variability and heterogeneity of the TC parameter (*cf.* Balling et al., 1992; Norden and Förster, 2006; Schütz et al., 2012a,b; Homuth et al., 2014). The importance of a realistic treatment of

the TC parameter in basin thermal reconstruction and hydrocarbon generation modelling was treated in Fjeldskaar et al (2006).

6.3 Temperature field

Despite the lack of large thermal anomalies, we observe significant lateral variability in the subsurface thermal structure across the Danish onshore areas. Large vertical and lateral temperature variations mainly result from regional and local geological variability and associated variations in thermal rock properties and heat flow. The isothermal maps show lateral variations within the approximate range of up to 30–45°C at depth of 2–5 km (increasing with depth, cf. Fig. 9 and electronic supplement). The regional variation of the deep background heat flow reflects the main tectonic features. Heat flow was set as *a priori* lower boundary condition (range 42–59 mW·m⁻²) and subsequently confirmed in the calibration procedure yielding insignificant adjustments (± 2 mW·m⁻²).

Areas of shallow crystalline rocks in the western part of the RFH and along the SKP generally show lower temperatures compared with the thick sedimentary succession of the DB. Here salt structure and associated deep troughs dominate the modelled temperature pattern. The observation of positive temperature anomalies above and in the upper parts of salt structures, and negative anomalies in, around and below their deeper parts is a well-known feature (cf. Balling et al. 1981, P. Balling et al., 2013; Jensen, 1983, 1990; Noack et al., 2010; Norden et al., 2012; Sippel et al., 2013). This effect, often referred to as the ‘chimney effect’, is a ‘refraction effect’ that is related to the high TC contrast between rock salt and the surrounding sediments. We see temperature anomalies of +20 to -15°C, which are similar to observations in the above-referenced studies. Higher temperatures in deep sedimentary troughs between surrounding areas of salt structures, or along crystalline basement highs, are known as ‘thermal blanketing effect’ and are caused by the relatively lower conductivity of the thick sediments, resulting in higher temperature gradients.

As a guide for geothermal exploration, we report the depth of the 45°C and 130°C isotherms (Fig. 12), often referred as approximate reference levels for the geothermal energy exploitation for heat and electricity production, respectively (Huenges et al., 2010). The isothermal level of 45°C varies significantly with a depth range between 750 and 1,750 m. The shallowest depth level is found at the temperature anomaly southeast of Aabenraa (southernmost Jutland, Fig. 12), close to the heating plant of Sønderborg. In the southern part of Denmark, this isotherm can be drilled at depth between 750 and 1250 m, whereas in the northern part, depth up to 1750 m need to be penetrated. These differences will have a significant impact on drilling costs. For the 130°C isotherm (range: 3.6–5.6 km), the depth pattern is minted by the large tectonic

features. Shallow depth below 4 km, are found only in the centre of the DB, whereas STZ/SKP and Ringkøbing High require depth of more than 4.8 km. However, at those depth, reservoirs may not be present, and if any, poor reservoir quality may be expected (e.g. Olivarius et al. 2015; Blöcher et al. 2016).

Figure 12: Depth to isotherm levels of 45°C (potential direct heating) [left] and 130°C (potential electricity production) [right].

A comparison with the model of Poulsen et al. (2017) shows in general quite similar temperature trends, but significant local differences are observed.

We recognize the more pronounced difference in a narrow zone along the southern margin of the STZ in northern Jutland. Here, at a depth of 2–3 km, Poulsen et al. (2017) model marked positive anomalies at up to 15–20°C higher than in adjacent areas and actually, the highest temperatures in the study area for these depths. Here, our model shows only marginally higher temperatures (by about 5°C). We found the highest temperatures further south in the central parts of the DB, partly associated with salt structures (Fig. 9), which are here implemented and modelled according to the improved seismic database and with greater model resolution. The reason for the higher temperatures, along the STZ in Poulsen et al., seems to be a combination of slightly higher background heat flow and slightly lower TC in the relatively thick low-conductivity Fjerritslev Fm (cf. Fig. 6), both elements producing higher temperature gradients. Unfortunately, for this relatively narrow zone, there is lack of good quality well temperatures for a comparison. Differences in the temperature levels for the Gassum Fm are, for the northern areas, partly related to these same reasons. Furthermore, we note that Poulsen et al. presented

mean formation temperatures, whereas our model displays values for the top level of the formation.

6.4 Heat-flow field

For each of the three tectonic units (DB, NGB, and STZ/SKP), consistent heat-flow values are found to vary only within relatively small limits. Since these determinations were based on temperature observation from depth larger than 1.5 km, values are likely not significantly affected by the long-term paleoclimate surface temperature variation between glacial and non-glacial periods. Any effect seems of the order of, or less than 2–3 mW/m² according to Majorovicz et al. (2008) and similar model results in Balling et al. (1981), and thus within uncertainty limits of current estimates. Furthermore, by introducing a transient surface-boundary temperature variation, reflecting such temperature variations, it is possible to compare, in addition to shallow temperatures, also modelled and observed heat flow, which shows consistency (Fig. 9). The overall picture considering previous studies and results from the surrounding areas also shows good agreement as discussed below.

The consistency between modelled heat flow and the derived new values of heat flow at deep well sites (Table 2 and Fig. 8) clearly points to a very limited effect from any bias in the log-derived TC depth-functions. If vertical component TC for clay-rich units of very low conductivity may be slightly overestimated, conductivity of quartz-rich sandstones may be slightly underestimated, as discussed above, resulting in generally good representative thickness-weighted harmonic TC mean values, applied for calculating site values of heat flow.

Danish Basin

Terrestrial heat-flow has been determined, onshore and offshore, in a number of previous studies in the DB (summarized in Balling, 1992). In difference to these, values from the present study are computed based on thermal-conductivity profiles from petrophysical well logs and an increased number of high quality corrected BHT data. Earlier studies focussed on the accurate determination of conductivities on drill-core samples and were then faced with the issue of upscaling.

Nevertheless, mean ($\pm 1\sigma$) (72 ± 3 mW·m⁻²) and range (65–76) from our study are in excellent agreement with the outcome from Balling (1992) [mean: 72 ± 5 , range: 65–75]. Almost identical values (difference < 3 mW·m⁻²) are found for wells Farsø-1, Hyllebjerg-1 and Voldum-1. Larger differences (6–9 mW·m⁻²) are revealed for Nøvling-1 and Rønde-1. Our new values from wells Jelling-1, Linde-1, Mejrup-1 show somewhat lower heat flow, averaging to 66 mW·m⁻², compared to 73 mW·m⁻² for the remaining wells. Both, mean and range are also in good

818 agreement with terrestrial heat-flow data from the North Sea (from North to South, ca. 100 km
819 offshore; well K-1: $75 \text{ mW}\cdot\text{m}^{-2}$, well R-1: $69 \text{ mW}\cdot\text{m}^{-2}$, well S-1: $72 \text{ mW}\cdot\text{m}^{-2}$; cf. Balling, 1992).

820 *North German Basin*

821 The new surface heat-flow values [mean: 81 ± 5 , range: 77–87, $n = 3$] for the Danish area of the
822 NGB show an excellent agreement with previous studies from Balling (1992) [mean: 81 ± 2 ,
823 range: 79–82, $n = 3$] and from Fuchs & Balling (2016b) [mean: 80 ± 5 , range: 72–84, $n = 8$].
824 New values of $78 \text{ mW}\cdot\text{m}^{-2}$ for the Ørslev-1 and Søllested-1 wells, in the very south-eastern part
825 of Denmark, are within uncertainty limits of the $82 \text{ mW}\cdot\text{m}^{-2}$ value reported for Ørslev-1 by
826 Balling (1992) and also in good agreement with values of 74–77 $\text{mW}\cdot\text{m}^{-2}$ measured ca. 100 km
827 southeast across the Baltic Sea along the German coastline (Norden et al., 2008; Fuchs &
828 Förster, 2010).

829 *Sorgenfrei-Tornquist-Zone/Skagerrak-Kattegat-Platform*

830 Significantly lower values of ca. $60 \text{ mW}\cdot\text{m}^{-2}$ observed for the STZ/SKP are in good agreement
831 with those reported in the adjacent tectonic units of the Baltic Shield ($50\text{--}60 \text{ mW}\cdot\text{m}^{-2}$ from:
832 Slagstad et al., 2009; Balling, 2013; Veikkolainen et al. 2017; Rosberg and Erlström; 2019).
833 Both tectonically and in terms of thermal structure, the STZ/SKP, and in particular the SKP,
834 constitutes a transition zone between the DB with thick sequences of Paleozoic to Cenozoic
835 sediments and the old Precambrian Baltic Shield. This tectonic transition is also evident from
836 seismological observations and models, demonstrating a marked increase in lithospheric
837 thickness, from about 100 km or less, in basin areas (DB and NGB) to more than 200 km in
838 adjacent shield areas in southern Sweden (cf. Hejrani et al., 2015; Köhler et al., 2015).

839 *Mantle heat flow*

840 For the model base at 15 km, heat flow extrapolated borehole observations (Table 2) averages
841 to approx. 51 ± 5 (DB), 59 ± 6 (NGB), and $42\pm3 \text{ mW}\cdot\text{m}^{-2}$ (STZ/SKP), respectively. Our model
842 crustal radiogenic heat production is $1.7 \mu\text{W}\cdot\text{m}^{-3}$ (for upper crust) and $0.4 \mu\text{W}\cdot\text{m}^{-3}$ for lower
843 crustal rocks. The radiogenic heat production for the remaining lower parts of the crust, down
844 to the depth of the Moho discontinuity at around 30 km (with crustal P-wave velocities of 6.4–
845 $6.9 \text{ km}\cdot\text{s}^{-1}$, Thybo, 2001; range of depth to Moho, 25–33 km in Artemieva, 2018) is likely to be
846 low, on average around $0.4 \mu\text{W}\cdot\text{m}^{-3}$ (cf. Balling, 1995; Norden et al. 2008). This results in an
847 estimate of heat flow at the crust-mantle boundary (q_{Moho}) averaging to 33 ± 7 ($Q_{25\%}\text{--}Q_{75\%}$: 31–
848 $37 \text{ mW}\cdot\text{m}^{-2}$) for the DB, 36 ± 5 for the NGB, and $29\pm6 \text{ mW}\cdot\text{m}^{-2}$ for the STZ/SKP. Data for DB
849 and NGB fit well to the modelled 35–40 $\text{mW}\cdot\text{m}^{-2}$ in profile sections in Balling (1995) (south-
850 eastern DB and western NGB) as well as with a similar range of values in the model of Norden
851 et al. (2008) for the eastern part of NGB towards the Baltic Sea. The low heat flow from the

mantle, estimated at $24 \text{ mW}\cdot\text{m}^{-2}$, for the Hans-1 well (Table 2) in the southern part of the Kattegat Sea between Denmark and Sweden, and the higher basin values, are in very good agreement with seismological results on differences crustal and lithospheric structure as mentioned above. Heat flow from the mantle is, as demonstrated in several studies (e.g. Balling, 1995; Balling, 2013; Artemieva, 2018), an important factor in controlling thermal structure of the crust-lithosphere-asthenosphere system, including thickness of lithosphere.

7.0 Summary and conclusions

- A 3D numerical deep basin and crustal temperature model that integrates borehole petrophysical and temperature observations has been developed for onshore Denmark. For the first time on a countrywide scale, a comprehensive analysis of well-log data was used as parameterization source for a temperature model.
- Excellent temperature predictions ($\text{rms} = 1.2^\circ\text{C}$, $\text{ame} = 0.7^\circ\text{C}$) are achieved by: 1) applying a data-driven characterization of rock properties and heat flow, and by 2) constraining the model to fit measured high-quality well-temperatures, by optimizing thermal conductivity, radiogenic heat production and background heat flow.
- Significant lateral subsurface temperature variations are related to the complex geological history (thickness variations and facies changes, salt structures, and strong topography of top crystalline crust). The observed variations in rock TC and background heat flow, yield significant variations in modelled temperature gradients and produces marked lateral temperature variations.
- Temperatures in the approximate range of $40\text{--}90^\circ\text{C}$ are found for the Gassum Fm. in most of the DB, which provides suitable conditions for low enthalpy geothermal heating. Temperatures above 130°C are observed for the Bunter Sandstone-Skagerrak Fms in the basin centre and, technically, offer the potential for geothermal electricity production. Integrated with information on reservoir hydraulic properties and facies changes, the presented temperature maps, and associated detailed digital information, will contribute to the planning and management of subsurface geothermal resources in Denmark and help preventing conflicts of use.
- The combination of new model and borehole heat-flow values show a consistent picture for the Danish and neighbouring regions. Relatively high mean values for the terrestrial surface heat flow, $72 \text{ mW}\cdot\text{m}^{-2}$ observed for the DB and $81 \text{ mW}\cdot\text{m}^{-2}$ for the northernmost onshore part of the NGB, are in a line with results from previous studies and are consistent with a tectonic and geodynamic setting closely related to the North Sea and

885 Central European basin systems. These values of (unperturbed) surface heat flow can
886 be considered as robust background data for any geothermal modelling in the region.

887 **8.0 Appendix A: Supplementary data**

888 Supplementary material related to this article can be found, in the online version, at doi:
889 <https://doi.org/10.1016/j.geothermics.2019.101722>.

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