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Research Article

Keywords: Subsurface modelling, Reservoir model design, 3D hydrostratigraphy, Northwest German Basin

Posted Date: September 23rd, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10917990/v1>

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Additional Declarations: No competing interests reported.

1 Hydrostratigraphic 3D subsurface grid modelling of the Northwest German Basin: combining 2 surface-based structural with voxel-based hydrostratigraphic modelling

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11 Abstract

12 Large-scale 3D subsurface models constitute, among others, the foundation for groundwater flow
13 simulations and management, geothermal potential assessment, carbon capture and storage (CCS)
14 initiatives, as well as site selection strategies for nuclear waste repositories. As part of a larger project
15 dealing with numerical predictions of subglacial meltwater erosion during future glaciations, we
16 present a flexible workflow that integrates surface-based structural modelling with voxel-based
17 hydrostratigraphic grid modelling to spatially model the complex fill of the Northwest German Basin.
18 The modelling workflow is applicable to other sedimentary basins with complex fills and
19 heterogeneous data coverage.

20 The workflow was applied to construct regional 3D subsurface grid models to 2,000 m depth in an
21 area of up to 50,000 km². For the model construction, we harmonised heterogeneous data sources,
22 including borehole data, geological cross-sections, and existing structural 3D models, and utilised
23 Permian to Quaternary hydrostratigraphic units. This approach enabled efficient property
24 interpolation and the representation of both extensive and spatially restricted lithofacies, such as those
25 associated with salt rim synclines and tunnel valleys. Model validation shows that the Nearest-
26 Neighbour interpolation can cope with unevenly distributed data when guided by the structural

27 framework model, and that the models reproduce relevant stratigraphic heterogeneities even where
28 data coverage is heterogeneous.

29 **Keywords**

30 Subsurface modelling, Reservoir model design, 3D hydrostratigraphy, Northwest German Basin

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33 **1. Introduction**

34 3D subsurface models are used for, among others, groundwater resource management, nuclear waste
35 disposal, geothermal energy production, and CO₂ storage. Many of these applications are not
36 restricted to local, site-specific processes, therefore requiring a regional, large-scale approach. For
37 example, large-scale and deep groundwater flow simulations under recent and past conditions
38 describe basin-wide processes that depend on a precise representation of the subsurface geology (e.g.
39 Hebig et al. 2012; Hermanowski and Piotrowski 2019; Frick et al. 2022; Tsypin et al. 2024). Site
40 selection for geological CO₂ storage requires the evaluation of large areas to determine the regions
41 with the highest potential (e.g. Xu et al. 2025). Three-dimensional subsurface models help to visualise
42 the often-complex subsurface geology and provide input data for numerical models (e.g. Sattler et al.
43 2022; Schimschal et al. 2025; Ahlers and Henk 2026).

44 Construction of (hydro-)geological subsurface models needs to be time- and cost-efficient,
45 particularly when addressing applied-research questions. However, these models often concern areas
46 with scattered and heterogeneous data coverage. Utilising multisource databases is necessary, which
47 increases the uncertainty of the entire dataset (e.g. Koch et al. 2014; Cao et al. 2024) and affects the
48 reliability of the results. The quality of a geological model can be limited by several factors, including
49 the quantity and nature of the input data, as well as the geological expertise of the model constructor
50 (Wang et al. 2022). Besides the quality of the borehole information, the spatial distribution of the
51 input data influences the reliability of a model drastically (e.g. Sun et al. 2019). Despite some recent
52 progress (e.g. Rojas et al. 2010; Enemark et al. 2019), there is no simple method for evaluating the

53 uncertainty effects of the geological models (Bredehoeft 2003, 2005; Refsgaard et al. 2012).
54 Estimating such uncertainties is therefore often ignored in groundwater applications (e.g. Bredehoeft
55 2003; Neuman 2003; Bredehoeft 2005; Carrera et al. 2005; Refsgaard et al. 2006; Refsgaard et al.
56 2012).

57 In traditional (hydro-)geological 3D subsurface modelling, a distinction is made between surface-
58 based and volume-based models. Surface-based models consist of interpreted surfaces stacked in
59 stratigraphic order (Caumon et al. 2009). Structural framework models are common surface-based
60 3D subsurface models (e.g. Hansen et al. 2007; Bombien et al. 2012; Sattler et al. 2022). They can
61 represent complex geometries, but their construction can be very time-consuming, and they do not
62 provide information about the properties of the represented model units (Turner 2006; Li et al. 2022).
63 Voxel-based models consist of a structured grid of volumetric pixels, known as voxels, which are
64 assigned to particular model units (Turner 2006). They enable representation of spatially limited
65 deposits and offer a data structure which facilitates fairly fast model construction, although
66 visualisation of geometrically complex features is limited (Turner 2006; Jørgensen et al. 2010; Li et
67 al. 2022). Hybrid models link the two approaches to combine the benefits of both. They depict the
68 geometry of stratigraphic boundaries and the properties of materials between these boundaries (e.g.
69 Jørgensen et al. 2010). However, the complexity of the hybrid models often makes model
70 implementation and updating challenging and requires substantial manual effort (Li et al. 2022).

71 Here we present a modelling workflow that enables construction of large hydrostratigraphic grid
72 models (approximately 50,000 km²) despite a complex subsurface geology and a heterogeneous
73 database. The workflow aims to resolve the following issues: i) integration of all available data from
74 multi-source databases, ii) challenging representation of spatially complicated depositional and
75 structural units, and iii) manageability, updatability and time efficiency of the model construction.
76 The models were built using the software package SKUA-GOCAD 22™ and are based on the
77 available large-scale structural models for the study area, GTA3D (LBEG 2013; *Niedersächsisches*
78 *Landesamt für Bergbau, Energie und Geologie*) and TUNB3D-NI (LBEG 2022b), and additional

79 borehole data and cross-sections. The constructed 3D subsurface models will be subsequently used
80 for numerical simulation of subglacial meltwater erosion and subglacial groundwater flow during
81 future glaciations, as constraining these processes is crucial for the site selection of nuclear waste
82 repositories.

83 **2. Geological framework of the study area**

84 The study area is located in the North German Basin (NGB), which is the largest sub-basin of the
85 Central European Basin Systems (CEBS; Littke et al. 2008). The formation of CEBS was initiated
86 during the Early Permian, following the establishment of an extensional stress field in the area (Littke
87 et al. 2008; Maystrenko et al. 2008). The North German Basin is divided into the Northwest German
88 Basin (NWGB) and the Northeast German Basin (NEGB), separated by the Altmark Swell (Gast et
89 al. 1998) (Fig. 1a). The NWGB hosts up to 8 km thick Permian to Cenozoic fill recording a multiphase
90 tectonic history of rifting, thermal subsidence and salt tectonics (van Wees et al. 2000). During a
91 thermal subsidence phase in the Late Permian, evaporites were deposited under arid conditions
92 (Stollhofen et al. 2008). The following Triassic succession of the NWGB is dominated by continental
93 to shallow-marine sedimentary rocks, including the Buntsandstein fluvial-aeolian sandstones, the
94 Muschelkalk carbonate and evaporite sequences, and the Keuper sabkha-related mudstones and
95 evaporites (Geluk and Röhlings 1997; Geluk 2005; Gast et al. 2010). In the Jurassic, shallow- to
96 marginal-marine environments led to the deposition of both clastic and carbonate rocks, with
97 sequences of mudstone, sandstone, and limestone reflecting recurring transgressive-regressive cycles
98 in an epicontinental sea (Baldschuhn et al. 2001; Scheck-Wenderoth and Lamarche 2005; Lott et al.
99 2010). The Cretaceous succession is dominated by open-marine carbonate rocks, particularly the
100 widespread chalk deposits of the Late Cretaceous, reflecting a long-lived transgression of a warm,
101 shallow epicontinental sea across the basin (Scheck-Wenderoth and Lamarche 2005; Voigt et al.
102 2008; Vejbæk et al. 2010).

103 During the Triassic and the Jurassic to Early Cretaceous, two generations of salt structures developed
104 in the NWGB (Mohr et al. 2005; Scheck-Wenderoth et al. 2008; Brandes et al. 2013; Warsitzka et al.

105 2019). The growth of salt structures is often accompanied by the development of secondary salt rim
106 synclines, due to depletion and thinning of the salt layer and the resulting subsidence at the Earth's
107 surface. These secondary salt rim synclines often provide accommodation space for sediments and
108 lead to the formation of thick sediment packages in the immediate vicinity of the salt structures (Best
109 et al. 1988; Kockel 1988; Allen and Allen 2013). The basin inversion in the Late Cretaceous
110 reactivated the movement of these salt structures, causing many to reach the surface (Scheck-
111 Wenderoth et al. 2008; Warsitzka et al. 2019). These salt structures comprise salt diapirs, salt walls
112 and salt pillows (Maystrenko et al. 2005; Kukla et al. 2008; Scheck-Wenderoth et al. 2008).

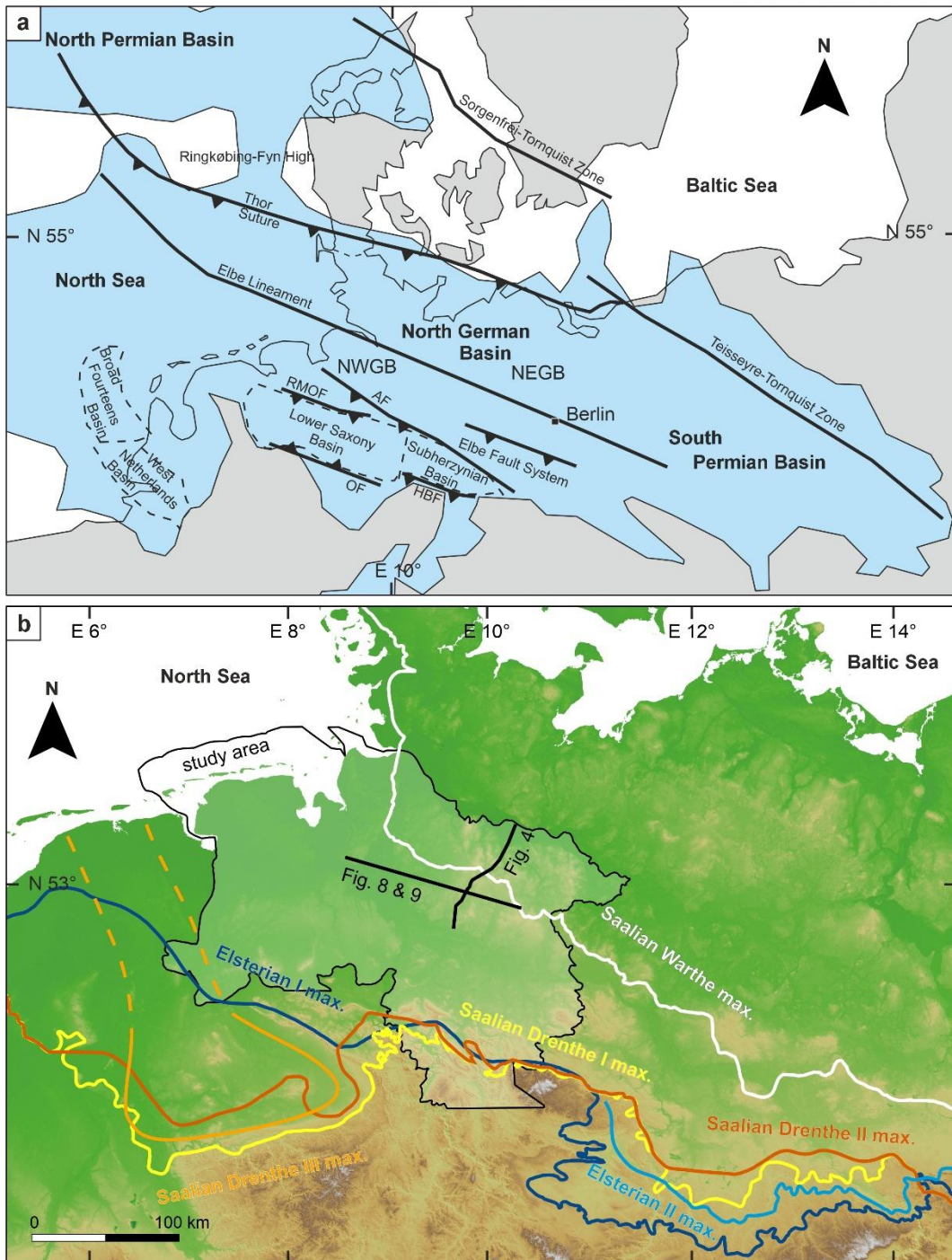


Fig. 1. (a) Structure of the North German Basin (modified after Scheck et al. 2002; Scheck-Wenderoth and Lamarche 2005; Brandes et al. 2013). NWGB = Northwest German Basin, NEGB = Northeast German Basin (cf. Gast et al. 1998). AF = Aller Fault, HBF = Harz Boundary Fault, OF = Osning Fault, RMOF = Reeder Moor Oythe Fault. **(b)** Overview map, showing the maximum extent of the Middle and Late Pleistocene ice sheets (modified after Ehlers et al. 2011; Lang et al. 2018; Soest et al. 2026).

The pattern of the Cenozoic sedimentation is strongly influenced by progressive uplift of the Variscan massifs at the southern basin margins, the Neogene uplift of the Fennoscandian Shield, and the

121 subsidence in the areas of the North German Basin and the North Sea Basin (Knox et al. 2010; Arfai
122 et al. 2014; Arfai et al. 2018). Secondary salt rim-synclines provided major accommodation space for
123 these Palaeogene to Neogene deposits (Best et al. 1988; Kockel 1988; Brandes et al. 2012; Osman et
124 al. 2013). The Palaeocene to Oligocene deposits depict an overall transgressive trend in the NGB
125 (Bachmann et al. 2008), leading to the deposition of primarily fine-grained marine sediments (e.g.
126 Gürs 2005; Standke et al. 2005; Janssen et al. 2018). The Miocene to Pliocene is characterised by an
127 overall regressive trend in the NWGB, interrupted by phases of sea level rise (Bachmann et al. 2008),
128 followed by deposition of alternating fluvial and marine sediments that can be lignite-bearing (e.g.
129 Gürs 2005; Standke et al. 2005; Janssen et al. 2018).

130 *Quaternary geology of the Northwest German Basin-* During the Middle and Late Pleistocene,
131 northern Germany was repeatedly overridden by the Fennoscandian ice sheets (e.g. Ehlers et al. 2011;
132 Roskosch et al. 2015; Lang et al. 2018; Soest et al. 2026). The ice advances of the Elsterian and late
133 Saalian Drenthe glaciation were the most extensive ones, reaching the central German uplands in the
134 south (Fig. 1b; e.g. Ehlers et al. 2011; Lang et al. 2018; Soest et al. 2026). During the Weichselian
135 glaciation, the ice did not extend beyond the Elbe River and did not reach the study area (e.g. Lüthgens
136 et al. 2010; Ehlers et al. 2011; Krauß et al. 2025).

137 During the Elsterian glaciation, deep subglacial tunnel valleys were incised by meltwater erosion.
138 These tunnel valleys can be several kilometres wide and up to 150 km long (e.g. Kuster and Meyer
139 1979; Ehlers and Linke 1989; Piotrowski 1994; Litt et al. 2007; Stackebrandt 2009; Breuer et al.
140 2023) and reach average depths of 200-300 m in northern Germany, but may locally be up to 600 m
141 deep (e.g. Kuster and Meyer 1979; Piotrowski 1994; Kuster and Meyer 1995; Stackebrandt 2009;
142 Steinmetz et al. 2015; Breuer et al. 2023; Soest et al. 2026). These tunnel valleys were partly
143 reactivated during the Saalian ice advances (e.g. Janszen et al. 2013). Weichselian tunnel valleys are
144 typically shallower, ranging from 30-80 m in depth (e.g. Jørgensen and Sandersen 2006; Kehew et
145 al. 2012), and occur primarily in northeastern Germany and Denmark (Jørgensen and Sandersen 2006;
146 Stackebrandt 2009). Tunnel valleys are commonly filled with meltwater deposits, till, and fine-

147 grained glaciolacustrine deposits referred to as “Lauenburg Clay Complex” deposited during
148 deglaciation in the underfilled Elsterian tunnel valleys (e.g. Ehlers et al. 1984; Jørgensen et al. 2010;
149 Lang et al. 2012; Janszen et al. 2013; Lang et al. 2015; Steinmetz et al. 2015; Soest et al. 2026).
150 During interglacials, fluvial and lacustrine deposition occurred in large parts of the study area (e.g.
151 Caspers et al. 1995; Litt et al. 2007; Lang et al. 2012; Janszen et al. 2013; Steinmetz et al. 2015;
152 Lauterbach et al. 2024). The sea level rise affected the coastal areas, and marine and marginal marine
153 sediments and peats were deposited (e.g. Streif 2004; Gibbard and Knudsen 2024). Throughout the
154 Weichselian glaciation, alluvial and aeolian deposition dominated (e.g. Böse 1991; Kasse 2002; Litt
155 et al. 2007; Meinsen et al. 2014; Winsemann et al. 2015; Lehmkuhl et al. 2016; Winsemann et al.
156 2022).

157 The transition from Pleistocene to Holocene was characterised by a rapid climatic shift from cold,
158 periglacial conditions to a stable, temperate environment (Streif 2004; Cohen et al. 2012). In the
159 coastal areas, marine, marginal marine deposits, and peat and bog formed (e.g. Behre 2004; Streif
160 2004). Further inland, aeolian, alluvial, and lacustrine deposits occur (e.g. Kasse 2002; Litt et al.
161 2007). These deposits can cover large areas but are often very thin (Streif 2004).

162 *Hydrogeology*- The hydrogeological properties of the stratigraphic units of the NWGB are relatively
163 well known (e.g. Manhenke et al. 2001; Reutter 2011; Ad-Hoc AG Hydrogeologie 2016; Elbracht et
164 al. 2016). The Cenozoic fill of the NWGB constitutes the most important aquifer systems for drinking
165 water supply in the northwest German lowlands (Ad-Hoc AG Hydrogeologie 2016; Elbracht et al.
166 2016). Buried tunnel valleys are important groundwater reservoirs due to their size and partly coarse-
167 grained infill (Elbracht et al. 2016). They are incised into the Neogene and Palaeogene sediments of
168 the North German Basin (e.g. Breuer et al. 2023; Lang et al. 2025) that also are important aquifers
169 and aquitards (Ad-Hoc AG Hydrogeologie 2016) reaching significant depths and thicknesses in
170 secondary salt-rim synclines (cf. Best et al. 1988; Kockel 1988). The Oligocene Rupelian clay is
171 considered the most important large-scale aquitard in the shallow subsurface (Hebig et al. 2012; Brose
172 and Hermsdorf 2017). However, it is known that the Rupelian clay is discontinuous in many areas

173 and it was affected by subglacial erosion. In several regions, tunnel valleys are cut into Rupelian clay,
174 which generates direct hydraulic contact between Quaternary and pre-Quaternary aquifers (Klinge et
175 al. 2002; Limberg et al. 2016).

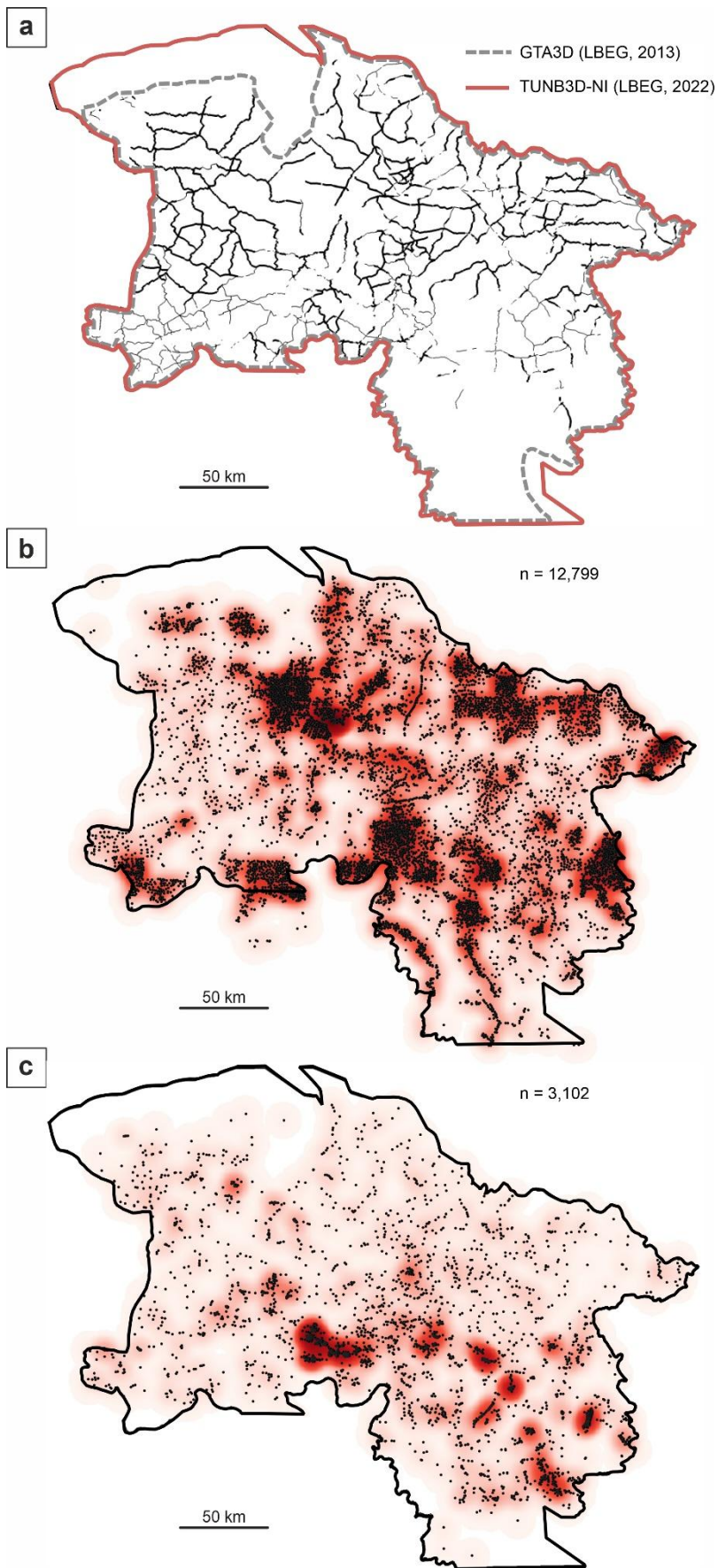
176 **3. Data preparation and model construction**

177 3.1 Database

178 The 3D subsurface models were constructed using a heterogeneous, multi-source database. This
179 dataset comprises existing structural 3D models (Fig. 2a; LBEG 2013, 2020, 2022b), 294 geological
180 and hydrogeological cross-sections (Fig. 2a; LBEG 2021), the Geological Map of Lower Saxony at
181 a scale of 1:500,000 (LBEG 2015), and borehole markers and logs from 15,901 boreholes derived
182 from the Lower Saxony Borehole Database (Fig. 2b, c; LBEG 2022a) and the Hydrocarbon Database
183 (LBEG 2022a).

184

185



186

187 **Fig. 2.** (a) Location of cross sections and surface-based structural and hydrostratigraphic 3D subsurface models used for
 188 model construction (LBEG 2013, 2021, 2022b). (b) Spatial distribution and density of borehole data across the study area

189 used for the construction of the Cenozoic structural model. The boreholes were selected from the regional borehole
190 databases (LBEG 2022a) based on the provided information (location, stratigraphy, and lithostratigraphy had to be
191 described). (c) Spatial distribution and density of borehole data across the study area used for the interpolation of the
192 properties of hydrofacies and lithology within the Neogene to Permian model units. The boreholes were selected from
193 the regional borehole databases (LBEG 2022a) based on the provided information (location, stratigraphy, and
194 lithostratigraphy had to be described).

195 3.2 Conceptual model

196 As the 3D subsurface grid models were constructed for the subsequent numerical modelling of
197 subglacial erosion and subglacial groundwater flow predictions during future glaciations, the
198 understanding of the distribution of well- and low-permeable deposits within the subsurface was
199 essential. The availability of meltwater at the ice-bed interface and its erosive potential strongly
200 depend on the hydraulic conductivity of the bed (Kehew et al. 2012). Therefore, our models need to
201 provide an overview of the distribution of lithologies and permeabilities in the subsurface, while
202 ensuring they remain manageable and not too complex for further numerical modelling, which
203 typically requires generalisation and simplification of data.

204 A conceptual model reduces the complexity of the regional geological setting and provides a
205 consistent overview of the properties of the subsurface. For this study, we defined a single conceptual
206 model for the whole study area, following the common strategy for large-scale subsurface modelling
207 (e.g. Brassington and Younger 2010; Izady et al. 2014). This approach ensures computational
208 efficiency and data manageability while maintaining a physically sound representation of the
209 subsurface hydrogeology.

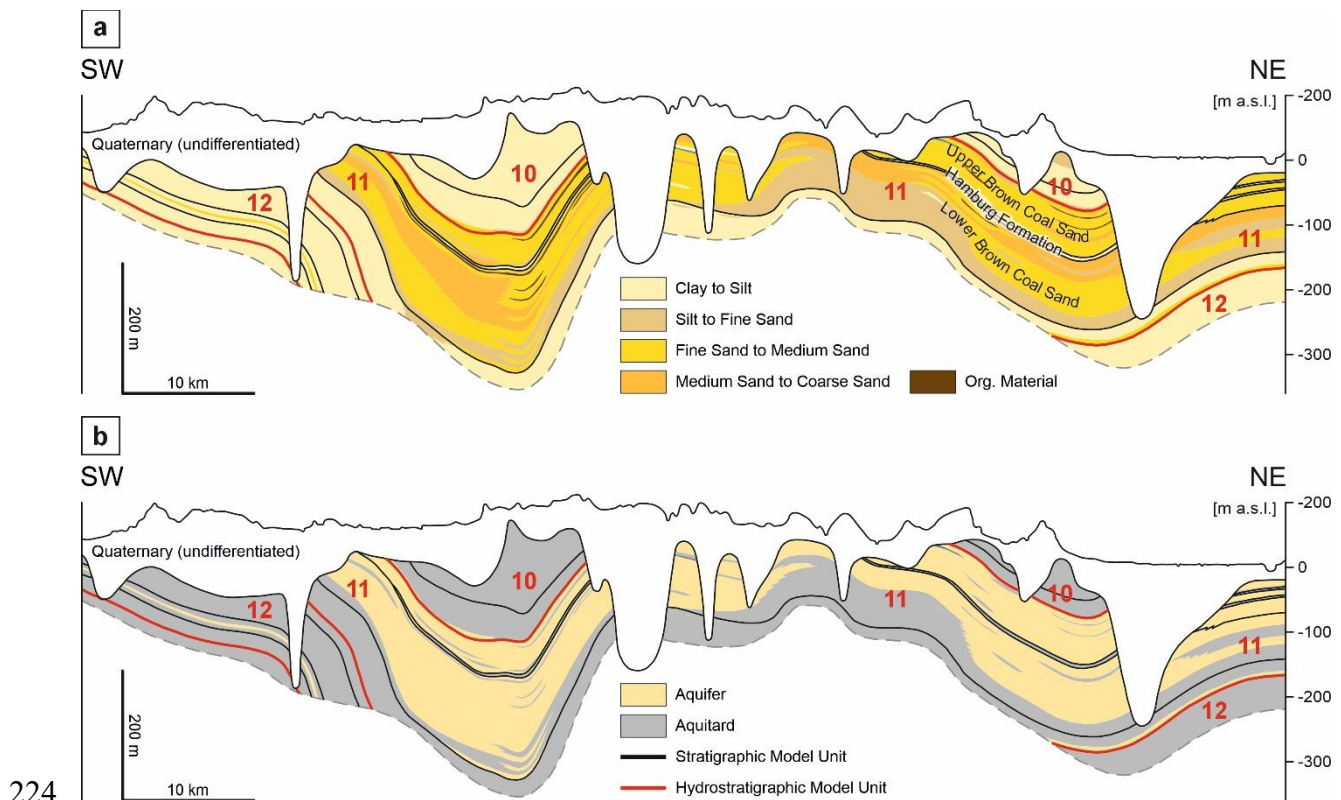
System	Hydrostratigraphic Model Unit		Lithology	Hydraulic conductivity [m/s]
Quaternary	1	Weichselian sand-sheet and dune deposits	Sand	>1E-5 – 1E-3
	2	Weichselian loess deposits	Clay, silt	>1E-7 – 1E-5
	3	Weichselian periglacial slope deposits	Clay, silt	>1E-7 – 1E-5
	4	Weichselian fluvial deposits	Sand, gravel	>1E-4 – 1E-3
	5	Saalian (Drenthe I+II) till	Clay, silt, sand, gravel	>1E-7 – 1E-5
	6	Saalian (Drenthe I+II) meltwater deposits	Sand, gravel	>1E-4 – 1E-3
	7	Elsterian till	Clay, silt, sand, gravel	>1E-7 – 1E-5
	8	Elsterian glaciolacustrine deposits	Clay, silt	>1E-7 – 1E-5
	9	Elsterian meltwater deposits	Sand, gravel	>1E-5 – 1E-3
Neogene	10	Pliocene to Middle Miocene deposits	Sand(-stone), gravel	>1E-5 – 1E-3
			Clay(-stone), silt(-stone), marl(-stone), coal (undiff.)	<1E-5
	11	Lower Miocene deposits	Sand(-stone), silt(-stone), gravel, coal (undiff.)	>1E-4 – 1E-3
			Clay(-stone), silt(-stone), coal (undiff.), marl(-stone)	>1E-7 – 1E-5
Palaeogene	12	Upper Oligocene to Middle Oligocene deposits	Sand(-stone), gravel	>1E-5 – 1E-3
			Clay(-stone), silt(-stone), marl(-stone), coal (undiff.)	<1E-5
	13	Lower Oligocene to Middle Eocene deposits	Sand(-stone), gravel	>1E-5 – 1E-3
			Clay(-stone), silt(-stone), marl(-stone), coal (undiff.)	<1E-5
	14	Lower Eocene to Upper Palaeocene deposits	Sand(-stone), gravel, rocks	>1E-5 – 1E-3
			Clay(-stone), silt(-stone), marl(-stone), coal (undiff.)	<1E-5
Cretaceous	15	Upper Cretaceous deposits	Sand(-stone), marl(-stone), limestone, chalk	>1E-5 – 1E-3
			Lime(-stone), chalk, marl(-stone), clay(-stone), ironore	>1E-7 – 1E-5
	16	Lower Cretaceous deposits	Sand(-stone), silt(-stone), limestone, marl(-stone)	>1E-5 – 1E-3
			Clay(-stone), marl(-stone), sand(-stone), silt(-stone), shale, evaporites	>1E-9 – 1E-5
Jurassic	17	Wealden to Upper Jurassic deposits	Sandstone, marlstone, limestone, dolomite	>1E-5 – 1E-3
			Claystone, shale, siltstone, marlstone, limestone, evaporites, trachyte	>1E-9 – 1E-5
	18	Middle Jurassic deposits	Sandstone, marlstone	>1E-5 – 1E-3
			Claystone, siltstone, iron stone, marlstone	>1E-9 – 1E-7
	19	Lower Jurassic deposits	Sandstone, limestone	>1E-5 – 1E-4
			Claystone, shale, siltstone, marlstone, coal (undiff.)	>1E-9 – 1E-7
Triassic	20	Upper Keuper deposits	Sandstone	>1E-5 – 1E-3
			Claystone, shale, siltstone, marlstone	>1E-9 – 1E-7
	21	Middle to Lower Keuper deposits	Sandstone	>1E-5 – 1E-3
			Claystone, marlstone, dolomite, evaporites, halite, coal (undiff.)	>1E-9 – 1E-5
	22	Muschelkalk to Upper Buntsandstein deposits	Sandstone, limestone, chalk	>1E-5 – 1E-3
			Claystone, marlstone, dolomite, evaporites, halite	>1E-9 – 1E-7
	23	Middle Buntsandstein deposits	Claystone, siltstone, sandstone	>1E-5 – 1E-4
	24	Lower Buntsandstein deposits	Limestone	>1E-5 – 1E-3
			Claystone, shale, siltstone, sandstone	<1E-5
P	25	Zechstein deposits	undiff.	<1E-5

210

211 **Fig. 3.** Simplified stratigraphic chart of the study area showing the main lithologies and hydraulic conductivities of the
212 hydrostratigraphic model units. The stratigraphic column is adapted from Menning (2018) and is not to scale. Hydraulic
213 conductivities are modified primarily after Reutter (2011), supplemented by data from Mattheß and Ubell (2003), Ad-

214 Hoc AG Hydrogeologie (2016), and Elbracht et al. (2016). Hydrostratigraphic units highlighted in yellow are classified
 215 as aquifers; those in grey are classified as aquitards; undiff. = undifferentiated

216 The conceptual model consists of 25 hydrostratigraphic model units covering Permian (Zechstein) to
 217 Quaternary deposits (Fig. 3), based on previous work by Reutter (2011), with additional information
 218 from Mattheß and Ubell (2003), Ad-Hoc AG Hydrogeologie (2016), and Elbracht et al. (2016).
 219 Hydrostratigraphic model units summarise stratigraphic units, which represent interconnected porous
 220 material with relatively uniform hydraulic properties (cf. Poeter and Gaylord 1990). The model units
 221 categorise stratigraphic units based on their hydrogeological properties into aquifers and aquitards
 222 (Fig. 4). Each hydrostratigraphic unit is given a range of hydraulic conductivity values (K-values)
 223 that are representative of the respective lithologies (modified after Reutter 2011; Fig. 3).

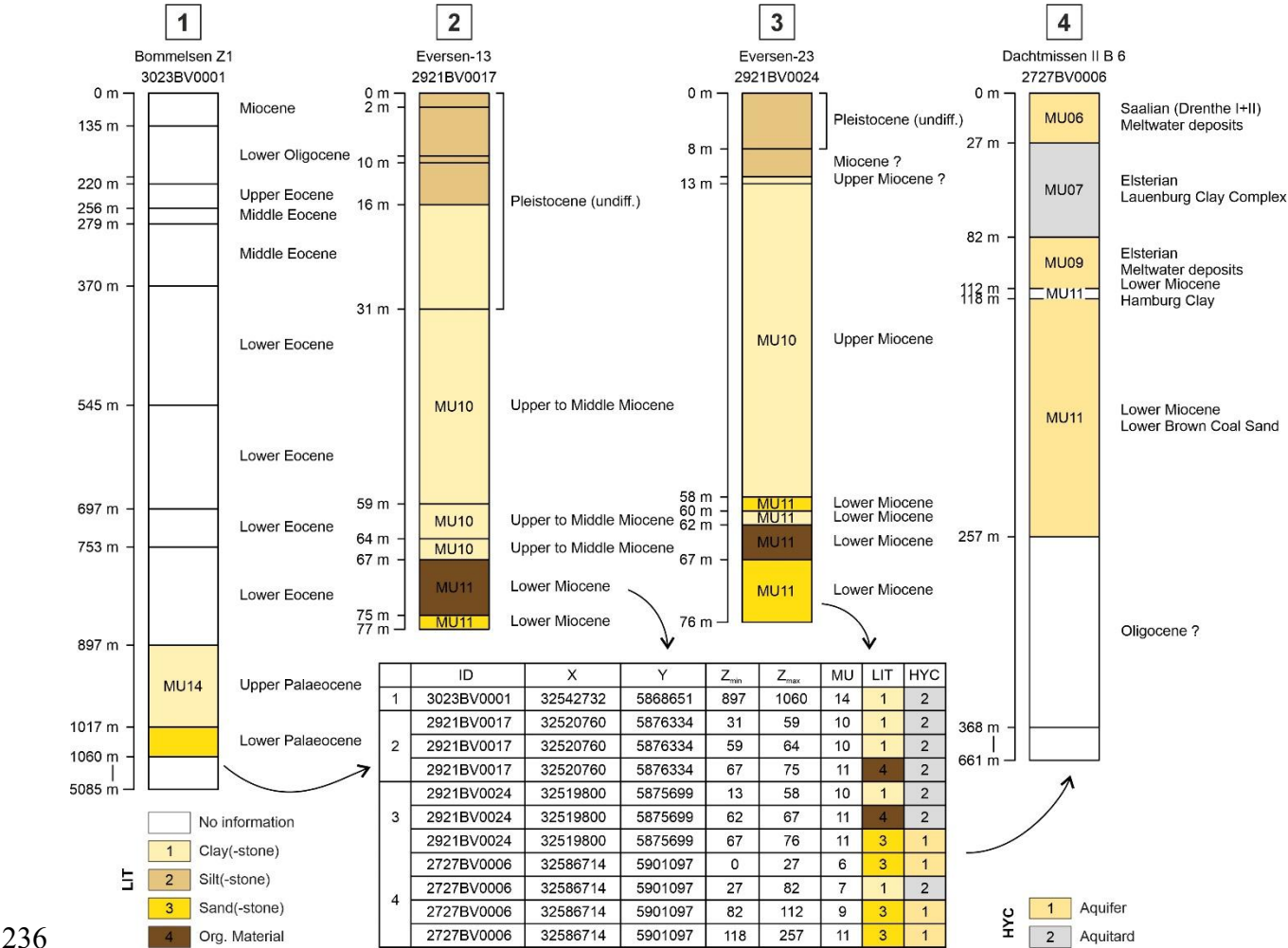


225 **Fig. 4.** Conceptual cross-section of the study area (modified after Kuster 2005), illustrating the simplification of (a)
 226 stratigraphic units into (b) hydrostratigraphic model units. Hydrostratigraphic units highlighted in yellow are classified
 227 as aquifers; those in grey are classified as aquitards (see Fig. 3 for details). Location of the cross-section in Fig. 1b.

228 3.3 Data preparation

229 The different datasets were harmonised and simplified according to the classification of model units
 230 presented in the conceptual model (Fig. 3 and Fig. 4). This was done partly manually and partly via

231 Python scripts. During the simplification process, only those sections within the boreholes that exhibit
 232 a minimum thickness of 10 m were considered. This simplification reduces stratigraphic precision
 233 while not compromising the overall quality of the model. It enables creation of a more manageable
 234 and practical subsurface model. Stratigraphic, hydrostratigraphic, lithological and hydrogeological
 235 information was translated into a simplified numerical classification code (Fig. 5).



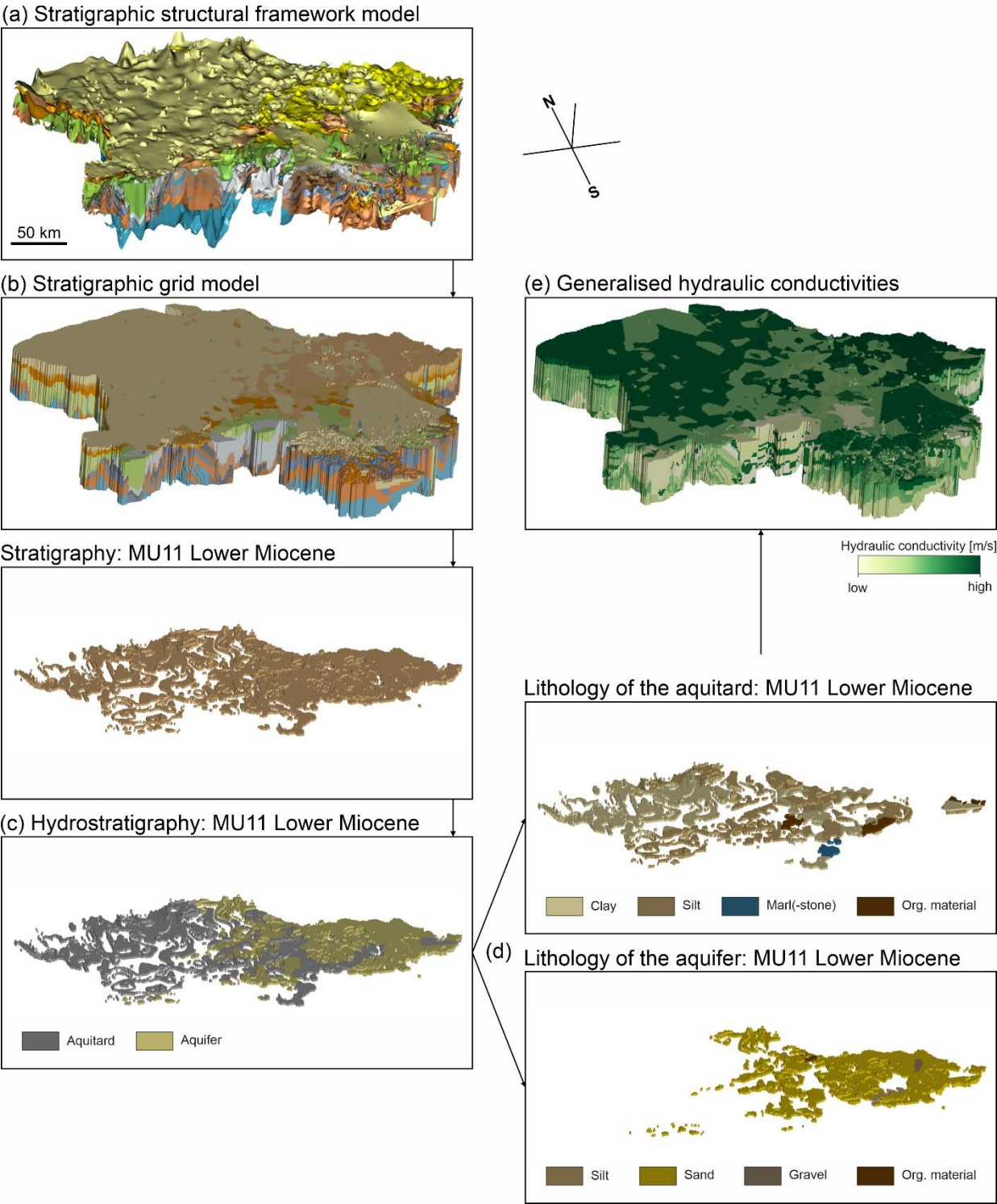
237 **Fig. 5.** Example of the process of reviewing the original borehole data and simplifying the input data for model
 238 construction (scheme adapted from Marquette et al. 2024). Only markers including information about stratigraphy and
 239 lithology could be considered during model construction. Stratigraphic (MU) and lithological information (LIT) from
 240 logs 1, 2 and 3 were translated into a standardised numerical classification code (see table), and the markers were assigned
 241 to the hydrostratigraphic classification (HYC). Log 4 illustrates what a generalisation of a borehole corresponding to the
 242 hydrostratigraphic classifications from Fig. 3 looks like. Only markers with a thickness above the chosen threshold
 243 considering the model resolution are considered. HYC = Hydrostratigraphic Class, LIT = Lithology, MU = Model Unit,
 244 undiff. = undifferentiated.

245 3.4 Model construction

246 Model construction was carried out using SKUA-GOCAD™ 22. This software was used because of
247 its integrated workflows (*Structure and Stratigraphy* workflow and *Reservoir Properties* workflow)
248 and for its implemented modelling approaches based on discrete smooth interpolation (DSI; Mallet
249 1989, 1992).

250 The subsurface models were developed using a layered-grid approach, combining surface-based
251 structural modelling with voxel-based property modelling (cf. Enemark et al. 2022). First, surface-
252 based structural framework models were constructed to establish the basal surfaces of the most
253 significant stratigraphic units in the research area (Fig. 6a). Two distinct structural framework models
254 were constructed: (1) a deep, regional-scale model encompassing Neogene to Permian units, and (2)
255 a shallow, high-resolution model focusing specifically on Quaternary deposits. We opted for two
256 separate structural framework models as the deep subsurface (Neogene to Zechstein) could be
257 modelled workflow-based, and the Quaternary depositional units required manual modelling due to
258 their geometric complexity. Faults were intentionally omitted from the structural models, meaning
259 that potential local changes in permeability along fault zones are not accounted for. This
260 simplification is common practice in regional-scale 3D subsurface models built for hydrogeological
261 assessments (Bense et al. 2013). The dichotomy of faults with contrasting effects on fluid flow, with
262 higher along-fault conductivity and limited across-fault transmissivity (Manzocchi et al. 2010), is
263 neglected because most faults in this part of the basin-fill are expected to be small and have a low
264 impact on the regional groundwater flow (cf. Grube 2019; Hardt et al. 2021). These framework
265 models then served as the structural basis for constructing stratigraphic grid models with varying
266 extensions and varying resolutions of $1000 \times 1000 \times 100$ m and $500 \times 500 \times 10$ m (Fig. 6b). In the
267 third step, the grid models were populated with properties such as hydrostratigraphy and lithology.
268 Within the grid models, properties like hydrostratigraphy and lithology were interpolated using
269 Nearest-Neighbour (NN) interpolation (Fig. 6c, d). In the last step, hydraulic conductivities based on

270 literature values were assigned to the hydrostratigraphic model units, which ultimately yielded a
 271 comprehensive, large-scale subsurface model (Fig. 6e).



272
 273 **Fig. 6.** Exemplary scheme showing the process of grid population with the different interpolation steps. (a) Layered
 274 structural model with basal stratigraphic surfaces. (b) Stratigraphic grid model of the Neogene to Permian model units.
 275 (c) Model Unit 11 Lower Miocene subdivided into an aquifer and an aquitard based on borehole data interpolation. (d)

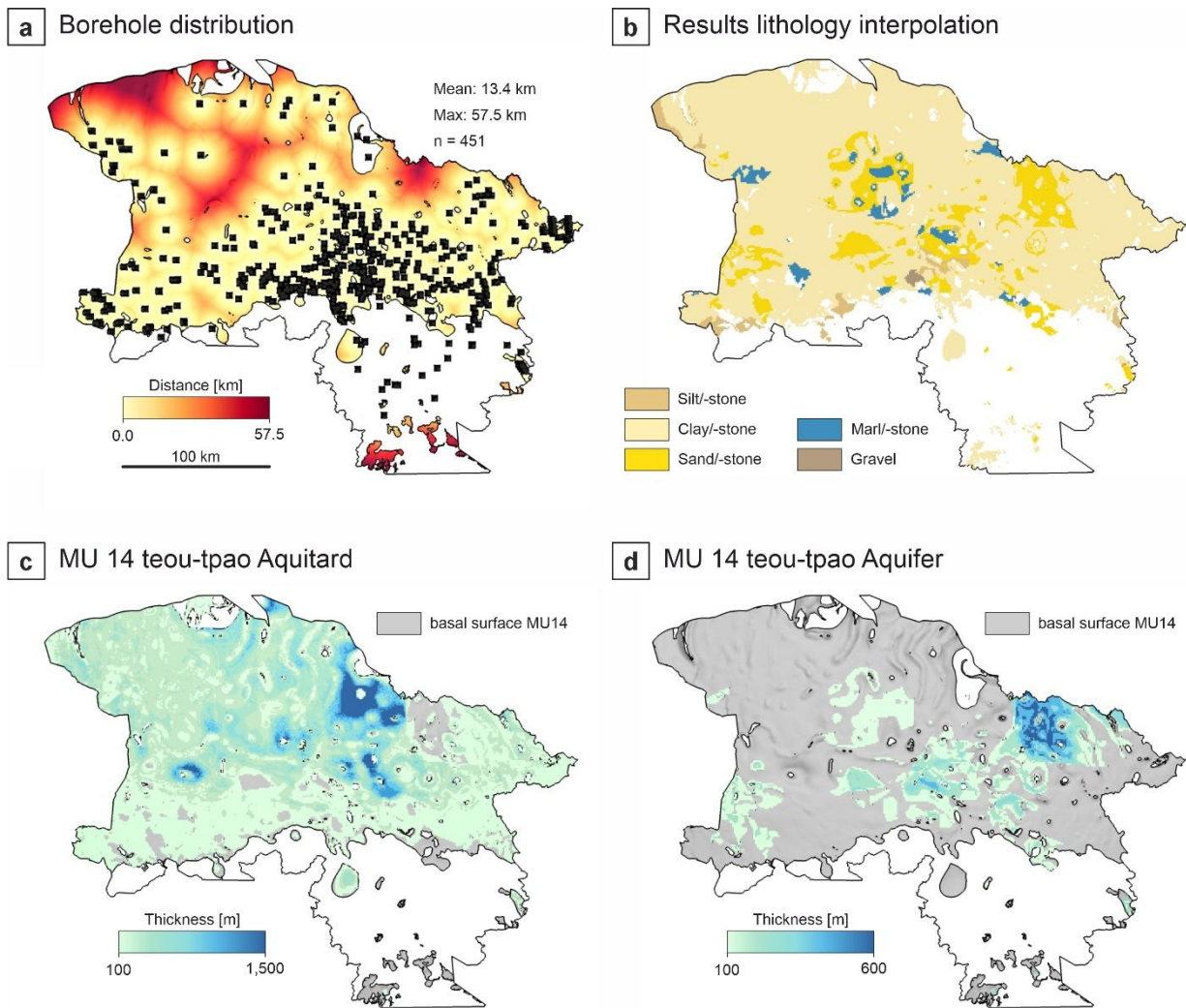
276 Further interpolation of lithologies within the hydrostratigraphic domains of the Lower Miocene. (e) Implementation of
277 generalised hydraulic conductivities based on the K-value ranges from the literature. See Table 1 for more information.

278 **4. Results**

279 4.1 Workflow execution and grid population quality

280 By conditioning the property population to the 25 distinct hydrostratigraphic model units (Fig. 3), the
281 constructed grid regions successfully guided the NN interpolation. Interpolating the
282 hydrostratigraphy and lithology within the grid offered greater flexibility for the reconstruction of
283 spatially restricted deposits (e.g. lithofacies spatially limited to secondary salt-rim synclines). These
284 deposits would have been neglected in an exclusively surface-based modelling approach, as the time
285 and effort required to reconstruct them in conventional models would have been too time-consuming.
286 The model quality was evaluated with reference to the data density distribution. The overall data
287 coverage is very good (Fig. 2c). However, when analysing the individual model units, it becomes
288 clear that the distribution of borehole data is spatially heterogeneous, reflecting the influence of
289 historic and prevailing exploration trends in the study area (Fig. 7a). This is where the (hydro-
290)stratigraphic subdomains within the grid guided the interpolation process. In areas with high data
291 coverage, the NN algorithm precisely reconstructed local lithological variations, capturing smaller-
292 scale heterogeneity. In data-sparse areas, the domain segregation ensured that the regional anisotropy
293 trends remained stable (Fig. 7b).

294



295

296 **Fig. 7.** Maps showing the input data and the results for the interpolation of the hydrostratigraphy and lithology of model
 297 unit 14 Upper Palaeocene to Middle Eocene. **(a)** Input data for the interpolation of Lithologies. The map illustrates areas
 298 of high data constraints and low data density, where grid properties are primarily driven by structural framework trends.
 299 MU = model unit. **(b)** Shows the distribution and thickness of the deposits with low hydraulic conductivities. It consists
 300 mostly of clay(-stone), silt(-stone) and marl(-stone). The minimum thickness of the aquitard is 100 m, the mean thickness
 301 is 299 m, and the maximum thickness is 1500 m. **(c)** Distribution and thickness of the deposits with high hydraulic
 302 conductivities. Mostly composed of sand(-stone). The minimum thickness of the aquitard is 100 m, the mean thickness is
 303 177 m, and the maximum thickness is 600 m. MU = Model unit.

304 Despite the heterogeneous database, the interpolation of hydrostratigraphic model units in the NWGB
 305 delivered robust and reproducible results. The constructed large-scale subsurface models are a
 306 realistic representation of the distribution and composition of different hydrostratigraphic units. The
 307 interpolation of hydrostratigraphy and lithology allows for a differentiated analysis of the

308 reconstructed model units. The resulting 3D models can be used for further analysis of the distribution
309 of deposits with different hydraulic conductivities within the study area.

310 In the following, model unit 14 Upper Palaeocene to Lower Eocene is examined as an example.

311 Within this model unit, deposits with lower hydraulic conductivity, including predominantly clay(-
312 stone), silt(-stone) and marl(-stone), are present in the entire model area, but reach greater thickness
313 of up to 1500 m mainly in secondary salt rim synclines in the NE of the study area (Fig. 7c). The
314 Upper Palaeocene to Lower Eocene with higher hydraulic conductivity, mainly consisting of sand(-
315 stone), are spatially limited to secondary salt rim synclines (Fig. 7d), reaching a thickness of up to
316 600 m.

317 The applied workflow may not be capable of fully capturing the complexities of real-world geology;
318 however, it incorporates all available data from the study area and thus delivers a robust
319 representation of the subsurface geology of the NWGB.

320 4.2 3D hydrostratigraphic configurations of the NWGB

321 Despite the limitations of the available data, the resulting models enable a comprehensive three-
322 dimensional visualisation of the lithology and hydraulic conductivities of the hydrostratigraphic
323 model units in the subsurface. The differentiated analysis of the model units based on their hydraulic
324 conductivity reveals that, especially for the Neogene to Palaeogene deposits, the highest aquifer
325 thicknesses are associated with the secondary salt rim-synclines. The aquifers are often isolated in
326 these depressions and are not always continuously distributed in the subsurface (Fig. 8).

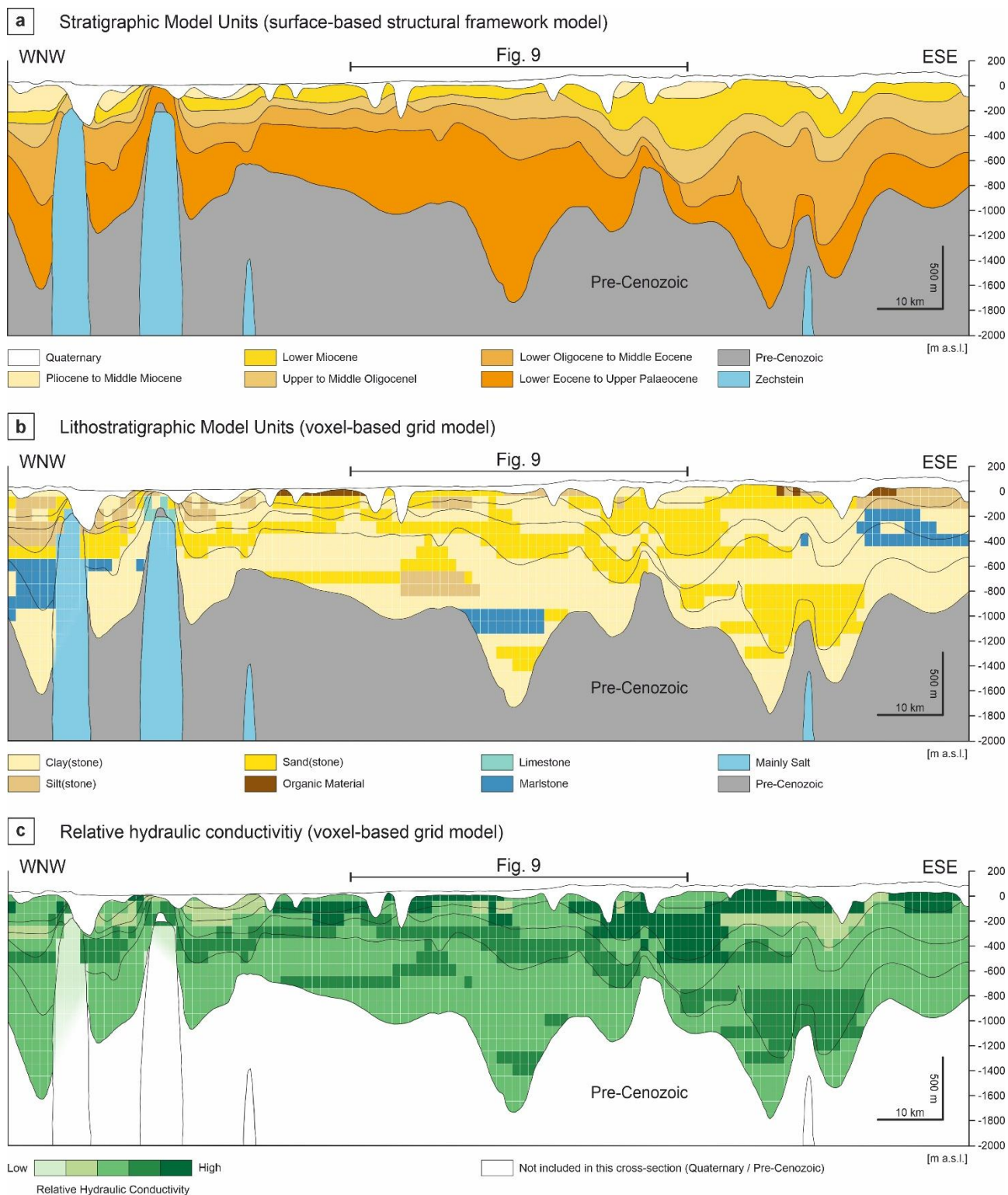


Fig. 8. Cross-section showing the distribution of (a) stratigraphic model units, (b) lithostratigraphy and (c) hydraulic conductivities derived from the lithostratigraphic units. Location of the cross-section in Fig. 1b.

The integration of higher-resolution Quaternary model units allows a three-dimensional analysis of lithological contacts. The Elsterian tunnel valleys cut deep into the Neogene to Palaeogene deposits. The inferred tunnel valley infill mainly consists of meltwater deposits with high hydraulic

conductivities, which allow for possible hydraulic windows between shallow Quaternary aquifers and deeper Neogene to Palaeogene aquifers (Fig. 9). The contact of depositional units with similar hydraulic conductivities allows for potential groundwater interchange there.

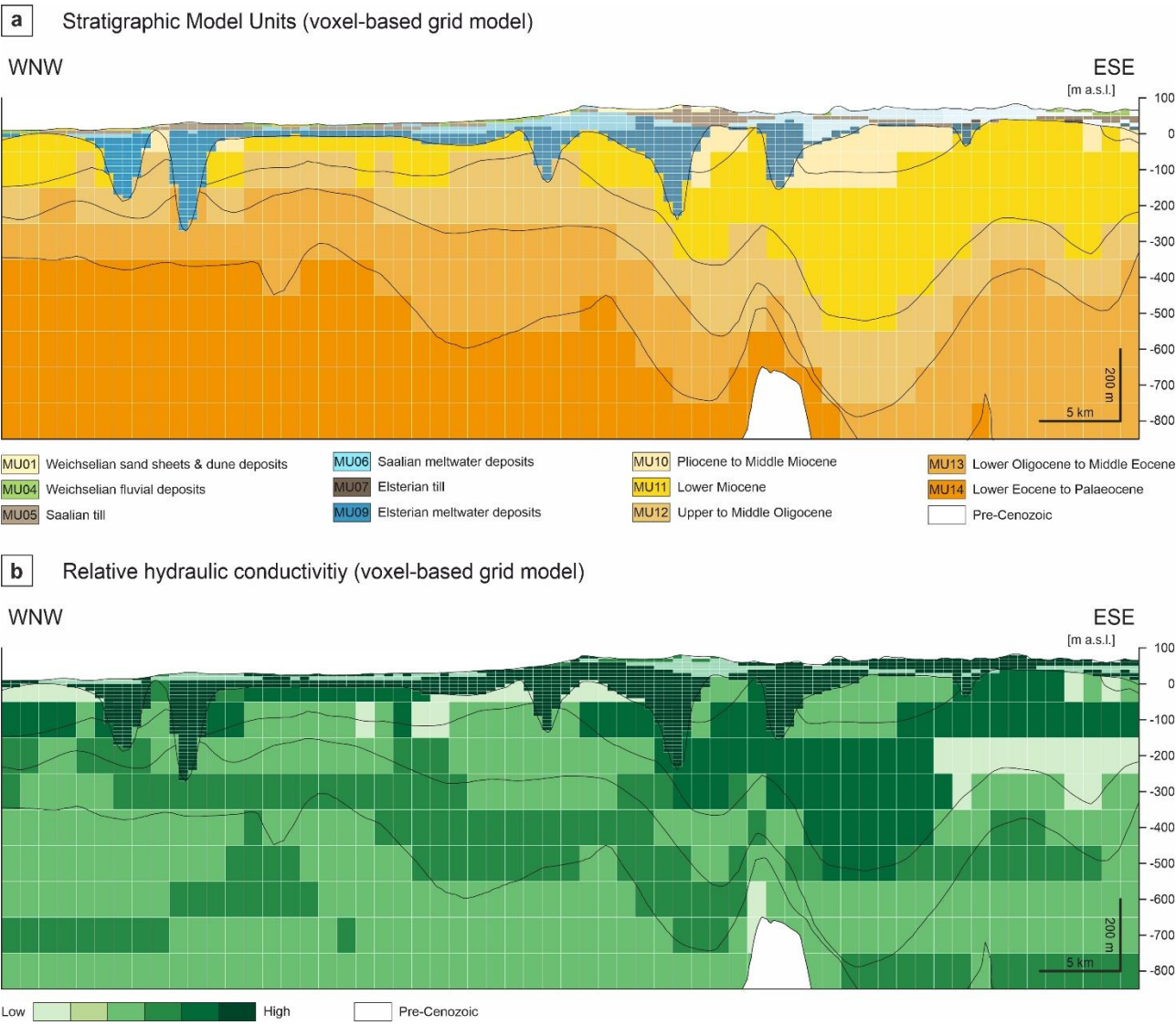


Fig. 9. Cross-section showing possible hydraulic connectivity between shallow Quaternary aquifers and deep Neogene to Palaeogene aquifers. Location of the cross-section in Figs 1 and 8.

5. Discussion

5.1 Model limitations

The development of large-scale 3D subsurface models requires a constant balance between geological detail and computational feasibility. In practice, regional models must often be simplified due to hardware limitations and the need to maintain functionality for numerical simulations (cf. Sattler et

al. 2022; Tsypin et al. 2024; Ahlers and Henk 2026). The hydrostratigraphical models presented in this study provide a reliable synthesis of the hydrogeological conditions in the NWGB, but the authors acknowledge that there are several limitations as discussed in the following.

Model resolution- Due to computational limitations and time constraints, the resolution of the presented models is limited to $1000 \times 1000 \times 100$ m to $500 \times 500 \times 10$ m (Fig. 10). Hardware limitations constitute one of the major restrictions in geological and hydrogeological modelling (e.g. Turner 2006; Yang et al. 2022; Shi et al. 2023). With the chosen resolution, we were able to reconstruct important structural features such as salt structures and their secondary rim synclines (Figs. 7 and 8) and depositional units such as spatially restricted glaciolacustrine deposits or tills (Fig. 9) in a reasonable timeframe. Other studies have demonstrated that good results in groundwater flow modelling can be achieved with similar resolutions (e.g. Piotrowski et al. 2009; Hermanowski and Piotrowski 2019). This suggests that the resolution selected for the 3D models is suitable for subsequent large-scale flow and erosion modelling in the study area. However, due to the selected grid resolution, certain important aquitards, such as the Hamburg Clay, are difficult to represent adequately in the model, given their often very limited thickness (Fig. 4).

Parameter	Model I	Model II	Unit	Comment
Coordinate Reference System	EPSG: 4647	EPSG: 4647	-	-
X (origin)	32324578	32324548	m	Geological setting
Y (origin)	5716274	5716274	m	Geological setting
Z (min)	900	890	m	Geological setting
Z (max)	-2,000	-2,000	m	Project specification
Model resolution (X)	1,000	1,000/500	m	Hardware limitation
Model resolution (Y)	1,000	1,000/500	m	Hardware limitation
Model resolution (Z)	100	100/10	m	Hardware limitation
Model extent (area of active cells)	50,762	46,153	km ²	Project specification
Model resolution (cells/direction)	351/272/30	351/272/30 702/544/290	cells	Hardware limitation
Total cells	2,864,160	2,864,160 110,747,520	cells	Hardware limitation
Active cells	1,044,889	1,044,889 1,058,500	cells	Hardware limitation

Fig. 10. Main parameters of the 3D subsurface grid models developed in this study.

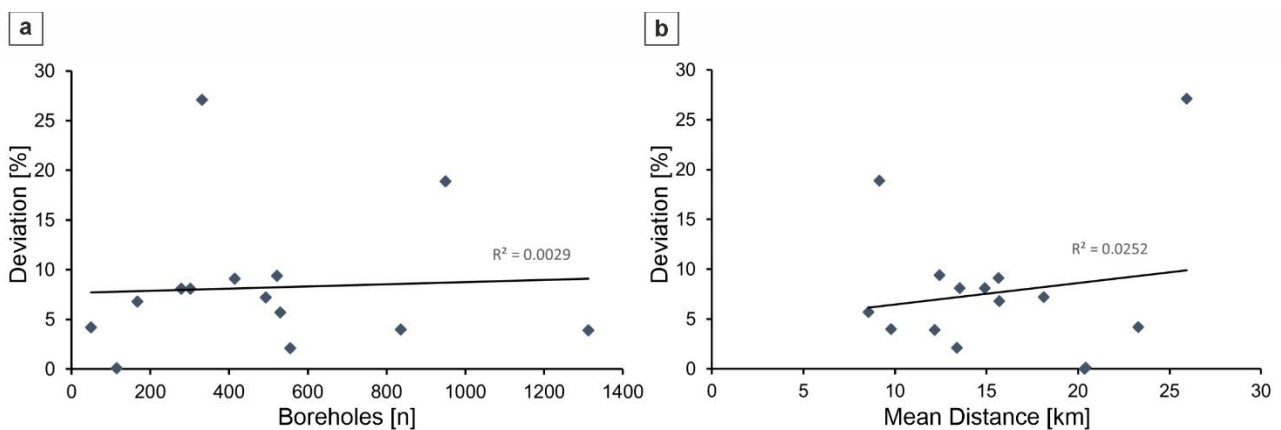
361 *Simplification of the regional geology*- For the generalisation of the complex regional geology, we
362 used hydrostratigraphic units (Fig. 3), a well-established and standard methodology in groundwater
363 research (e.g. Barfod et al. 2018; Åberg et al. 2021; Marquette et al. 2024; Mouloudi et al. 2025;
364 Åberg et al. 2026). We used hydrostratigraphic definitions that were already defined in previous
365 studies in our area (Manhenke et al. 2001; Reutter 2011) and demonstrated that these units provide a
366 robust framework that yields geologically and hydraulically meaningful results. Large-scale models,
367 such as the one used by Tsypin et al. (2024) for a similarly sized region, often employ a much higher
368 degree of generalisation to maintain performance. In such regional studies, complex sedimentary
369 successions such as those of the Quaternary are frequently represented as single, simplified units with
370 uniform properties (e.g. Brandt et al. 2024; Tsypin et al. 2024; Ahlers and Henk 2026). Applying a
371 workflow that contains the separation of the grid models into distinct hydrostratigraphic domains can
372 significantly reduce computational processing times during property population. This ultimately
373 allows for the integration of a higher level of spatial detail and geological resolution within the
374 individual model units and ensures that features critical for subglacial erosion and hydraulic
375 connectivity remain represented without compromising the model's computational efficiency.

376 *Data limitations*- The accuracy and reliability of 3D subsurface models are substantially influenced
377 by both the spatial distribution and the quality of the available input data (e.g. Sun et al. 2019; Zhang
378 et al. 2026). The main source of input data for the models constructed in this study were existing
379 structural framework models (Fig. 2a; LBEG 2013, 2022b), cross-sections (Fig. 2a), and borehole
380 data (Fig. 2b, c). However, the results show that the data coverage in the study area is good enough
381 for model construction and the available datasets were sufficient to enable modelling of the respective
382 units. This has already been shown by other studies in the same study area (e.g. Sattler et al. 2022;
383 Meinsen et al. 2026). Nevertheless, additional data acquisition in specific regions and especially the
384 integration of seismic datasets would further improve the spatial resolution and reliability of the
385 models.

386 5.2 Evaluation of the applied grid population method

387 In recent years, artificial intelligence (AI)-supported methods for grid population, such as machine
388 learning (ML) or deep learning (DL), have become increasingly popular in geoscientific applications.
389 Well-established geological statistical and probabilistic methods struggle with capturing complex
390 large-scale stratigraphic variability (Sinding-Larsen et al. 2025), highlighting the urgent need for AI-
391 supported approaches, such as ML and DL, that can offer robust and confident end-to-end solutions
392 for 3D subsurface modelling (e.g. Kaplan and Topal 2020; Marzan et al. 2021; Erdogan Erten et al.
393 2022; Abdelrahman et al. 2024). However, ML and DL algorithms demand high-quality, high-
394 precision datasets to be effectively trained (Cao et al. 2024; Zhou and Shi 2025). In addition, some
395 advanced ML algorithms are computationally intensive and time-consuming, limiting their feasibility
396 for practical geological applications (Zhou and Shi 2025).

397 The available data in our study area were insufficient not only for the effective application of AI
398 approaches, but in part also inadequate for conventional geostatistical methods such as kriging.
399 Therefore, NN interpolation was selected for property interpolation due to its straightforward
400 implementation, computational efficiency, and limited hardware requirements. It is a tested and quick
401 method for the construction of geological 3D subsurface models (e.g. Bullejos et al. 2022; Martín-
402 Martín et al. 2023; Du et al. 2024; Komara et al. 2024).



404 **Fig. 11.** Correlation between (a) the number of data points and the deviation between input data and interpolation results,
405 and (b) the average map distance between data points and the deviation between input data and interpolation results. In
406 both charts, the coefficient of determination (R^2) indicates that there is no correlation.

407 The interpolation results of the hydrostratigraphic model units for the large-scale, low-resolution
408 models show an average deviation of $\pm 8.2\%$ relative to the borehole data. The NN interpolation of
409 the lithologies for the large-scale, low-resolution models shows an average deviation of $\pm 5.0\%$
410 relative to the borehole data. This deviation can be attributed to poor data coverage in certain areas
411 of the region and over- or underrepresentation of model units due to their varying thicknesses within
412 the boreholes. The NN algorithm is sensitive to the spatial distribution of the input data (e.g. Bullejos
413 et al. 2022), although our models show no clear correlation between the deviation and the number of
414 markers per model unit (Fig. 11a) or the mean distance between the single data points per model unit
415 (Fig. 11b). We found that NN interpolation provided robust and rapid results, making it an efficient
416 choice for constructing large-scale models, where data consistency and processing speed are
417 paramount. This aligns with previous work highlighting the efficiency of NN interpolation for the
418 construction of geological and hydrogeological models (e.g. Bullejos et al. 2022; Martín-Martín et al.
419 2023; Du et al. 2024; Komara et al. 2024). Nonetheless, it is reasonable to assume that implementing
420 AI-supported algorithms could have further enhanced the quality of the property distribution,
421 especially in areas with sparse data basis or higher geological heterogeneity.

422 5.3 Model findings and implications for modelling subglacial groundwater flow of future glaciations

423 Although the presented models already capture a high degree of complexity, they are based on certain
424 assumptions and simplifications. These should be taken into account when interpreting the
425 implications of the subsequent studies. A detailed examination of the grid population results
426 demonstrates the quality of the lithologic interpolation within the stratigraphic units. The Neogene to
427 Palaeogene depositional patterns have been significantly influenced by syndepositional salt
428 dynamics. As the secondary salt rim synclines subsided, they created a high, spatially limited
429 accommodation space, which resulted in strong thickness variations of Palaeogene and Neogene
430 deposits in northern Germany (e.g. Best et al. 1988; Kockel 1988; Kuster 2005; Brandes et al. 2012).
431 These spatially restricted deposits often come with significant modelling challenges due to their
432 complex geometries and the fact that they are often insufficiently captured by borehole data. Our

models confirm the existence of hydrogeological connectivity through preferential flow paths between shallow Quaternary aquifers and deeper Neogene to Palaeogene aquifers (Figs. 8 and 9), as previously suggested (e.g. Tsypin et al. 2024).

6. Conclusions

The developed workflow can be used to construct 3D subsurface grid models with varying resolutions and can be applied to any area where borehole data are available. Although the accuracy of the 3D model is still highly dependent on data density and quality, we show that the workflow produces robust results even in areas with spatially heterogeneous data coverage. The presented workflow combines surface-based structural modelling with voxel-based property modelling, enabling structural control on the interpolation of grid properties such as hydrostratigraphy and lithofacies. This structural control guides the interpolation process and helps to produce robust results in geologically complex areas and is able to reproduce key features controlling groundwater flow and aquifer connectivity.

These 3D subsurface grid models serve as a reliable foundation for the subsequent numerical simulation of meltwater erosion during future glaciations in the research area. The models are also applicable for a range of modern hydrogeological applications, including sustainable groundwater resource management, assessment of aquifer vulnerability, geothermal energy development, and risk evaluation concerning water quality and supply. The models provide essential parameters such as lithology, hydraulic conductivity, and the spatial distribution of aquifers and confining layers. Furthermore, the workflow supports flexible model updating and adaptation, allowing rapid incorporation of new data and evolving requirements in response to ongoing societal and environmental challenges.

Overall, by facilitating the development of robust, adaptable, and data-integrated geological models, the workflow offers substantial benefits for addressing current and future hydrogeological issues

457 relevant to society, such as safeguarding water resources, ensuring environmental protection, and
458 supporting climate adaptation measures.

459 **Acknowledgements**

460 We thank the Bundesgesellschaft für Endlagerung mbH (BGE) for financial support (Reference
461 Number STAFuE-21-01-Klei), the Niedersächsisches Landesamt für Bergbau, Energie und Geologie
462 (LBEG) for providing geological datasets, and AspenTech for providing SKUA-GOCAD™ 22
463 within their Academic Programme. The study benefited from discussions with Jörg Elbracht and Grit
464 Griffel (LBEG), and Christophe Prijac (AspenTech). We thank Yeliz Genc and Malte Hoffmann for
465 assistance with borehole data preparation.

466 **Funding**

467 This work was funded by the Bundesgesellschaft für Endlagerung mbH (BGE) under the grant
468 number STAFuE-21-01-Klei.

469 **Competing Interests**

470 The authors declare no competing interests.

471 **Author Contributions**

472 RF: Investigation, Data preparation, Visualisation, Writing – original draft. MH: Data preparation.
473 PH: Validation, Writing – review & editing. GJ-O: Writing – review & editing. JP: Funding
474 acquisition, Project administration, Supervision, Validation, Writing – review & editing. CB:
475 Supervision, Validation, Writing – review & editing. JW: Funding acquisition Project administration,
476 Supervision, Validation, Writing – review & editing

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