REPORT

Contract: COSMA-1, D 2.0
Final version, **Date: 12.11.2013**

Cicerostr. 24
D-10709 Berlin
Germany
Tel +49 (0)30 536 53 800
Fax +49 (0)30 536 53 888
www.kompetenz-wasser.de

Hydrogeological and static structural geological model implementation

- Technical report -

COSMA-1, D 2.0

by

L. Thomas, T. Taute, M. Schneider (Freie Universität Berlin)

E. Schöne, L. Röhmann, T. Kempka, M. Kühn (Deutsches GeoForschungsZentrum GFZ, Potsdam)

for

Kompetenzzentrum Wasser Berlin gGmbH

Preparation of this report was financed in part through funds provided by

Berlin, Germany

2013

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Title
Technical report: Hydrogeological and static structural geological model implementation - Modeling Scenarios; COSMA-1, D 2.0

Authors
L. Thomas, T. Taute, M. Schneider (Freie Universität Berlin)
E. Schöne, L. Röhmann, T. Kempka, M. Kühn (Deutsches GeoForschungsZentrum GFZ, Potsdam)

Quality Assurance
H. Schwarzmüller (KWB)
N. Quisel (VERI)
B. David (VE DTO)

Publication / Dissemination approved by technical committee members
Boris David, Veolia Eau DT
Andreas Hartmann, KWB
Michael Kühn, GFZ
Michael Schneider, FUB
Emmanuel Soyeux, VERI

Deliverable number
D 2.0

Final version ☒
Date: 12.11.2013

Geological **CO_2** **S**torage and Other E**m**erging Subsurface **A**ctivities
- Protection of Groundwater Resources, Phase 1 -

COSMA-1, D 2.0

Technical Report on hydrogeological and static structural geological model implementation

FU Berlin: Lutz Thomas, Thomas Taute, Michael. Schneider

GFZ, Potsdam: Ellen Schöne, Lina Röhmann, Thomas Kempka, Michael Kühn

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1 Introduction

The overall goal of the project Cosma-1: “Geological CO_2 storage and other emerging subsurface activities” is the assessment of potential impacts of subsurface activities on shallow aquifers used for drinking water production.

The first two deliverables (D 1.1 and D 1.2) dealt with general approaches for risk assessment and a description of potential hazards and hazardous events, which might be a risk for shallow freshwater aquifers, as well as lessons learned from existing geothermal energy production and storage sites in Germany.

This Technical Report describes the activities of the second phase of the project COSMA-1 and focuses on the compilation of geological and hydrogeological background data (average values) and the development of a simplified conceptual hydrogeological model for a setting typical for the Northern German Sedimentary Basin.

The hydrogeological model of the Cenozoic includes Quaternary and Tertiary aquifers down to the layer beneath the Rupelian clay. On this basis, a numerical model with the program Modflow (PMWIN 5.3) was implemented as no complex geometries had to be considered.

The structural geological model of the target formation for underground utilisation, the Detfurth Formation (Middle Bunter), incorporates four different fault systems with nine faults in total enclosing the area of interest.

Further, a concept for modeling the interaction between deep, consolidated, saline aquifers with unconsolidated freshwater aquifers in a setting typical for the Northern German Sedimentary Basin was developed. This included the model selection, model parameterization, definition of boundary conditions and implementation in hydrogeological flow model software packages.

In the further course of the project, a scenario analysis will be performed by using the numerical hydraulic model of the Middle Bunter and the simplified numerical groundwater model of the Cenozoic. The numerical models will be used to assess the key parameters, having an impact on the upconing of deeper saline groundwater beneath the well fields of water works (in shallow aquifer) due to imposed pressure signals.

2 Cenozoic model

The conceptual hydrogeological model for the Cenozoic should contain the basic stratigraphic and lithologic units, which are characteristic of the Northern German sedimentary basin.

After consultation with all involved project partners and stakeholders, it was agreed that the hydrogeological model should represent a "worst case"- scenario, which includes windows within the Rupelian clay as well as deep glacial erosion channels which allow an ascent of salt water into the shallow freshwater aquifers. Therefore, the model does not represent the real situation within the deeper subsurface of a defined location, but possible geological conditions in the sense of worst-case scenarios. Nevertheless, stratigraphy, lithology and hydrogeological units of the model are typical for the Northern German Sedimentary Basin and were derived from geological and stratigraphical profiles and drilling logs.

2.1 Geological situation

Tertiary

In the considered region, a continuous sedimentation in the Cenozoic began with the Middle-Oligocene Septaria- or Rupelian clay, a marine facies, which is prevalent throughout the northern German lowlands (Pekdeger et al. 1998). The Rupelian clay with a partial thickness of over 100 m is an important aquitard, which separates the deep saline water and the fresh water aquifers of the Cenozoic (Gocht 1964). Due to glacial erosion of the Elsterian, the Rupelian clay was locally reduced in its primary thickness to a considerable amount. At some places, the Rupelian clay is totally eroded, especially where deep glacial erosion channels occur.

The marine deposits of the middle Oligocene are followed by shallow marine sandy deposits of the Upper Oligocene, which are also called Cottbus layers. Above the glauconitic, partly silty fine sands of the lower Cottbus layers, the sedimentation continued with the upper Cottbus layers, a sequence of 40 to 60 m thick mica containing fine sands (Frey 1975). Concordant to the Cottbus layers are the terrestrial sands of the Miocene, which are occasionally interspersed with lignitic clays and silts and lignite deposits (Frey 1975).

Quaternary

Within the study area, three glacial periods (Elsterian, Saalian, Weichselian) and two interglacial periods (Holsteinian and Eemian) can be distinguished. The glacial deposits are characterized by the deposition of silt and glaciofluvial sands and gravels, as well as tills and clays, and during the interglacials by sedimentation of organic silt, peat, coarse sand and gravel.

Among the Pleistocene sediments, the deposits of the Elsterian represent those with the maximum thicknesses, with an average of about 50 m (Frey 1975) and more than 190 m in deep subglacial erosion channels (Wurl 1995).

Above the Elsterian sediments are the terrestrial deposits of the Holsteinian interglacial, a fluvial - limnic environment, with a thickness of about 20-50 m. At the base, there is usually coarse sand and gravel. The main deposits of the Holsteinian interglacial are muds, rich in organic matter and fossils, clays and silts. The average altitude of the Holsteinian interglacial is located around the present sea level (0 m above sea level).

The sediments of the Saalian glacial, a sequence of glacial till, glaciofluvial sands and scattered glaciolacustrine clays and silts, are widely distributed (Kallenbach 1993).

The lacustrine organogenic and fine clastic sediments of the Eemian interglacial mostly were locally bounded on basins (Lippstreu 1995). An overprinting by the Weichselian glacial is the cause of the isolated distribution of the Eemian sediments.

Because of that, the sediments of the Saalian glacial mostly form together with the overlying Weichselian sediments a coherent package of layers of similar lithofacies with an average thickness of about 50 m. During the Weichselian, today's land surface was finally formed.

In the Holocene, peats, sapropel and calcareous muds were deposited in the sinks and basins of the late Pleistocene land surface.

Table 1 gives an overview of the stratigraphic sequence of the model area.

Table 1: Overview of the stratigraphic sequence of the model area (modified after Kallenbach 1980, Kloos 1986, Wurl 1995): Cenozoic and layers beneath Rupelian Clay.

Era	Period	Epoch	Stage	Petrography	Thickness
Cenozoic	**Quaternary**	Holocene		Sand, mud, peat	max. 25 m
		Pleistocene	**Weichselian** (glacial) Eemian (interglacial) **Saalian** (glacial) Holsteinian (interglacial) **Elsterian** (glacial)	Till, rubble, gravel, sand, silt Clay, mud, peat, silt	max. 250 m
	Tertiary	Pliocene		-----------------------	Hiatus
		Miocene		Sand, gravel, silt, lignite	max. 280 m
		Oligocene	Chattian Rupelian	Cottbus Layers (sand, silt, clay) Rupelian Clay	40-60 m 80-100 m
		Eocene		-----------------------	Hiatus
		Paleocene		-----------------------	Hiatus
Mesozoic	**Cretaceous**	Upper		Lime marl, clay, sandstone	0-90 m
		Lower		Sandstone, clay	0-60 m
	Jurassic	Upper (Malm)		Limestone, marl, clay	0-150 m
		Middle (Dogger)		Sand- and Siltstone	0-200 m
		Lower (Lias)		Sandstone, clay, marlstone	0-300 m

2.2 Hydrogeological model

The first step in establishing a hydrogeological model is the compilation of all available geological and hydrogeological background data of the region of interest. Therefor published and unpublished data from previous work (e.g. Pekdeger et al. 1998, Wurl, 1995, Limberg & Thierbach, 1997, 2001, Manhenke et al., 1995, Manhenke et al. 2001) were taken into account as well as geological profiles and borehole data.

Based on these data, together with hydrogeological maps (1:50.000 – HyK 50), hydro-geological profiles and bore logs with petrographical drilling profiles, a conceptual hydro-geological model of a selected region with a model scale of 10 km x 10 km as a basis of a numerical model was created. This model includes Quaternary and Tertiary aquifers and aquicludes down to the layer beneath the Rupelian clay (Tab. 2). The regarded geological profiles (see Fig. 1) show, based on deeper drillings, marl, sandstone and claystone of Jurassic or Cretaceous age beneath the Rupelian clay.

The main objective was the assignment of distinct hydraulic units to aquifer complexes. The differentiation of aquifers and aquicludes, the estimation and assignment of permeabilities as well as the thicknesses of aquifers and aquicludes based on stratigraphy, lithology and petrography of the different layers.

Within the model area, five different hydraulic units or aquifer complexes (GWL 1 – GWL 5), separated by aquicludes, could be identified. Table 2 shows the different hydraulic units of the regarded model area, their petrography and stratigraphy as well as their average permeabilities, based on literature research. As a result, a conceptual hydrogeological model typical for the northern German sedimentary basin was created.

A geological profile, typical for the model region, is shown in figure 1.

The Abbreviations (Code) in Table 2, Table 3 and Figure 1 are as follows:

Y = overburden, qh = Quaternary Holocene, qw = Quaternary Weichselian, qsWA = Quaternary Saalian (Warthe-phase), qsD = Quaternary Saalian (Drenthe-phase), qhol = Quaternary Holsteinian, qe= Quaternary Elsterian, tmiBRo = Tertiary Miocene upper Briesker layers, tmiBRu = Tertiary Miocene lower Briesker layers, tmiMIu = Tertiary Miocene lower Mittenwalder layers, tmiMO = Tertiary Miocene Molliner layers, tolo = Tertiary upper Oligocene (Chatt), tolCO = Tertiary Oligocene Cottbus layers, tolCOo = Tertiary Oligocene upper Cottbus layers, tolRT = Tertiary Oligocene Rupelian clay, tolRA = Tertiary Oligocene Rupelian Basissand, tolSWo = Tertiary Oligocene upper Schönewalder layers, teo = Tertiary Eocene, Jur = Jurassic, Cret = Cretaceous.

Table 2: Differentiation of hydraulic units as aquifer complexes with average permeabilities (modified after Limberg & Thierbach 2001)

Aquifer (L) / Aquiclude (H)	kf [m/s]	kf [m/s] - average	Petrography	Code	Hydraulic unit (GWL)
0	10^-2 -10^-9		overburden, waste	y	
H 1	10^-5 - 10^-9		peat, silt	qh	GWL 1
L 1.1	10^-2 - 10^-4		sand, gravel	qw, qh	qw-qh
L 1.2	10^-2 - 10^-4	3,0E-03	sand, gravel	qw, qh	
L 1.3	10^-2 - 10^-4	2,8E-03	sand, gravel	qw	
H 2	10^-5 -10^-7		till	qw	
L 2	10^-3 - 10^-4	2,6E-03	sand, gravel	qsWA-qw	
H 3.1	10^-5 - 10^-9		till	qsWA	GWL 2
L H 3	10^-2 - 10^-4	2,1E-03	sand, gravel	qsD – qsWA	qhol-qw
H 3.2	10^-5 - 10^-9		till / silt, clay	qsD	
L 3.1	10^-2 - 10^-4	2,1E-03	sand, gravel	qhol – qsD	
H L 3	10^-5 - 10^-9		clay, silt	qhol	
L 3.2	10^-2 - 10^-4	8,4E-04	sand, gravel	qe - qhol	
H 4	10^-5 - 10^-9	1,0E-09	till / silt, clay	qe	GWL 3
L 4.1	10^-2 - 10^-4	6,8E-04 bis 4,6E-04	sand, gravel	qe	tmi - qhol
L 4.2	10^-2 - 10^-5	4,5E-04	sand, gravel	qe	
L 4.3	10^-3 - 10^-5	7,0E-04	sand	tmiBRo	
H 5	10^-5 - 10^-9		clay, silt	tmiBRu	
L 5	10^-3 - 10^-5	1,4E-04	sand	tmiBRu	
H 6	10^-5 - 10^-9	1,0E-08	clay, silt	tmiMIu	GWL 4
L 6	10^-3 - 10^-5	6,6E-04	sand	tmiMO, tmiMI	tolCO – tmi
L 7	10^-4 - 10^-5	5,9E-05	sand	tolo, tolCO, tolCOo	
H 8	10^-5 - < 10^-9	1,0E-09	clay, silt	tolRT, tolo	
L 8	10^-3 - 10^-5		sand	tolRa, tolSWo, teo	GWL 5
					teo-tolRa/Jur//Cret

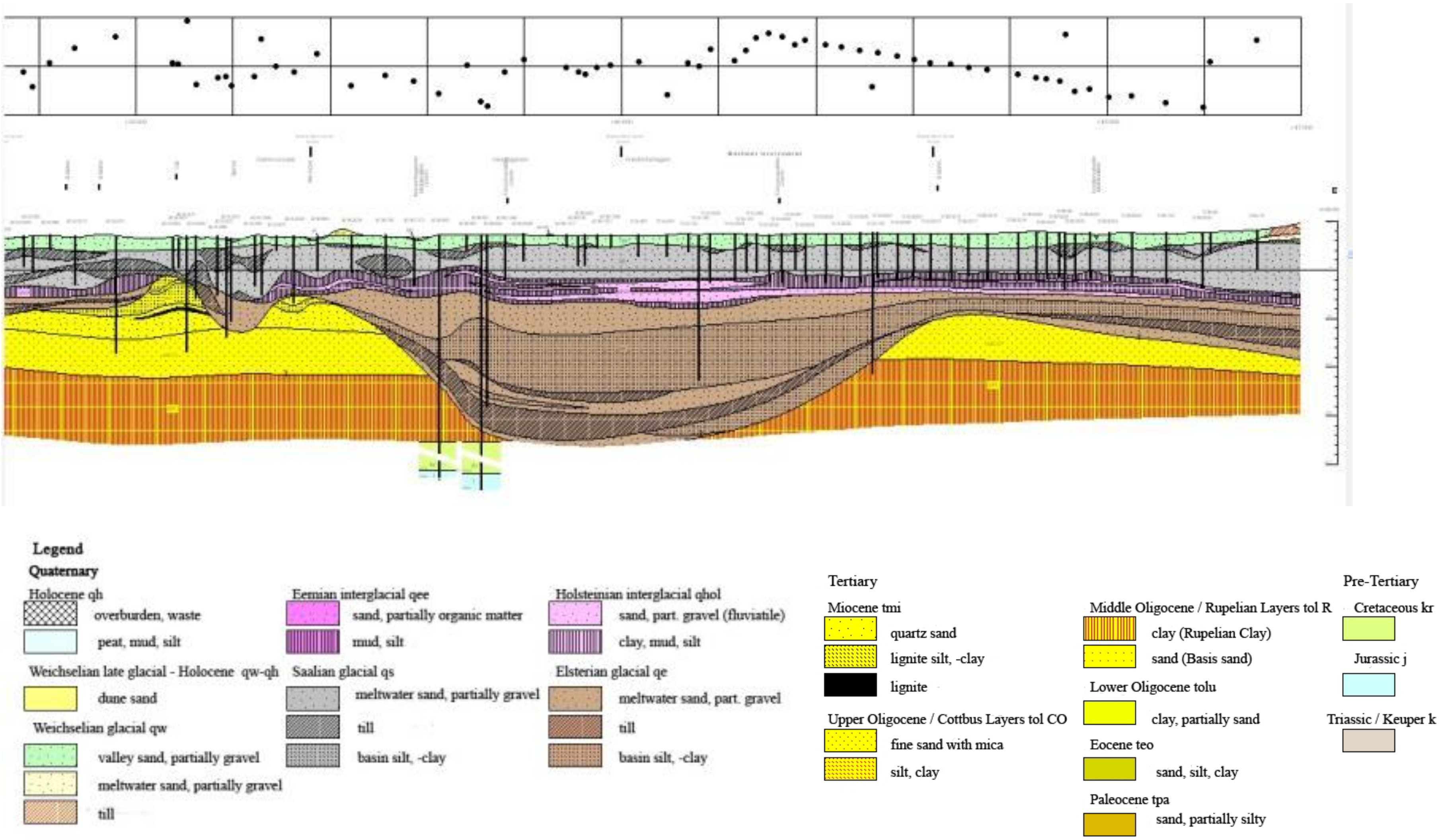

Fig. 1: Schematic geological profile (W-E) of the model region with the location of boreholes in a plan view (upper box) within a distance to the profile line of +/- 500 m (modified after Limberg et al. 2009).

The data (x,y,z-values) of the model region were digitised, and surface plots of the different layers were created, using the Kriging method, with a linear semi-variogram model and an anisotropy ratio of 1, as gridding procedure.

Examples of the surface plots of the model region are given as ground surface (Fig. 2), base of Quaternary (Fig. 3) and surface plot of the Rupelian clay (Fig. 4).

The surface plots are in a very good accordance with previously published and unpublished work as well as available geological profiles and borehole logs. The nearest neighbour statistics of the output grid of the surface of the Rupelian clay for example shows a median absolute deviation of 8 (Delta z).

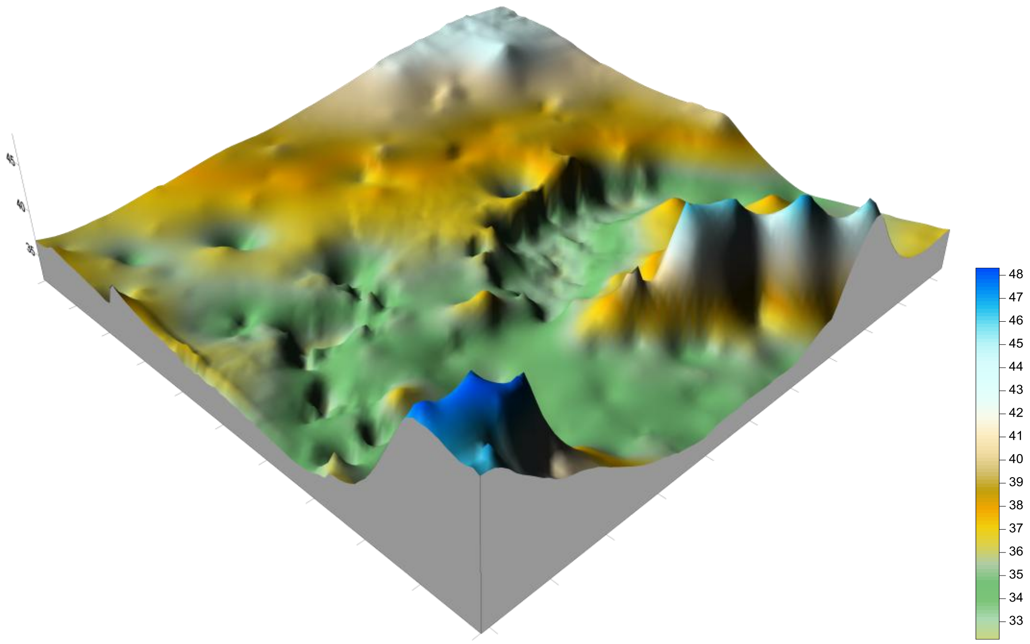

Fig. 2: Surface plot (ground surface) of the model region; scale in m NN.

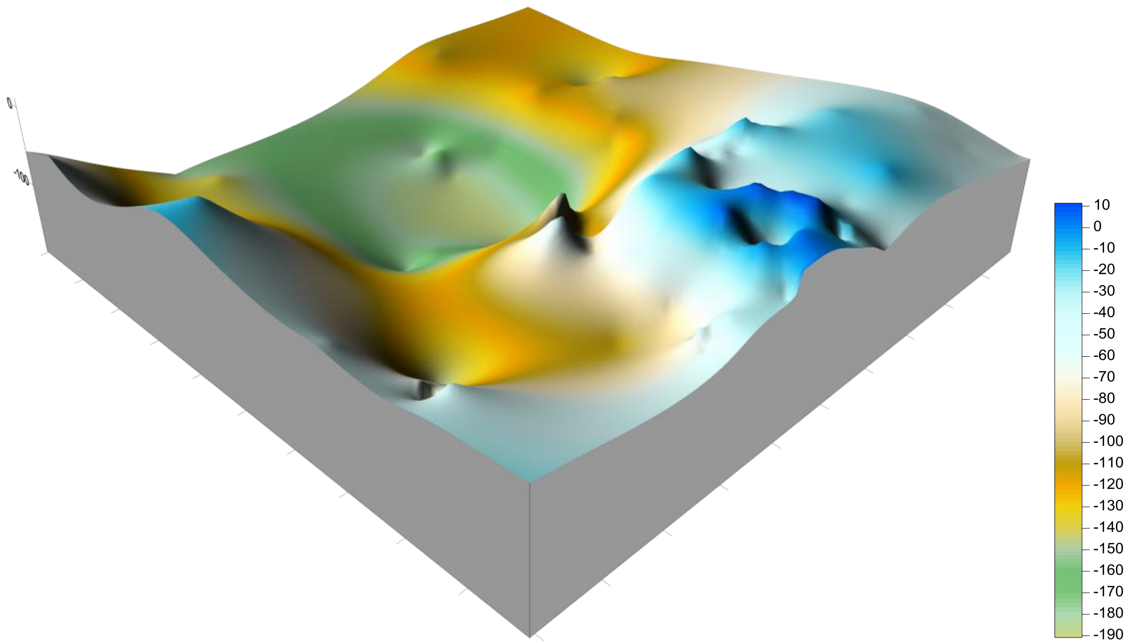

Fig. 3: Surface plot of the base of Quaternary. Scale in m NN.

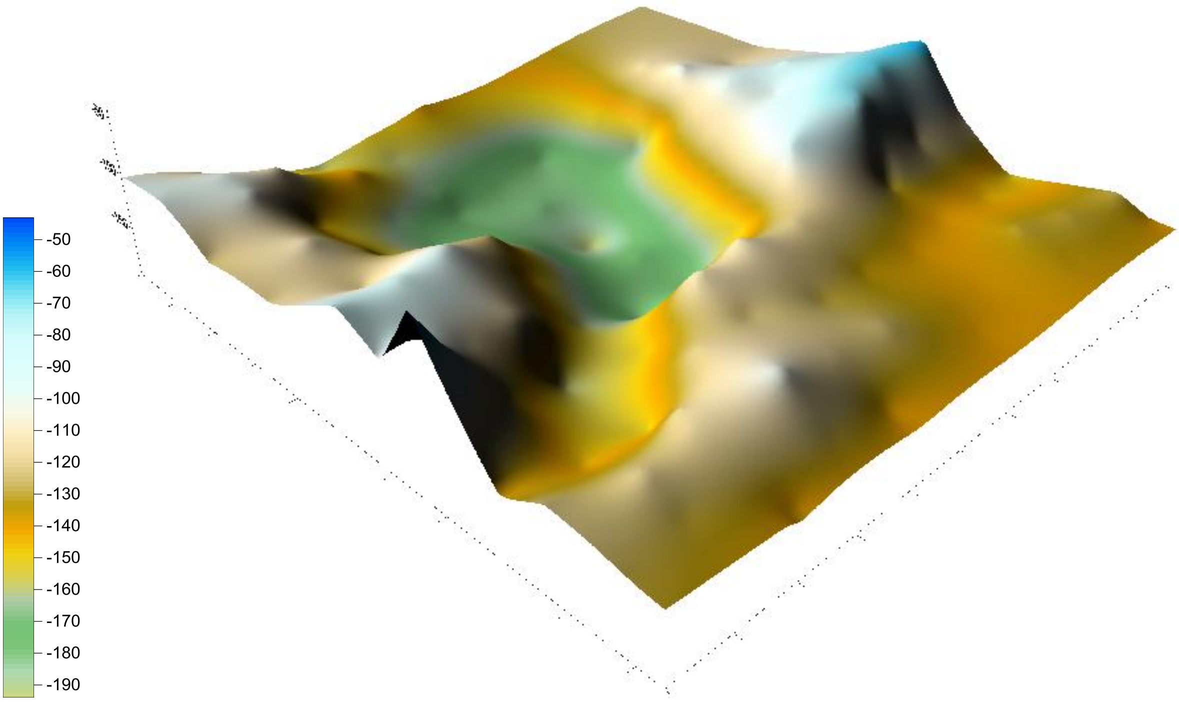

Fig. 4: Surface plot of the top of Rupelian clay (Layer 8 of the numerical model). Scale in m NN.

2.3 Implementation in a numerical model

The conceptual hydrogeological model is the basis for the numerical model, implemented in ModFlow (PMWin 5.3), using a 3D finite differences numerical method.

For computational reasons, the model was limited to an area of 10 x 10 km. It contains a total of ten layers with five aquifers as hydraulic units, separated by five aquicludes.

Since only worst case scenarios should be considered, the boundary conditions were set as no flow and closed conditions.

Table 3 gives an overview of the implementation of the conceptual hydrogeological model in a numerical model with the parameterization of the different layers.

Tab. 3: Schematic conceptual hydrogeological model with parameterization of the layers

Model Layer	**Hydraulic unit (Thickness)**	**Type**	**kf [m/s] (average)**	**Layer type**	**Strati-graphy**
I	GWL 1 (~ 25 m)	Aquifer	3.0E-03	unconfined	qw-qh
II	(~ 10 m)	Aquiclude	1.0E-09		
III	GWL 2 (~ 50 m)	Aquifer	2.0E-03	confined / unconfined	qhol-qw
IV	(~ 10 m)	Aquiclude	1.0E-09		
V	GWL 3 (~ 20 m – ~ 150 m)	Aquifer	6.0E-04	confined	tmi-qhol
VI	(~ 15 m)	Aquiclude	1,0E-09		
VII	GWL 4 (~ 80 m)	Aquifer	6.0E-04	confined	tolCO-tmi
VIII	(~ 100 m)	Aquiclude (Rupelian)	1.0E-09		
IX	GWL 5 (~10 m)	Aquifer	1.0E-04	confined	teo-tolRa Jur/Cret
X	(~ 50 m)	Aquiclude	1,0E-09		Jur/Cret

For implementing the 3D conceptual hydrogeological model into the numerical ModFlow software package (PMWin 5.3), the Kriging method as the gridding tool was applied, using a linear semi-variogram model and an anisotropy ratio of 1. As a search method in ModFlow (PMWin 5.3), octant with 1 data per sector was chosen. The grid size was defined as 100 x 100, resulting in a total of 10.000 nodes.
The parameterization of the hydraulic parameters for the numerical model is given in table 4.

Tab. 4: Parameterization of hydraulic parameters for the numerical model of the Cenozoic

Model layer	Horizontal hydraulic conductivity [m/s]	Vertical hydraulic conductivity [m/s]	Effective porosity (estimated)	Thickness [m]
I	3.0 E-03	3.0 E-04	0.25	25
II	1.0E-09	1.0E-10	0.05	10
III	2.0E-03	2.0E-04	0.25	50
IV	1.0E-09	1.0E-10	0.03	10
V	6.0E-04	6.0E-05	0.25	20 - 150
VI	1.0E-09	1.0E-10	0.03	15
VII	6.0E-04	6.0E-05	0.25	80
VIII	1.0E-09	1.0E-10	0.01	0 - 100
IX	1.0E-04	1.0E-05	0.25	10
X	1.0E-09	1.0E-10	0.03	50

For the scenario modelling, the recharge will be set to 122 mm/a as a mean annual value, and the groundwater extraction rate as total average per year to a value of 1.7 m^3/ s, derived from water-works extraction rates.

3 Deep structural geological model

Geology of the Northeast German Basin (NEGB)

The Northeast German Basin (NEGB) is part of the Southern Permian Basin (Brink, 2005). Moreover, the NEGB is a sub-basin of the North German Basin (cf. Fig. 5). The NEGB is limited to the south by the Elbe Lineament and to the north by the Tronquist-Teisseyre-Zone (cf. Fig. 6). To the west, the basin is bordered by the North Sea and to the east by the Polish Trough (Vosteen et al., 2004).

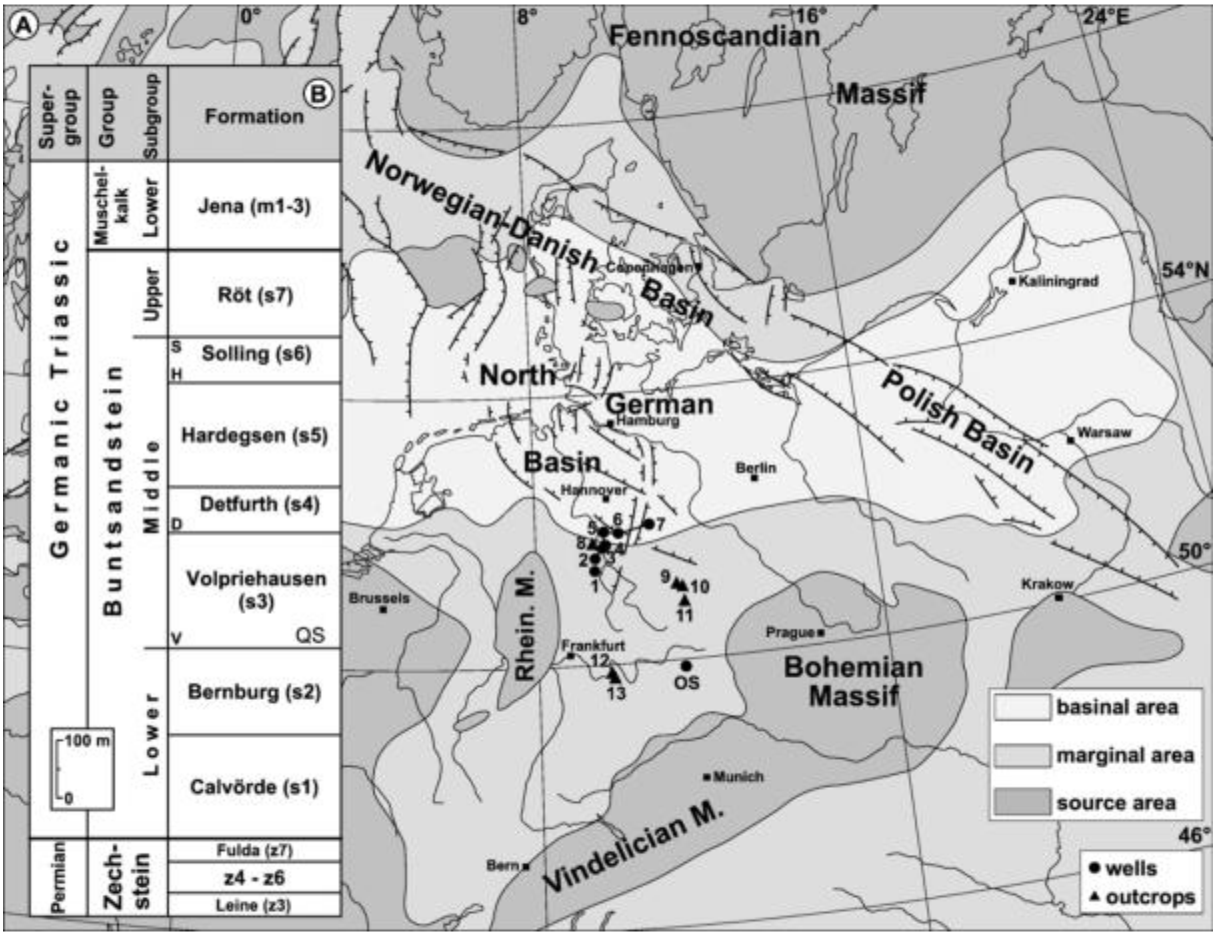

Fig. 5: A: Paleogeographical map of Bunter from the Central European Basin and its sub-basins. B: Lithostratigraphy of the Upper Zechstein to Lower Muschelkalk in Central Germany (Szurlies, 2007).

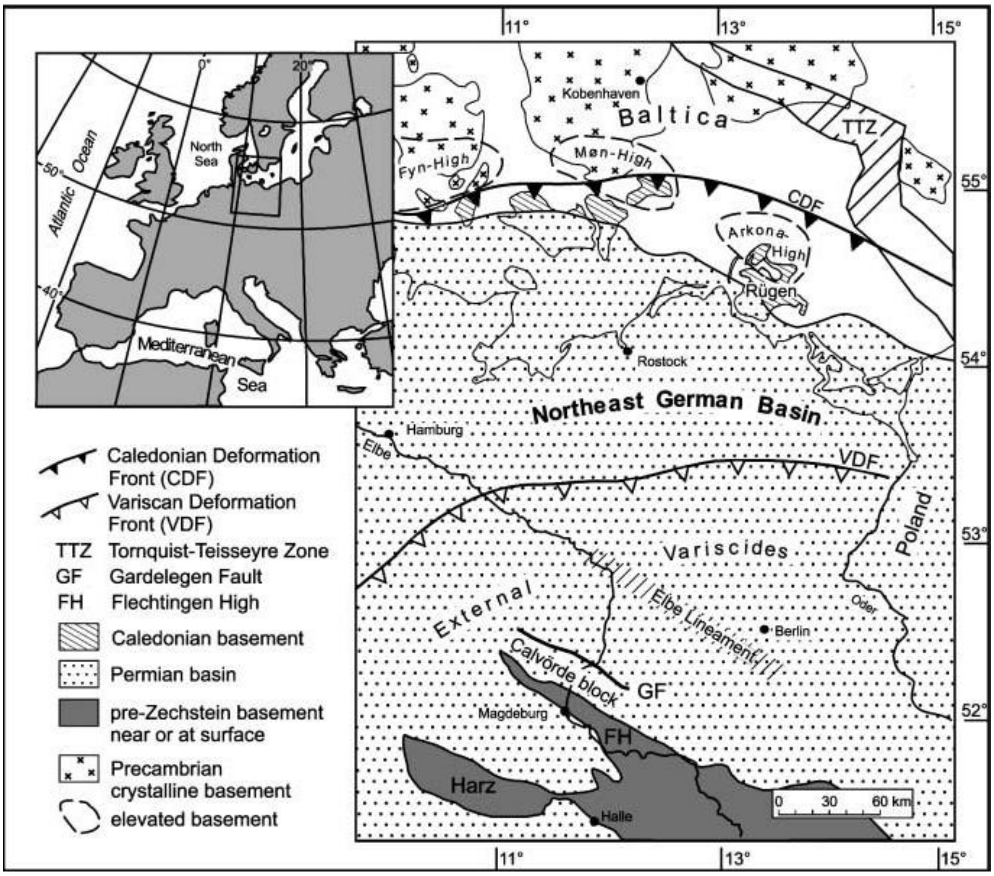

Fig. 6: Main tectonic elements of the Northeastern German Basin (Kossow et al., 2000)

For the deep reservoir model, an area with a lateral extent of 100 km x 100 km was chosen. A structural geological model was developed in order to allow for multi-phase flow simulations using the numerical simulator TOUGH2-MP/ECO2N (Pruess 2005, Zhang et al. 2008). The goal of these simulations will be the assessment of pressure perturbation in the used reservoir, Detfurth Formation in our case, and brine displacement along potentially open faults. The simulation results will then be provided to FU Berlin for an assessment of shallow aquifer salinization by brine migrating upward from the deep reservoir.

The basin started to form between the latest Carboniferous and the Early Permian (Tesmer et al., 2007). This period of time was characterized by the Caledonian and Variscan orogenies which strongly influenced underlying basement by multiphase deformation (Kossow et al., 2000). The Permian to Quaternary basin infill approaches up to 8,000 m in total thickness in the Central NEGB. The basement of the NEGB consists of Permo-Carboniferous volcanics (Scheck et al., 1999). Basically, the overlying sediments consist of clastic deposits and represent aeolian, fluvial and shallow-lake deposits.

After the Variscian orogeny the basin was filled with Permian deposits. First, the continental dominated Rotliegend was deposited in the eastern part of the State of Brandenburg followed by marine deposition (Zechstein) of carbonates and evaporates. With a thickness of more than 1,500 m and a low porosity and permeability, the Zechstein acts as a hydrogeological barrier (Williamson et al., 1997).

Transgression and regression of the Tethys controlled the sedimentation of the Mesozoic (Tesmer et al., 2007). Furthermore, the Mesozoic was characterized by salt mobilisation which was associated with flow processes in the Zechstein formation (Stackebrandt et al., 2004). These flow processes formed anticlines, which may act as potential storage sites.

Terrestrial red-bed sequences (Lower Triassic: Buntsandstein) were deposited at the beginning of Triassic (Vosteen et al., 2004). The formation Buntsandstein has a thickness of 700 m to 800 m and consists of clastic sediments originating from the Bohemian Massif south of the State of Brandenburg. The oldest rock sequence of the 200 m thick Middle Buntsandstein forms the Volpriehausen formation, followed by Detfurth, Hardegsen and Solling formation. The Upper Buntsandstein is a 180 m thick clay, anhydrite and evaporite sequence. It overlies the Middle Buntsandstein and represents a low permeable seal.

Transgression of the Tethys induced a shallow marine facies of carbonates (Middle Triassic: Muschelkalk). In the following phase of regression during Late Triassic (Keuper), terrestrial sediments were deposited. With the end of the Triassic, the infill of the basin was almost completed. Furthermore, the evolution of the basin is characterized by several stages of subsidence with its main phase during Triassic times. After Scheck et al. (1999), the NEGB developed out of five main stages of basin evolution. The first stage was introduced by an initial rift phase during Late Carboniferous to Early Permian. A second phase is characterized by a maximum subsidence from the Early Permian to Middle Triassic. After that, a phase of basin differentiation followed from Middle Triassic to Cretaceous. During Late Cretaceous, a stage of inversion occurred. During Cenozoic times, a final subsidence phase arose in the NEGB (Scheck et al., 1999).

The selected anticline exposes a depositional gap of Late Triassic (Upper Keuper), Jurassic and Upper Cretaceous. Thus, deposits from Palaeocene and Eocene follow in the geological sequence in the NEGB. The sediments of these epochs consist mainly of clay and sandstone.

Detfurth Formation as potential reservoir

The Detfurth formation has a total thickness of 60 m and offers suitable conditions for e.g. CO_2 storage. The Detfurth sandstone is 23 m thick and the reservoir top of the chosen Mesozoic anticline at a depth of about 1,100 m. 37 m of the Detfurth formation comprise a low permeable sequence which is located above the potential storage formation. Based on typical geometries, the anticline is assumed to have an east-west extension of about 20 km and an extension with north-south orientation of 5 km. The Detfurth sandstone is parameterized by a porosity of 15 % to 18 % and a permeability of 200 mD to 600 mD (Vattenfall, 2009).

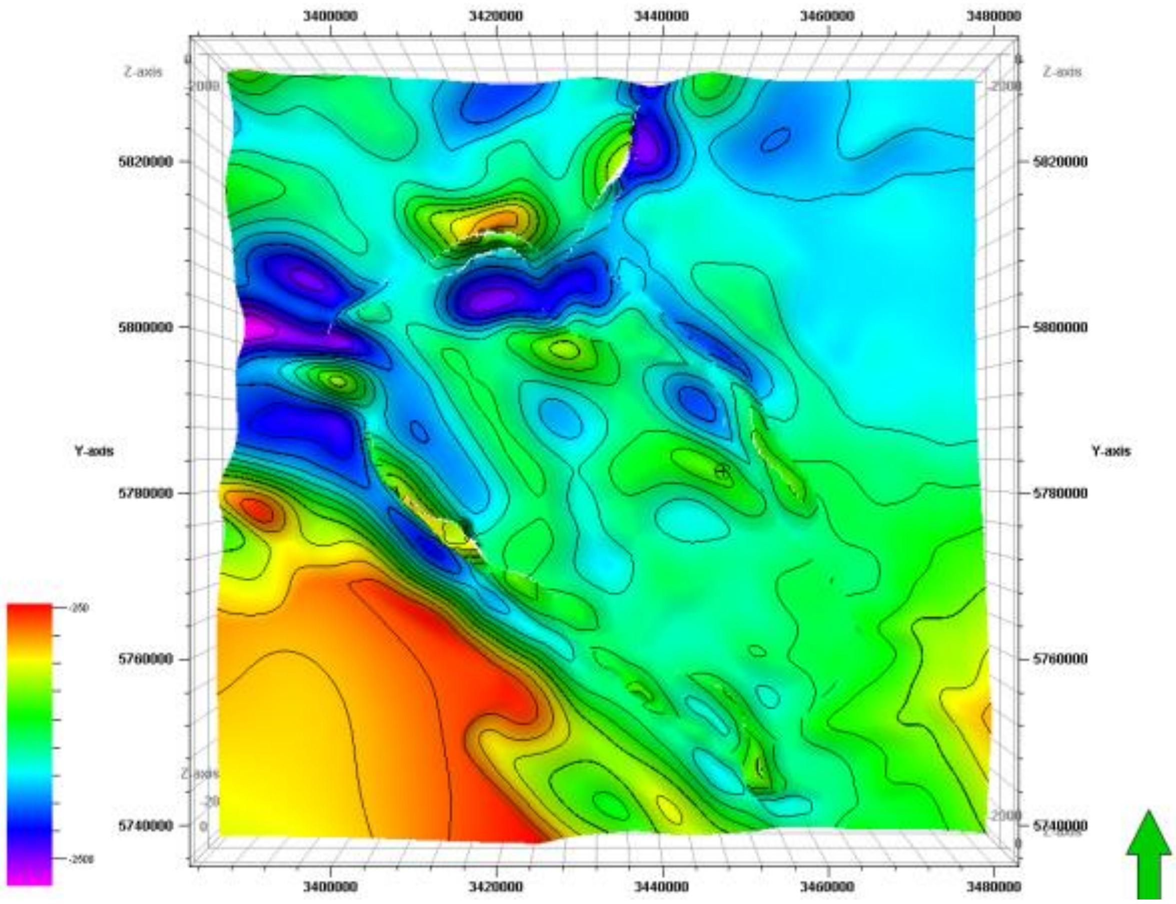

Fig. 7: 3D Structural geological model including the top horizon of Detfurth formation. Model 5 times superelevated.

Implementation of the structural geological model

The Petrel software package (Schlumberger, 2011) was used to build up the 3D structural geological model (Röhmann, 2013). For that purpose, depth contour lines of the Zechstein-

Top (cf. Fig. 8) were imported and digitalized using the Petrel software package, and subsequently adjusted to the depth and thickness of the Detfurth formation (cf. Fig. 7). The modelling area has an areal extent of 100 km x 100 km and a maximum thickness of 1,700m. The 3D model includes the Detfurth storage formation as well as fault elements, which extend to the base of the Rupelian clay (cf. Fig. 8).

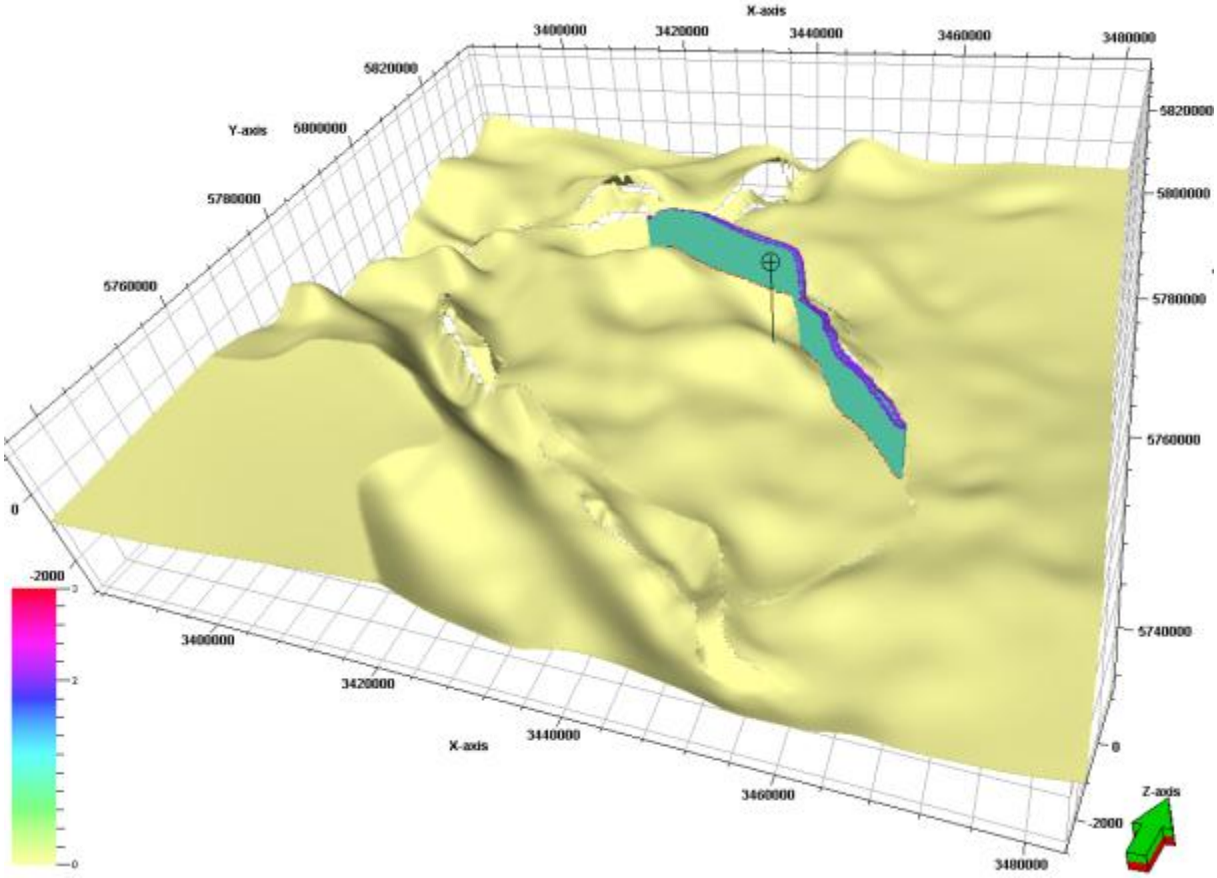

Fig. 8: 3D model with active elements (Detfurth formation and closest fault of the first fault system) as well as the position of the injection well, vertical exaggeration factor is 5).

Geological faults

The model comprises four fault systems, which enclose the CO_2 selected injection site (cf. Fig. 9). One fault system is oriented NW-SE and situated about 5 km east of the southwest dipping anticline. Another fault zone extends west to the anticline and has the same orientation, but is dipping northeast. A third SW-NE orientated fault zone passes north of the anticline and is dipping southeast. South of the anticline is the fourth fault zone cutting the NEGB. All fault systems are mostly constituted of normal faults, except of the first mentioned fault zone, which features reverse faults in some parts (Röhmann et al., 2013).

A total of nine faults are considered in the study area. For the investigations, all faults are expected as vertically impermeable, except the closest fault of the fault system addressed above. This fault (length 120 km) is assumed to be located in the sphere of influence of the pressure elevation due to CO_2 injection in selected storage site. Permeable (400 mD, equals to about $4e^{-13}$ m^2) elements were set next to the fault to investigate potential upward brine migration through the fault zone.

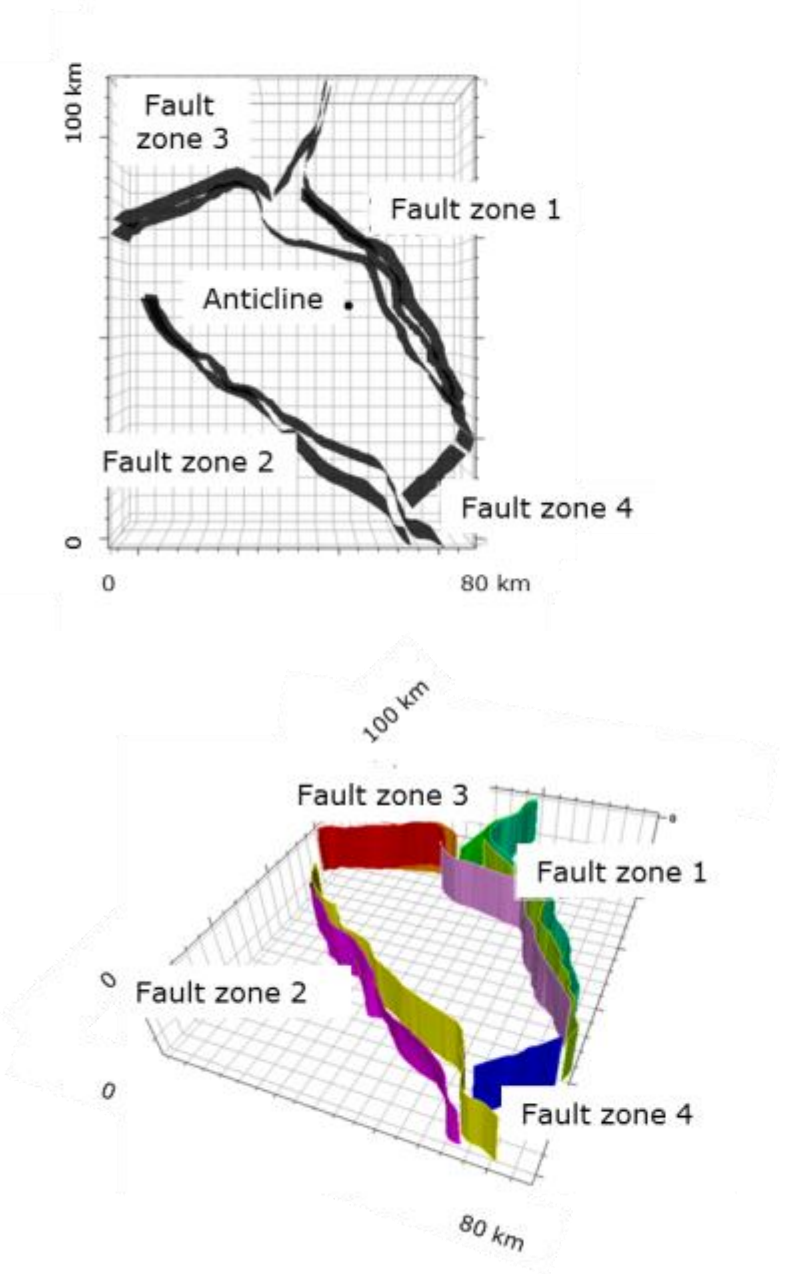

Fig. 9: Faults that build up the four fault systems enclosing the hypothetical CO_2 storage anticline (Röhmann, et al. 2013).

Model gridding

In order to implement the 3D geological model into the multi-phase flow simulator, it is necessary to discretize the geological model in respect to the general grid convergence criteria of the simulator. For this reason, the model was initially gridded using the Petrel software package. To realize the workflow, the geometry of the structural framework was transferred to the gridding process including all geological horizons, additionally defining the grid increment (Röhmann et al., 2013). Hereby, a lateral discretisation of 250m x 25 m with about 4.6 m (Detfurth formation) and about 28 m (fault elements) in vertical direction was assigned creating a 3D grid. This resulted in a total of 8.8 million elements (nx = 400, ny = 400, nz = 55), whereby 832,600 elements were determined as being active. The Detfurth formation contains 800,000 elements (nx = 400, ny = 400, nz = 5), while the fault is composed of 32,600 elements.

Parameterization of salinity, temperature and pressure was carried out to implement a representable 3D model of the study area as discussed by Tillner et al. (2013). The distributions of these parameters are plotted in Fig. 10 and Table 5. Model boundaries are assumed to be closed by implementation of the Neumann "no-flow" condition at the boundary elements, whereas the top elements of the fault were multiplied with a pore volume factor of 1010 in order to represent an overlying aquifer below the base of the Rupelian clay (Dirichlet boundary condition).

Table 5:. Initial model parameterization.

	Reference value at 1,000 m depth	Gradient
Salinity	0.25 (kg/kg)	$2.5e^{-4}$ (kg/kg-m)
Temperature	45 (°C)	$3e^{-2}$ (°C/m)
Pressure	1.0135e7 (Pa)	$1e^{4}$ (Pa/m)

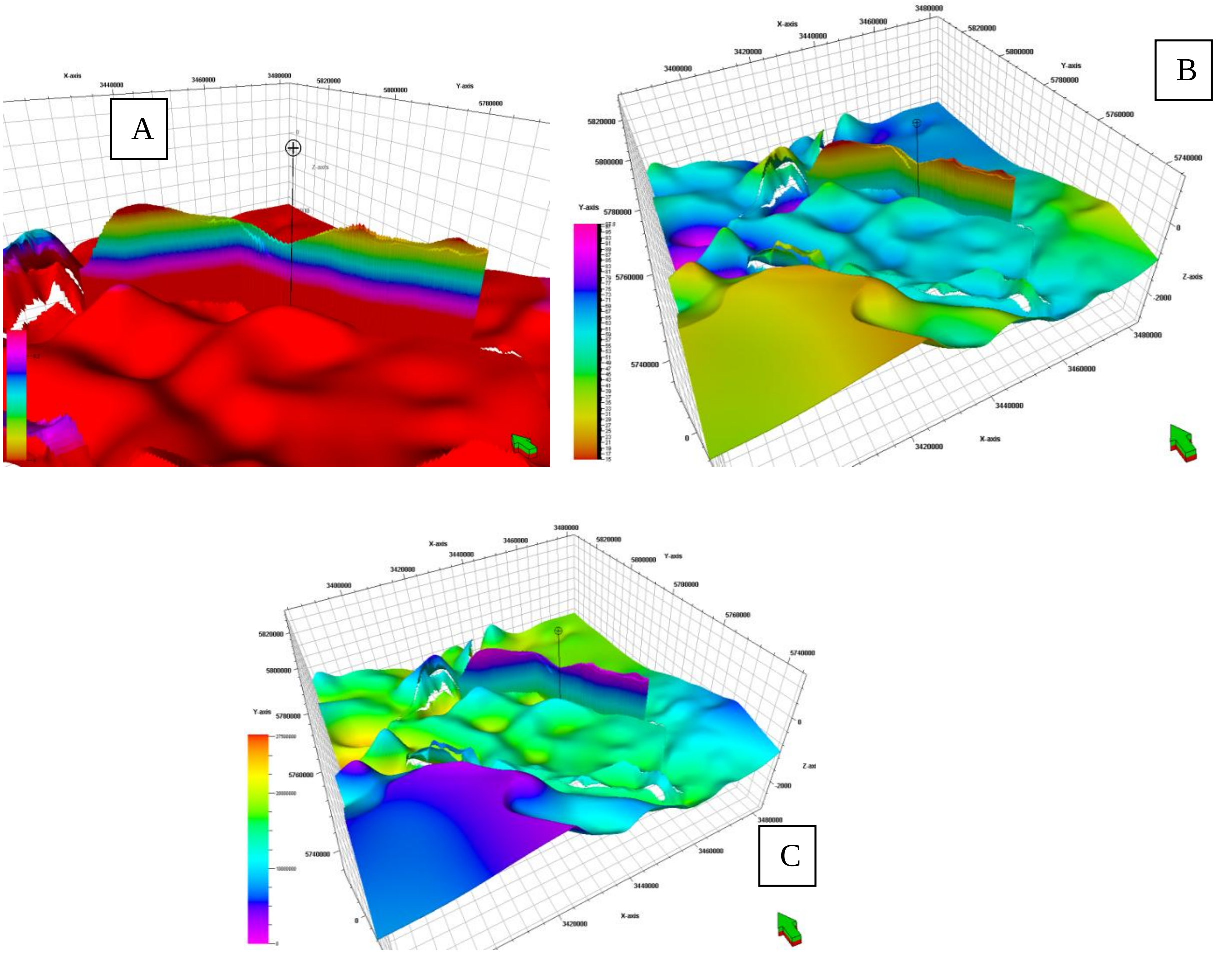

Fig. 10: Initial settings for the 3D model. A: Salinity, B: Temperature, C: Pressure (vertical exaggeration factor is 10).

4 Summary and outlook

At the FU Berlin, based on literature research, (hydro)geological profiles and borehole logs, a simplified conceptual hydrogeological model of the Cenozoic was created, representing a typical geological situation in the North Eastern German Sedimentary Basin (NEGB). The spatial data of the different hydraulic units are implemented in a numerical model, using Modflow (PMWin 5.3) as software package.

Increased pressure gradients due to CO_2 injection and related volume transfer derived as output data from the deep structural model of the GFZ will be used as input data for the Cenozoic model in order to assess a potential upconing of saltwater into shallow freshwater aquifers.

The GFZ implemented a structural geological model of the target formation for underground utilisation – the Detfurth Formation – in the NEGB. The model developed has an areal extent of 100 km x 100 km and incorporates four different fault systems with nine faults in total enclosing the area of interest. Thereby, an anticline developed during salt-tectonic processes was envisaged as potential location to store greenhouse gases underground. The resulting geological model was gridded and parameterised according to available literature data to prepare it for subsequent dynamic flow simulations.

The next steps comprise the implementation of a numerical multi-phase flow model to account for CO_2 injection into the selected anticline for assessment of brine displacement via the closest fault of fault system 1. For this purpose, the model is first equilibrated with regard to the local regional pressure and salinity gradients. Subsequently, the deep reservoir and fault model (GFZ) is going to be coupled to the FUB shallow aquifer model for quantification of saline water intrusion into freshwater aquifers. We envisage using brine mass flow via the fault as a coupling parameter between these two models to ensure maintaining mass and energy balances during the coupling process. A validation of the model coupling will be carried out using the total system mass balances of both numerical models.

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