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**OUTLINE****EDITOR'S INTRODUCTION****CASE STUDY 21-1: THE USE OF 3-D MODELS TO MANAGE THE GROUNDWATER RESOURCES OF THE LOWER GREENSAND CONFINED AQUIFER, HERTFORDSHIRE AND NORTH LONDON, ENGLAND**

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**CASE STUDY 21-2: REGIONAL 3-D MODELS OF BREMEN, GERMANY: MANAGEMENT TOOLS FOR RESOURCE ADMINISTRATION**

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# 1 CHAPTER 21: APPLICATION THEME 4: REGULATORY SUPPORT

## 2 EDITOR'S INTRODUCTION

3 The support of regulation and management of subsurface uses is a new but rapidly growing use of 3-D  
4 geological models. To date, the primary regulatory use of 3-D geological models has been to support  
5 groundwater resource management (Chapters 6 and 19). More recently, 3-D models have been used for  
6 geothermal resource assessment and management; Chapter 20 provides three geothermal case studies  
7 and summarizes additional recent developments. Regulation and management issues also influence the  
8 use of models for geohazard mitigation (Chapter 22) and infrastructure (Chapter 23). Chapters 3 and 16  
9 explore in some detail the various interactions between geological information (and models) and the  
10 urban planning issues surrounding societal desires for environmental protection, resilience, and  
11 sustainability. Chapter 14 provides additional information on the interactions between 3-D geological  
12 models and 4-D process models

13 Regulation of the subsurface is evolving in many countries, and the use of appropriate  
14 technologies to define and assess alternative solutions to societal goals is increasingly becoming  
15 recognized as an inherent part of urban planning and resource management processes. Chapter 18 has  
16 three case studies of 3-D models for urban planning, including Glasgow where a long-term collaboration  
17 between the British Geological Survey and Glasgow City Council has resulted in establishment of a  
18 contractual requirement to deposit and share data in a knowledge exchange network "Accessing  
19 Subsurface Knowledge (ASK)", which provides links to a broad range of stakeholders who either use  
20 and/or generate subsurface data within any stage of the city development process (Bonsor, 2017). The  
21 use of 3-D models is particularly important in the very rapidly growing cities of south-east Asia (see Case  
22 Study 18-3, which describes a model for Dhaka, Bangladesh).

23 The first case study describes how a 3-D geological model provided by the British Geological  
24 Survey assists Environment Agency of England and Wales (EA) in assessing alternative sources of water  
25 supplies in the Hertfordshire and North London (HNL) area where the current groundwater withdrawals  
26 are adversely affecting the baseflow of several streams originating in the Chalk Group aquifer. The  
27 model supports the EA with appropriate responses to demands by public water suppliers and large  
28 industrial users for new licenses to abstract water from the Lower Greensand Group confined aquifer as  
29 an alternative water source to meet their business needs.

30 The second case study describes the regulatory uses of 3-D geological models by the Federal  
31 State of Bremen, the smallest of the three German city states, which consists of the two cities Bremen  
32 and Bremerhaven. Located in northwestern Germany, this densely populated industrial area  
33 experiences a wide range of subsurface problems related to building construction, transportation and  
34 water supply infrastructure improvements, and utilization of geothermal energy sources. These  
35 activities are influenced by contaminated soils and waste deposits at many locations, the risk of flooding  
36 due to storm events and, over a longer term, a rising sea level and associated ground water salinization.  
37 In response to these concerns, the Geological Survey for Bremen has developed a 3-D geological model  
38 of the subsurface Quaternary units and upper Tertiary units. This model and a derived steady-state  
39 groundwater flow model support government administrative actions, planning for construction projects,  
40 and issues related to groundwater use and geothermal development. Products derived from these  
41 models are provided to public and private sectors, partially through a web-service.

## 42 **CASE STUDY 21-1: THE USE OF 3-D MODELS TO MANAGE THE GROUNDWATER** 43 **RESOURCES OF THE LOWER GREENSAND CONFINED AQUIFER, HERTFORDSHIRE** 44 **AND NORTH LONDON, ENGLAND**

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### 49 **1. INTRODUCTION**

50 The Hertfordshire and North London ('HNL') area of England is currently water-stressed; provision of  
51 adequate water supplies while balancing ecologic and economic goals is challenging. The Chalk Group  
52 aquifer is the major groundwater source; current groundwater withdrawals are adversely affecting the  
53 baseflow of several streams originating in areas underlain by chalk. The Environment Agency, in its role  
54 as a public regulatory body, is implementing a comprehensive program of investigations and actions to  
55 return the HNL area to a sustainable abstraction regime. Public water suppliers and large industrial users  
56 are being compelled to look for alternative water sources to meet their business needs. The Lower  
57 Greensand Group confined aquifer, despite its higher development costs and lower yields, is becoming  
58 an increasingly important alternative source.

59 The Environment Agency must consider the concerns and interests of all user-groups when  
60 arriving at licensing decisions. Several water suppliers have recently requested the Environment Agency  
61 provide new licenses to abstract water from the Lower Greensand Group confined aquifer. Currently,

62 the Environment Agency has no formal strategy for managing abstractions from the Lower Greensand  
63 Group confined aquifer; each application decision is on a case-by-case basis. Existing hydrogeological  
64 knowledge of the HNL area is relatively limited. Better knowledge would help achieve the Environment  
65 Agency goal of enhanced, sustainable development of the Lower Greensand Group confined aquifer.  
66 The Environment Agency commissioned the British Geological Survey ('BGS') to construct a 3-D  
67 geological and hydrogeological model of the Lower Greensand Group aquifer (Figure 21-1).

68 =====

69 Figure 21-1 NEAR HERE

70 Fig. 21-1. Location of the model area, including the bedrock geology, boreholes used and principal cross-section  
71 location [Contains Ordnance Survey data © Crown Copyright and database rights 2017]

72 =====

## 73 2. GEOLOGICAL SETTING

74 Bedrock in the HNL study area consists of a suite of Mesozoic to Cenozoic marine sedimentary rocks  
75 (Table 21-1) that dip gently to the southeast (Hopson *et al.*, 1996; 2008). The Lower Greensand Group  
76 aquifer within the model area consists of the Woburn Sands Formation, a Cretaceous shallow marine  
77 sandstone; it is supplemented by several minor sand formations (Hopson *et al.*, 2008). These sands are  
78 confined where relatively impermeable formations above the Lower Greensand Group form aquicludes.  
79 A varied sequence of shallow Quaternary deposits (Table 21-2) overlies a NE-SW trending outcrop zone  
80 of the Lower Greensand Group. This creates an important recharge zone for the Lower Greensand  
81 Group. A buried glacial channel, termed the 'Hitchin Buried Valley' extends in a southerly direction in  
82 the area around Hitchin (Hopson *et al.*, 1996). Filled with over 100 m of glacial deposits, it extends into  
83 the underlying bedrock formations, creating an important hydrogeological feature.

84 =====

85 TABLES 21-1 and 21-2 NEAR HERE

86 TABLE 21-1. Simplified bedrock stratigraphy of the Lower Greensand Group model area with  
87 hydrogeological properties (Youngest first).

88 TABLE 21-2. Stratigraphic sequence and hydrogeological characteristics of surficial deposits in the Lower  
89 Greensand Group outcrop area; they influence aquifer recharge rates.

90 =====

## 91 3. DEVELOPING THE 3-D LOWER GREENSAND GROUP SUBSURFACE MODEL

92 The 3-D geological model of the Lower Greensand Group aquifer (Figure 21-2) was developed by  
93 following the borehole and cross section approach for model construction discussed in Chapter 10. The  
94 GSI3-D software currently used by the BGS (Kessler *et al.*, 2009) developed the 3-D model. However,  
95 data preparation and model visualization utilized additional software, including Microsoft® Access, Esri®  
96 ArcGIS, and GroundHog® desktop (Wood *et al.*, 2015). The model was constructed with six bedrock units

97 and sixteen Quaternary surficial units (Table 21-3). Model units represent critical hydrogeological  
 98 characteristics of the geologic model area; permeable bedrock units with no hydraulic connectivity to  
 99 the Lower Greensand Group confined aquifer are undifferentiated in the model. The model includes  
 100 Quaternary surficial deposits where they influence the hydrogeology of the Lower Greensand Group  
 101 recharge zone.

102 =====

103 Figure 21-2 NEAR HERE

104 Fig. 21-2. A) Location of the geological cross-sections; B) 3-D fence diagram of the model cross-sections; C)  
 105 Example of three cross-sections, A and B being ‘principal’ cross-sections, and C being an example of a ‘helper’  
 106 cross-section

107 =====

108 Table 21-3 NEAR HERE

109 TABLE 21-3. Generalized Vertical Section (GVS) for use in the GSI3-D modeling process

110 =====

### 111 **3.1 Data Selection and Preparation**

112 Lithological and geophysical borehole records held in the BGS database are the primary source of  
 113 subsurface information. Thirty-four geophysical logs helped define geological unit boundaries. Lithologic  
 114 borehole logs were of variable quality; many predated the 1950s and so contained obsolete terms or  
 115 inaccurate measurements. Moreover, they were not optimally placed; many are shallow borings. There  
 116 is a paucity of information in the southeastern model area. Several areas have clusters of shallow  
 117 boreholes. The model is based on 203 representative boreholes selected from 20,546 boreholes within  
 118 the model area. Key stratigraphic surfaces were defined using GroundHog® desktop GIS software  
 119 (Wood *et al.*, 2015) materially assisting the definition of key stratigraphic surfaces. The Ordnance Survey  
 120 Terrain 50 Digital Terrain Model (Ordnance Survey Limited, 2017) defined the topography; DigMap-50, a  
 121 digital BGS geological map at 1:50,000 scale (British Geological Survey, 2017a) defined the spatial  
 122 extents of geological units. Both datasets were converted to 50 m grids for use in the model. GSI3-D  
 123 controlled the model stratigraphic relationships using a digital Generalized Vertical Section (Table 21-3).

### 124 **3.2 Model Construction**

125 The model extends from the surface to a depth of 500 m below Ordnance Datum and covers an area of  
 126 2,349 km<sup>2</sup> (907 square miles). The model was constrained by 20 interpreted geological sections; 10  
 127 sections were oriented NW-SE and 10 sections NE-SW (Figure 21-2). This orientation of the sections  
 128 roughly follows the regional dip and strike. Five geological cross-sections from the nationwide geological  
 129 fence diagram UK3-D (British Geological Survey, 2017b) were used to guide model development. The  
 130 model initially was formed as a 3-D fence diagram (Figure 21-2B). Outcrop locations defined by

131 DiGMapGB-50 (British Geological Survey, 2017a), supplemented by digitized sub-crop limits, and defined  
 132 the lateral extents of each geological unit. Base surfaces of alluvium and head deposits were defined by  
 133 assuming a thickness for each unit within its extent. This procedure accurately represented these units  
 134 while avoiding additional cross sections.

135 An iterative process was employed to convert the network of cross sections into a completed 3-  
 136 D model (Figure 21-3). Adjustments were required in areas that did not conform to expected geological  
 137 conditions. In these locations, new ‘helper’ cross-sections were developed to constrain geological units  
 138 and produce a satisfactory model.

139 =====

140 Figure 21-3 NEAR HERE

141 Fig. 21-3. A) The calculated geological model; B) Close up of the 3-D calculated surficial geology of the Lower  
 142 Greensand Group outcrop/recharge zone

143 =====

#### 144 4. MODEL PRODUCTS

145 The completed 3-D model was used to produce several digital products for the Environment Agency and  
 146 the groundwater user community. Initial outputs included some 2-D derived products that could be  
 147 used by standard GIS software, including:

- 148 • ASCII grids of the tops, bases and thicknesses of the geological units;
- 149 • ESRI shapefiles of the lateral extents (‘geological envelopes’) of each geological unit;
- 150 • Procedures defined by Lelliott *et al.* (2006) produced a “hydro-domain map” which provides users  
 151 with a 2-D characterization of the hydrogeological properties of the intercalated surficial deposits in  
 152 the recharge area (Figure 21-4).

153 The completed 3-D model was provided to the Environment Agency accompanied by the free  
 154 BGS ‘Lithoframe viewer’ which allows viewing, investigation, and query of the 3-D geological model with  
 155 a simple GIS-type interface (Waters *et al.*, 2015).

156 =====

157 Figure 21-4 NEAR HERE

158 Fig. 21-4. A) “Hydro-domain map” of the Lower Greensand Group outcrop zone; B) “Hydro-domain”  
 159 characterization.

160 =====

161 Further output products were specifically related to the hydrogeology. Attributes defining the  
 162 aquifer designation, the flow mechanism, and the productivity characteristics of each geologic unit  
 163 (shown in Tables 21-1, 21-2 and 21-3) allowed the model and sliced virtual cross sections to be colored  
 164 to define important geohydrological considerations (Figure 21-5). A full scientific report (Cripps *et al.*,

165 2017) contains further hydrogeological information and provides a succinct summary of current  
166 hydrogeological knowledge for this area.

167 =====

168 Figures 21-5 NEAR HERE

169 Fig. 21-5. A) Location map identifying example cross-section outlined below; B) Example geological cross-section  
170 showing: Geology (top); Aquifer Designation (middle); and Flow Mechanism, Productivity (bottom).

171 =====

## 172 **5. APPLICATIONS OF THE 3-D MODEL AT THE ENVIRONMENT AGENCY**

173 The Lower Greensand Group model provides a summary of the state of current geological and  
174 hydrogeological knowledge of the Lower Greensand Group in the model area. Water level data from the  
175 Environment Agency Cam-Bedford-Ouse (CBO) MODFLOW numerical groundwater model (ENTEC UK  
176 Ltd., 2007), was added to the GSI3-D geological model. This provided a crucial link in the decision-  
177 making process. It allowed the water table or potentiometric surface for each aquifer to be computed  
178 and displayed, providing for better management of the confined Lower Greensand Group aquifer as a  
179 water resource.

180 The Environment Agency is now embracing the use of 3-D models for improved decision-making  
181 at catchment and regional scales. The 3-D models are being used internally to educate staff and enhance  
182 their understanding of subsurface geology implications. The Environment Agency uses 3-D models to  
183 communicate with stakeholders to explain complex geological issues in a format readily understood by  
184 non-experts.

185 In addition to the LGS aquifer mode, a simplified 3-D geology model of the Chalk Group aquifer  
186 in the HNL area was developed by the Environment Agency as an additional tool to improve stakeholder  
187 understanding of existing numerical groundwater models (Figure 21-6). The 3-D chalk model has  
188 successfully communicated complex issues of groundwater and surface water interactions to various  
189 non-specialist audiences interested in maintaining sustainable balances among ecologic and economic  
190 goals. The chalk model permits the 3-D visualization of the chalk geology of the HNL area while  
191 simultaneously illustrating three static groundwater level scenarios: long term average, 2001 flood level,  
192 and 2006 drought level. These scenarios allow individuals to relate their experiences of past extreme  
193 climatic events with potential groundwater resource use and management practices. The model has also  
194 been used to explain how groundwater resources can be protected from human activities and  
195 influences.

196 =====  
197 Figure 21-6 NEAR HERE  
198 Fig. 21-6. A) Calculated model of the River Chess catchment area, showing bedrock Cretaceous strata (different  
199 green colors) and Quaternary Surficial deposits (all other colors). (Farrant *et al.*, 2016). B) Location map of the  
200 Chess catchment model (blue) within the Lower Greensand Group (LGS) model area (red).  
201 =====

202           In the upper reaches of the River Chess catchment, groundwater abstractions for public water  
203 supplies are apparently contributing to low river flows. To support hydrogeological investigation of this  
204 situation, the Environment Agency, in conjunction with both Thames Water and Affinity Water,  
205 commissioned the BGS to build a 3-D geological model (Farrant *et al.*, 2016). The model produced an  
206 improved understanding of the stratigraphic variations in the chalk, its spatial variability in the  
207 catchment, and how this influences aquifer response to abstraction. The model has allowed refinement  
208 of the Southwest Chilterns groundwater model over the River Chess catchment and improved model  
209 calibration in this area.

## 210 **CASE STUDY 21-2: REGIONAL 3-D MODELS OF BREMEN, GERMANY:** 211 **MANAGEMENT TOOLS FOR RESOURCE ADMINISTRATION**

212 *Björn Panteleit and Katherina Seiter*  
213 *Geological Survey for Bremen (Geologischer Dienst für Bremen – GDfB)*

### 214 **1. INTRODUCTION**

215 The Federal State of Bremen is the smallest of the three German city states. Located in northwestern  
216 Germany, it consists of the two cities Bremen and Bremerhaven. The city of Bremen is located along the  
217 Weser River, about 60 km inland from the port city of Bremerhaven, located at the mouth of the Weser  
218 River. This densely populated industrial area experiences a wide range of subsurface problems related to  
219 building construction, transportation and water supply infrastructure improvements, and utilization of  
220 geothermal energy sources. These activities are influenced by contaminated soils and waste deposits at  
221 many locations, the risk of flooding due to storm events and, longer term, a rising sea level and  
222 associated ground water salinization.

223           In response to these concerns, the Geological Survey for Bremen (Geologischer Dienst für  
224 Bremen – GDfB) was commissioned to develop a 3-D geological framework model of the subsurface  
225 Quaternary units complemented by upper Tertiary units for the Federal State of Bremen. The model was  
226 constructed in two parts (Figure 21-7). The 3-D model for the city of Bremen was completed in 2011  
227 containing five principal stratigraphic units; the 3-D model for Bremerhaven was completed in 2014  
228 containing six principal stratigraphic units.



229 =====

230 Figure 21-7 NEAR HERE

231 Fig. 21-7. 3-D geological framework model of Bremen and Bremerhaven. Units from oldest to youngest (bottom to  
 232 top): 5, 6 fluvial and marine Tertiary sediments; 4 Elsterian glacial deposits; 3 Lauenburger glacio-lacustrine  
 233 deposits; 2 Weichselian/Saalian glacial deposits; 1 Anthropogene/ Holocene deposits. Units 5 and 6 are combined  
 234 for the Bremen model. (Seiter & Panteleit, 2016)

235 =====

236 The 3-D geological framework model and a derived steady-state groundwater flow model  
 237 support government administrative actions, planning for construction projects, and issues related to  
 238 groundwater use and geothermal development. Products derived from these models are provided to  
 239 public and private sectors, partially through a web-service.

## 240 2. GEOLOGICAL SETTING

241 Bremen is located in the northern German lowlands; specifically, on the marshy lowlands of the Aller-  
 242 Weser valley. The 3-D geological models are restricted to the Quaternary glacial and post-glacial  
 243 Holocene deposits and complemented by upper tertiary units. The tertiary units are derived from the  
 244 Geotectonical Atlas (GTA) issued by the LBEG (Landesamt für Bergbau, Energie und Geologie, Federal  
 245 State of lower Saxony). Thus, the models contain four basic stratigraphic quaternary units and two  
 246 (Bremerhaven), respectively one (Bremen) tertiary unit. (Table 21-4) which are from top to bottom : 1)  
 247 Anthropogene/ Holocene Unit, 2) Weichselian/Saalian glacial deposits, 3) glacio-lacustrine Lauenburger  
 248 unit, 4) Elsterian glacial deposits, 5) middle Miocene to Pliocene fluvial and marine deposits and 6)  
 249 lower Miocene marine deposits, which forms the lower boundary of the models. Glacial melt-water  
 250 eroded these Tertiary deposits, forming buried valleys, up to 360 m below sea level in Bremen and 244  
 251 m below sea level for Bremerhaven, that were subsequently filled with sand, clay, and tills from three  
 252 glacial cycles. These buried valleys are important groundwater sources which are partially protected  
 253 from contamination from near-surface activities by the overlying predominantly clayey Holocene  
 254 deposits.

255 =====

256 Table 21-4 NEAR HERE

257 TABLE 21-4. Simplified Quaternary and upper Tertiary stratigraphy of Bremen.

258 =====

259 The near-surface anthropogenic deposits include sands, which have been transported for  
 260 building construction, road building, or filling of abandoned harbor basins with a maximum high above  
 261 sea level of 40 in Bremen and 26 m in Bremerhaven. Debris layers from bombed buildings are  
 262 ubiquitous. Waste deposits exist in some landfills and at a surface waste disposal site. The natural  
 263 Holocene deposits include peat and organic clays in combination with fluvial and dune sands. The

264 underlying Weichselian and Saalian glacial deposits contain gravel layers resulting from glacial valley  
265 drainage systems; the bulk of these deposits consist of sand interfingering with lenses of till. The  
266 Elsterian glacial deposits were modelled as two units: The Lauenburger unit consisting of fine glacio-  
267 lacustrine deposits, and an underlying unit composed of coarser glacial deposits, mostly sands and  
268 occasional interfingering till deposits.

### 269 **3. DEVELOPMENT OF 3-D SUBSURFACE MODELS**

270 Over the past 150 years, various construction and resource activities in Bremen have resulted in about  
271 95,000 boring records being archived by the GDfB. These boreholes range in depth from building  
272 inspections of a few meters to deep gas exploration wells. These borehole records were digitally coded,  
273 interpreted, and stored to form a GDfB borehole database. In addition to borehole locations and  
274 lithologic descriptions, many records include information on the screening depth of observation wells,  
275 geophysical parameters (gamma ray or resistance logs), groundwater chemistry data, measured water  
276 levels, and groundwater extraction rates (for production wells).

#### 277 **3.1 Geological Framework Model**

278 Construction of the 3-D geological framework model was performed using the GOCAD 3-D modeling  
279 software by Paradigm. Data preparation and interpretation a GIS and GeODin (Fugro Consult GmBH)  
280 software was used to manage and interpret the information held in the GDfB borehole database. The  
281 extracted information was imported into GOCAD.

282 The 3-D geological framework model was designed to support the development of a discrete-  
283 element steady-state groundwater flow model. This method of groundwater flow simulation required  
284 layers to extend continuously across the entire model domain. Thus, the model contains a base layer  
285 (base Miocene) and six continuous hydrostratigraphic units corresponding the four Quaternary units and  
286 two tertiary units defined in Table 21-4.

287 Once the horizons defining these six hydrostratigraphic units were spatially located in the 3-D  
288 geological framework model, it was discretized into a regular 100 x 100 m grid (S-Grid in GOCAD). To  
289 allow for further evaluation, each hydrostratigraphic unit was divided vertically into a number of layers  
290 defined according to the thickness of the unit and its heterogeneity (Table 21-5). Thus, the vertical  
291 resolution of the model varies with the thickness of each stratigraphic layer and is not constant  
292 throughout the model (Figure 21-8).

293 =====

294 Table 21-5 NEAR HERE

295 TABLE 21-5. Descriptions and characteristics of 3-D model horizons and component units.

296 (Modified from Panteleit *et al.*, 2013)

297 =====

298 Figure 21-8 NEAR HERE

299 Fig. 21-8. Modified example of GOCAD S-Grid. (Seiter & Panteleit, 2016)

300 =====

301 In preparation for the groundwater flow modeling, the 3-D grid model was “parameterized” –  
 302 the lithologic character of each cell was assigned appropriate parameter values. Interfingering lenses  
 303 found within the units can now be identified by the differences in their hydraulic conductivity and  
 304 defined in GOCAD as “regions.” This allowed inhomogeneities to be identified within specific  
 305 stratigraphic units. The gridded parameter models were transferred to the USGS MODFLOW software  
 306 (USGS, 2005), which offers an integrated modeling environment for the simulation of groundwater flow,  
 307 transport and reactive processes.

308 =====

309 Figure 21-9 NEAR HERE

310 Fig. 21-9. Flow diagram of stepwise model construction. Numbers correspond to steps defined in the text.

311 (Modified from Panteleit *et al.*, 2013)

312 =====

313 In summary, the model construction involved a six-step process (Figure 21-9). The six steps are  
 314 as follows:

315 Step 1: Spatial configuration of cross sections: GIS technology was used to define desirable locations for  
 316 121 geological cross sections, 48 for the Bremerhaven area and 73 for the city of Bremen. Data queries  
 317 identified about 1150 of the deepest *reference boreholes*; these defined preferred cross-section  
 318 intersections. Cross sections were oriented to represent the deep Elsterian melt-water channels.  
 319 Throughout the construction process the borehole data were quality checked and assigned a quality  
 320 rating ranging from class Q1 (the best quality data, reference boreholes) to Q5 (data unsuitable for  
 321 modeling). Boreholes with a total depth of more than 25 meters and associated geophysical logs were  
 322 particularly suitable as reference data points and thus given a high-confidence classification (Q1).

323 *Gamma-ray* and resistivity *geophysical logs* were used to *determine the tertiary –quaternary transition.*

324 Step 2: Stratigraphic interpretation and construction of cross sections: All potential *reference boreholes*  
 325 were subjected to further stratigraphic interpretation using the GeODin software (Fugro Consult GmbH,  
 326 2016). Digital cross sections were constructed by correlating stratigraphic boundaries identified in  
 327 *reference borehole logs* to define the base of each hydrostratigraphic unit. Interfingering lenses had top

328 and bottom horizons digitized. The digital cross sections and selected borehole horizon markers were  
329 stored in a special database.

330 Step 3: Incorporation of “free wells”: More than 34,000 deep boreholes and wells and were not used to  
331 construct the cross sections. These wells, defined as “free wells”, provided valuable additional control to  
332 the definition of the stratigraphic surfaces. The petrographic descriptions of each layer in these “free  
333 wells” assessed and assigned quality ratings from Q2 to Q4 according to their quality. A Q4 rating was  
334 assigned to boreholes with stratigraphic horizons identified solely from geophysical logs; a Q5 rating was  
335 assigned to boreholes with information deemed unsuitable for the model construction process.

336 Step 4: Construction of stratigraphic horizons: The *reference boreholes* and associated digitized horizon  
337 vertices on the cross sections were set as “control nodes” during the construction of each horizon in  
338 GOCAD. They were not allowed to move during the interpolation process and stratigraphic horizons  
339 were forced to pass through their locations. In contrast, interpreted horizon vertices from the cross  
340 sections and stratigraphic positions identified in the imported *free wells* were used as “control points”.  
341 *Control points* influence the geometry of the interpolated surfaces according to user-defined criteria,  
342 but the horizons do not have to absolutely match them. Based on these “control nodes” and “control  
343 points”, horizons were modelled using the GOCAD DSI (Discrete Smooth Interpolation) procedure  
344 (Mallet, 1992; 1997). The resulting surfaces were relatively smooth, with minimal deviations from *control*  
345 *points*. Misinterpretations of borehole stratigraphy resulted in obvious surface irregularities; when  
346 observed, the borehole interpretations were corrected and the surface recalculated. The model base  
347 horizon (top of the Tertiary) had less available borehole information, so information from regional maps  
348 was used to guide its interpolation. The ground surface forms the top of the model. A 25 m resolution  
349 Digital Elevation Model (DEM) defined the ground surface.

350 Step 5: Construction of stratigraphic grids: The hydrostratigraphic horizons defining the model units  
351 were converted to a regular stratigraphic 100 x 100 m grid (GOCAD S-grid) by vertically associating the  
352 top and base horizons of each unit and dividing the distance between them into several layers according  
353 to the thickness of the unit and its heterogeneity (Figure 21-10A). Thus, the vertical resolution of the  
354 model varies, and Table 21-5 provides the range of the vertical resolution for each layer. To maintain  
355 continuous layers across the model, where a unit does not exist; it was defined as being 0.1 m thick.

356 Step 6: Parameterization of grid cells: In preparation for the groundwater flow modeling, each cell in the  
357 3-D grid model was assigned appropriate parameter values based on its stratigraphic unit and property  
358 values stored for each well-log in the GDfB borehole database. This “parameterization” of the model

359 converted lithologies to values of heat conductivity, permeability, or remediation potential (Figure 21-  
360 10B). These parameters were interpolated within the hydrogeological units from well-log observations  
361 imported into GOCAD using DSI and 3-D kriging operations supported by GOCAD.

362 =====

363 Figure 21-10 NEAR HERE

364 Fig. 21-10. Extract of the gridded geological framework model, showing: A) hydrostratigraphic units; B)  
365 parameterized hydraulic permeability model with values interpolated from borehole data. (Panteleit *et al.*, 2013)

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### 367 **3.2 Groundwater Flow Model**

368 A 3-D steady-state discrete-element regional groundwater flow model was developed using the 3-D  
369 geological framework model described in the previous section. The flow modeling was accomplished  
370 using MODFLOW with different graphical user interfaces as PMWIN (Chiang, 2005) or the open source  
371 FREEWAT platform for QGIS (Rossetto, 2015) and necessary pre- and post-processors. The flow model  
372 has 38-layers, corresponding to the number of layers defining the units in the geological framework  
373 model, and has the same 100 x 100 m grid size.

374 A gateway developed by McDiarmid (2011) allowed the rapid data transfer of parameterized  
375 GOCAD grid models to MODFLOW. Panteleit *et al.* (2013) provide details of the model hydraulic  
376 parameters. Each cell was assigned a hydraulic conductivity based on the “parameterization” derived  
377 from the lithologic borehole description (Fuchs, 2010). Vertical hydraulic conductivity was valued at  
378 nine-tenth the horizontal hydraulic conductivity by model calibration. Effective porosity, initial heads  
379 and boundary conditions were applied to the model by analyzing external sources. Modeled  
380 groundwater levels were verified by about 843 observation wells and water gauges. Groundwater levels  
381 are controlled by drainage in the low-lying agricultural areas and the water level of the river Weser.

### 382 **3.3 Higher-Resolution Local Geological Framework Models**

383 Several smaller areas experience severe groundwater contamination. In order to evaluate and manage  
384 these pollution plumes, a series of local and higher-resolution 3-D geological framework models were  
385 developed for these areas, including Bremen (Figure 21-11). These models have in general the same  
386 hydrostratigraphic units as the Bremen model, but have a finer grid resolution of down to voxels of 2.5 x  
387 2.5 x 0.2 m. They also were based on more detailed interpretations of inherent heterogeneity conditions  
388 within the hydrostratigraphic units. Local groundwater flow modeling was performed using  
389 parameterized versions of these models.

390 =====

391 Figure 21-11 NEAR HERE

392 Fig. 21-11. Refined 3-D geological framework models for local areas with specific groundwater contamination  
393 problems. Four local areas are shown. (Seiter & Panteleit, 2016)

394 =====

### 395 **3.4 Stochastic Simulations of Heterogeneity**

396 To model the transport and reaction of a contamination plume in the heterogenic Holocene deposits  
397 flow modeling described in the previous section was not able to adequately define the contamination  
398 plume. Analysis of the extent and potential future growth of the plume required a more detailed  
399 definition of subsurface heterogeneity. Using observed boreholes, stochastic simulations (see Chapter  
400 13) of the 3-D distribution of clay lenses produced a series of equally-likely subsurface models (Figure  
401 21-12). In areas with insufficient or irregular distributed observations, stochastic simulations were  
402 developed from a combination of actual boreholes and randomly-placed virtual boreholes (Figure 21-  
403 12B).

404 =====

405 Figure 21-12 NEAR HERE

406 Fig. 21-12. Examples of detailed evaluations of subsurface conditions using stochastic modeling of heterogeneity:  
407 A) model based on 216 actual wells; B) model based on 216 actual wells and 218 virtual wells. (Seiter & Panteleit,  
408 2016)

409 =====

410 These stochastic simulations of aquifer heterogeneity formed the basis for a series of  
411 parameterized grid model that permitted multiple assessments of the extent and growth of  
412 contaminant plumes. The transport and reaction model MT3D, accessed through PMWIN, performed  
413 these assessments. The model solutions compare very closely to the measured data or the observed  
414 contamination plumes.

### 415 **4. APPLICATION OF THE MODELS**

416 While geology and the models are certainly 3-D, typical users prefer 2-D derivative products, generally  
417 maps, printed or online. Some applications, based on a 3-D evaluation of the appropriate model, have  
418 produced user-friendly maps with distinctive topics such as “potential for enhanced rainwater  
419 infiltration” or “thermal conductivity and possible depth limitations for borehole heat exchangers”  
420 (Figure 21-13). True 3-D applications, such as groundwater flow-model results, are designed for use by  
421 expert users; thus, these applications are supplied with restrictions to specific user groups.

422 =====  
423 Figure 21-13 NEAR HERE

424 Fig. 21-13. Examples of three 2-D open-access web-based application maps. (A) Potential for enhanced rain water  
425 infiltration – based on near-surface permeability and depth to water; (B) Building ground quality – based on  
426 organic soils and location of marsh areas; (C) Geothermal conductivity – an important parameter for assessing  
427 geothermal potential. (Seiter & Panteleit, 2016)  
428 =====

429 Many 2-D derivative products are provided free-of-charge for use by any interested person  
430 through open-access via the World Wide Web. These products provide quick information for such topics  
431 as:

- 432 • **Potential for enhanced rain water infiltration:** To enhance the groundwater recharge and minimize  
433 impacts of heavy rain events, residents are charged reduced sewage water fees if they infiltrate  
434 collected rain water directly onto their property (Figure 21-13A).
- 435 • **Building ground quality:** In Bremen, building site quality is often adversely impacted by compaction  
436 of peat layers or highly organic clay soils. Disposal of these soils is expensive due to oxidation of  
437 pyrite and production of acid contamination. The Holocene units in the 3-D geological framework  
438 model were analyzed to produce a 2-D map showing the thickness of organic rich sediments (Figure  
439 21-13B).
- 440 • **Geothermal potential:** The Bremen area is increasingly using shallow geothermal systems with heat  
441 exchangers (commonly probes) down to a depth of up to 250 m (see Chapter 22 for examples of 3-D  
442 models supporting geothermal assessments). Information on geothermal conductivity (Figure 21-  
443 13C) and basic groundwater flow-rates are provided as web-based maps.
- 444 • **Corrosive groundwater:** In some areas of Bremen, the groundwater is corrosive to concrete due to  
445 the high levels of ammonia, magnesia, and sulfate, or low pH. The Bremen borehole database  
446 provided information on corrosive potentials; these are displayed as data points by a web-map  
447 service.
- 448 • **Flooding risk:** There is a risk of flooding by the Weser River. A map was produced that defined areas  
449 below the highest documented flood level and locations of identified flood deposits.

450 Additional 3-D evaluations, based on appropriate models, are designed for use by enterprises  
451 and/or consulting engineers, who can utilize detailed subsurface information and the geological  
452 framework to develop more detailed groundwater flow models (Panteleit *et al.*, 2013). Potential  
453 applications include:

- 454 • Improved leakage inspection of sewer systems.

- 455 • Installation of industrial production wells.
- 456 • Design of large geothermal heat exchanger systems.

457           Some data and evaluation services are only available for government administrators, so are  
458 provided online with a restricted access. The 3-D models provide a strong management tool for:

- 459 • Evaluating groundwater or geothermal production well requests.
- 460 • Evaluating restrictions in groundwater catchment areas to protect public water supplies.
- 461 • Assuring the supply of raw materials for the construction industry.
- 462 • Assessing the impact of climate change on groundwater availability (Panteleit *et al.*, submitted).
- 463 • Establishing limits for temporary artificial changes in groundwater levels.
- 464 • Incorporating 3-D geologic and hydrogeologic parameters in land use planning.
- 465 • Forecasting flow paths when monitoring contaminated areas.

## 466 **5. CONCLUSIONS**

467 In Bremen, a large number of relatively deep boreholes supported the development of 3-D geological  
468 framework models and derived groundwater flow models. These permit a wide range of geological  
469 evaluations. Model development required a strict digital coding of the borehole data and a logical  
470 verification of geologic interpretations. Model construction involved 3-D development of cross sections  
471 used implicit modeling procedures, employed by GOCAD, to define the 3-D stratigraphic surfaces rapidly  
472 and efficiently.

473           The Bremen 3-D geological framework models and derived groundwater flow models  
474 successfully provided better and easily accessible management tools for spatial information. Many  
475 products are provided as 2-D maps offered free-of-charge to the public, industry, and government  
476 administrators through web-services. More sophisticated 3-D products support enhanced planning and  
477 design support to construction projects, geothermal installations, and groundwater resource  
478 evaluations. Additional analyses with contaminant transport and reaction models permit the enhanced  
479 monitoring and prediction of the extent of contamination plumes over time.