Arbeitsbericht NAB 13-25

Hydrogeological model Nördlich Lägern

July 2014

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Nationale Genossenschaft
für die Lagerung
radioaktiver Abfälle

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Zusammenfassung

Der vorliegende Bericht dokumentiert Simulationen zu den lokalen Grundwasserzirkulationsverhältnissen im potenziellen Standortgebiet Nördlich Lägern mittels eines 3D hydrogeologischen Modells. Das hier beschriebene Modell umfasst eine Grundfläche von 258 km² um das Gebiet Nördlich Lägern von der Geländeoberfläche bis zu einer Tiefe von ca. 1160 m. Das Modell umfasst 19 hydrogeologische Einheiten vom Quartär bis zu den Gesteinen der Anhydritgruppe. Störungen von regionaler Bedeutung (Teile der Mandach-Überschiebung, Siglistorf Antiklinale und Baden-Irchel-Herdern Lineament) sind ebenfalls im Modell abgebildet. Die Geometrie ist aus einem regionalen geologischen Modell entnommen, das in Gmünder et al. (2013a) dokumentiert ist. Die für das lokale Modell erforderlichen lateralen Randbedingungen werden aus einem regionalen, die gesamte Nordwestschweiz umfassenden, hydrogeologischen 3-D Modell abgeleitet (siehe Gmünder et al. 2013b).

Die lokalen hydrogeologischen Verhältnisse im Standortgebiet werden massgeblich von den hydraulischen Eigenschaften der Störungen geprägt. Um deren Einfluss auf die Grundwasserzirkulation systematisch zu analysieren, wurde eine Sensitivitätsstudie mit 4 verschiedenen Basisfällen und umfangreichen Parametervarianten durchgeführt. In den 4 Basisfällen wurden die regionalen Störungen als geringmächtige vertikale Strukturen mit komplementären hydraulischen Eigenschaften (permeable fault – along flow/cross flow, sealing fault, throw only) implementiert, welche die sedimentären Schichtpakete fragmentieren. Zusätzlich wurde im Rahmen von weiteren Parametervarianten die Bedeutung einzelner hydrogeologischer Einheiten als potenziell wasserführende Systeme untersucht.

Zusammenfassend kann festgehalten werden, dass es durch die tonreichen Gesteine des Dogger und oberen Lias zur Ausbildung eines oberen und unteren Grundwasserstockwerks kommt. Eine Grundwasserzirkulation zwischen den beiden Stockwerken kann praktisch nur über die Störungen ausserhalb des Standortgebiets erfolgen, sofern diese permeabel sind.

Das obere Grundwasserstockwerk beinhaltet den Malm Aquifer, die lokal wasserführenden Schichten des Hauptrogenstein/Spatkalk (soweit vorhanden), und als potenziell wasserführendes System das Sissach-Member ('Brauner Dogger', Einheit BD5). Es zeigt sich, dass der Grundwasserfluss im oberen Grundwasserstockwerk stark durch die Topographie und die hydrogeologischen Eigenschaften der Störungen beeinflusst wird und es zumeist zur Ausbildung (sub-) hydrostatischer Drücke kommt. Die Hauptinfiltrationsgebiete liegen im Süden entlang des südlichen Teils der Lägern, während im Norden die Infiltrationszonen entlang der Flüsse und/oder entlang der Aufschlüsse der jeweiligen Aquifere liegen. Die Exfiltrationsgebiete liegen alle innerhalb, bzw. nur knapp ausserhalb des Modelliergebiets.

Das untere Grundwasserstockwerk beinhaltet die hydrogeologischen Einheiten Arietenkalk (als potenziell wasserführendes System nur in den Sensitivitätsfällen implementiert), Keuper Aquifer sowie den Muschelkalk Aquifer. Im Allgemeinen zeigen die Simulationen artesische Drücke in den Einheiten des unteren Grundwasserstockwerks. Allerdings kommt es zu einem Druckausgleich des unteren mit dem oberen Grundwasserstockwerk, wenn die Störungen als (vertikal) durchlässige Störungen betrachtet werden. Die Fliessrichtungen im unteren Grundwasserstockwerk sind nicht, bzw. nur noch sehr bedingt von der Topographie abhängig, hier dominieren die hydrologischen Eigenschaften der Störungen und die regionalen Infiltrationsgebiete den Grundwasserfluss.

Ein Vergleich der errechneten Grundwasserpotenziale mit den (wenigen) vorhandenen gemessenen Potenzialen zeigt, dass aufgrund der Simulationen keiner der Basisfälle ausgeschlossen bzw. als weniger wahrscheinlich bewertet werden kann.

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1 Introduction

1.1 Project Background

The Sectoral Plan Deep Geological Repositories/SGT (SFOE 2008) is the Swiss road map to establish repositories for radioactive waste. SGT/Stage 1 with focus on the selection of geologically suitable regions (Nagra 2008) led to the proposal of the six geological siting regions for the L/ILW repository (Südranden, Zürich Nordost, Nördlich Lägern, Jura Ost, Jura-Südfuss, Wellenberg) and the three geological siting regions for the HLW repository (Zürich Nordost, Nördlich Lägern, Jura Ost). Four different host rock formations are assessed as part of the L/ILW program (Opalinus Clay, 'Brown Dogger', Effingen Member, Helvetic Marls). The Opalinus Clay is the proposed host rock formation for the SF/HLW/ILW program.

SGT/Stage 2 requires the selection of at least two siting regions for each repository type (L/ILW and HLW). As a quantitative decision basis for the site selection process, provisional safety analyses studies are to be performed for all relevant repository configurations.

Comprehensive geoscientific data bases have to be prepared for the comparison with respect to, the so-called geodata sets for safety assessment. In this context, conceptual and numerical models of the groundwater flow conditions are elaborated on different scales of interest, ranging from the regional scale to the immediate vicinity of the proposed repository. The proposed numerical analyses of groundwater flow are divided into two work packages:

- WP 1/Regional scale modelling, aimed at evaluating the regional groundwater flow and therewith possible recharge and discharge areas of the regional aquifer systems and at specifying the hydraulic boundary conditions for the local scale models;
- WP 2/Local scale modelling, aimed at evaluating the local groundwater flow conditions in the different siting regions. Including the identification of possible local recharge and discharge areas and path lengths.

For the local scale models (WP2), four hydrogeological local models, based on a three dimensional geological model, were built. Fig. 1-1 shows the location and model extent of the four local model areas defined for the geological sites Jura-Südfuss (local model JS), Jura Ost (local model JO), Nördlich Lägern (local model Nördlich Lägern), Zürich Nordost combined with Südranden (local model ZNO-SR). For the site Wellenberg, a local scale hydrogeological model has previously been established (see e.g. Nagra 1997).

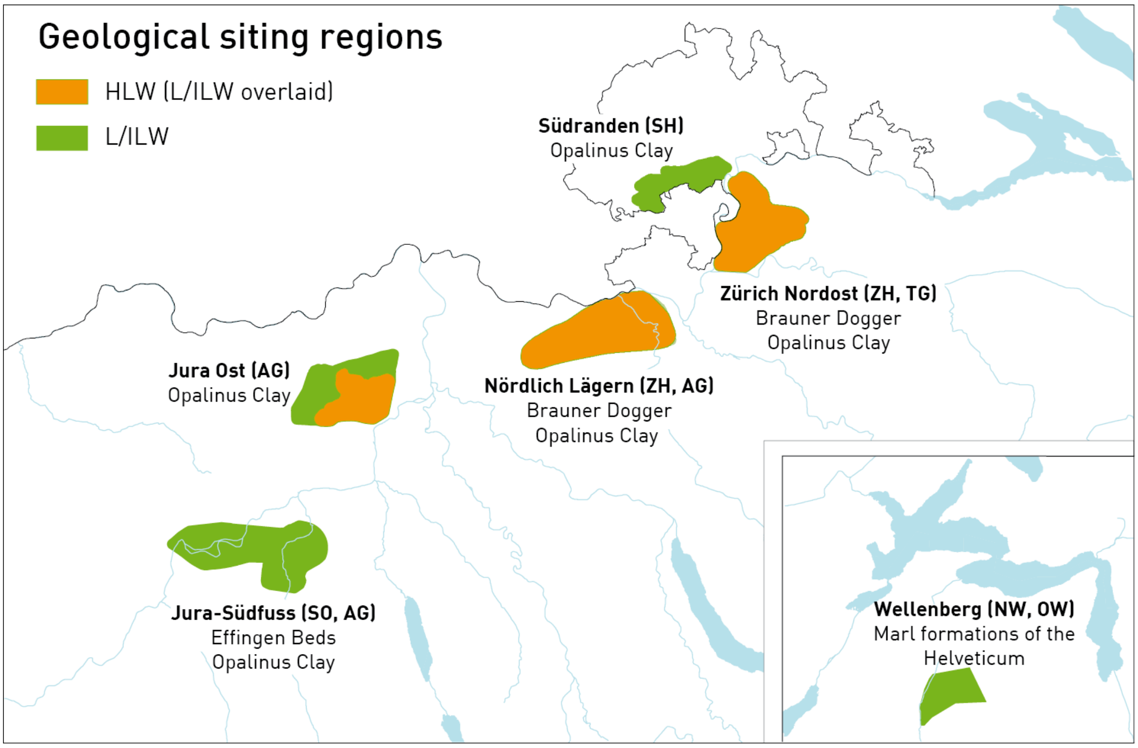


Fig. 1-1: Potential Siting Regions and Host Rocks for Geological Disposal of Low- and Intermediate-Level (L/ILW) and High-Level (HLW) Radioactive Waste in Switzerland.

(After Nagra 2008).

The general objectives of the local scale models (WP 2) are aimed at characterizing the local groundwater flow conditions in the different siting regions at present and for relevant long-term evolution scenarios:

- **Evaluation of host rock performance as a flow barrier** (incl. adjacent confining units): Assessment of conceptual and parametric uncertainties with respect to the role of water conducting features and the confining units
- **Evaluation of local/regional aquifer systems**: Assessment of hydraulic interactions between regional (WP 1) and local aquifer systems and identification of potential discharge paths. Estimation of effective hydraulic properties
- Visualizations of the hydrogeological conditions in support of communication of systems understanding;
- Supply of input for site specific hydraulic gradients and fluxes in the host rock;

The general objectives marked in bold are subdivided into site specific issues addressing the key questions to be solved for the individual siting regions (see next chapter).

1.2 Objectives for the Local Scale Model Nördlich Lägern

For the hydrogeological local scale model Nördlich Lägern described in this report a set of objectives has been defined prior to the modelling. The main interest lies in the main regional aquifers and to some extent also in the local transmissive units and their flow field and transport paths, including possible recharge and discharge areas and in the lower and upper confining units of the host rock formations and their role as flow barriers. For the aforementioned characterizations, the regional faults, namely the Siglistorf Anticline and the Baden-Irchel-Herdern Lineament, may play an important role. Depending on the properties of the faults (e.g. as impermeable barriers or as regions with low or medium transmissivities), they can have large effects on the overall flow field.

The site specific objectives can therefore be divided into related groups:

- The impact of regional faults on the local hydrogeological situation needs to be characterized. Two regional fault zones have been implemented in the local scale model domain that cross cut and offset the proposed host rocks and the confining units. Depending on the hydrogeologic properties of these faults, they influence local gradients as well as flow paths and therewith discharge and recharge areas/locations.
- The hydraulic interaction between local and regional aquifer systems and potential discharge and recharge areas need to be characterized and identified. In addition, vertical gradients within the host rock itself and/or horizontal gradients within the regional and local aquifer systems are important for a full characterization and safety assessment of the siting region. Since the aforementioned interaction may depend to a large degree on the hydraulics of the fault zones, they cannot be assessed independently.

Since the role of the local transmissive units for the local hydrogeology and/or the conductivities of the regional scale faults in the model domain are largely unknown, sensitivity analyses with respect to the transmissivity of the local units and the fault system have been performed.

2 Regional and Local (Hydro)geological Setting

2.1 Regional Setting

2.1.1 Regional Geological Setting

The area of investigation (here the area of the siting region Nördlich Lägern, see Fig. 2-2A) is located within the northern Alpine foreland of Northern Switzerland. The tectonic setting is of interest for hydrogeological simulations because faults that have developed during the different tectonic stages may influence the regional and local hydrogeological setting, depending on their conductivity. In the following, the main fault systems of the different tectonic units (see Fig. 2-1) are shortly described. An extensive review of the tectonic setting is given in e.g. Madritsch et al. (2012) and will not be repeated here.

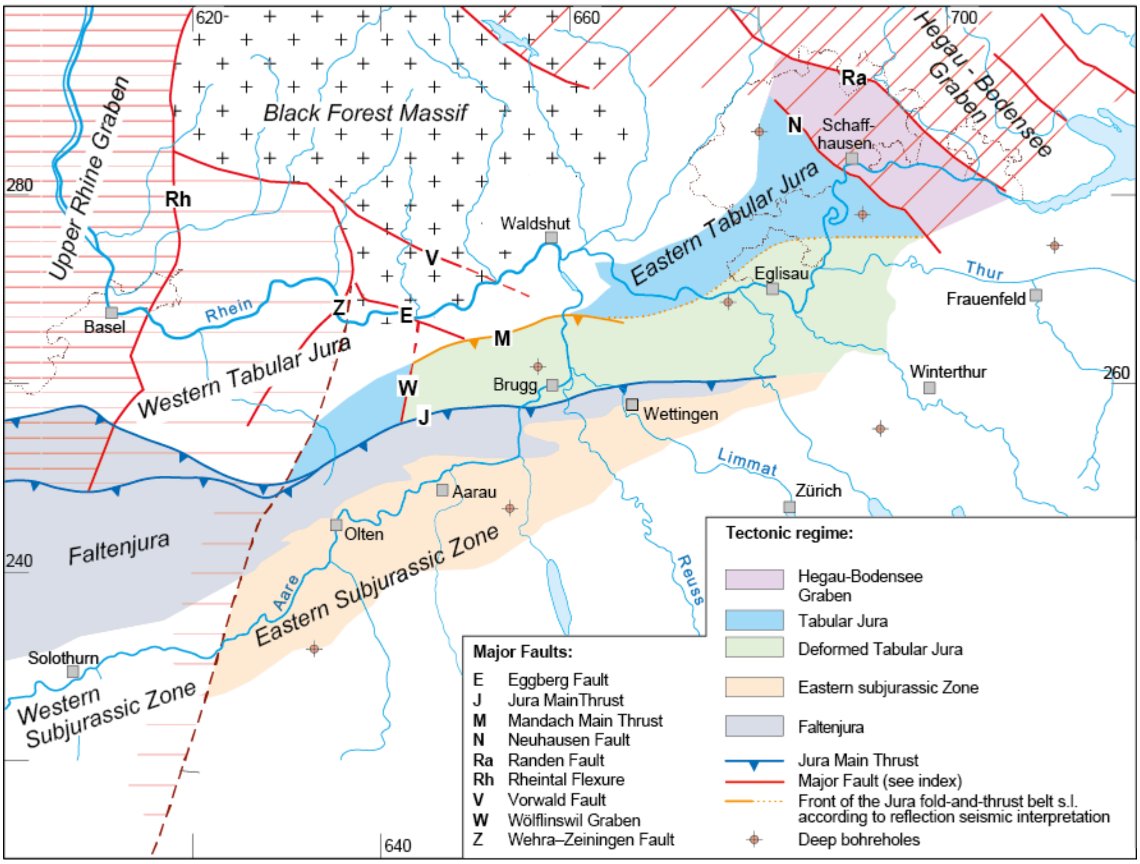


Fig. 2-1: Tectonic Sketch Map of the Wider Study Area Illustrating the Main Tectonic Units of the Region and the Major Fault Structures.

See Madritsch et al. (2012) for a detailed discussion (modified from Madritsch et al. 2012).

The Folded Jura, also called Jura Fold-and-Thrust Belt, is characterized by dominantly ENE-WSW striking folds and thrusts that are occasionally cut by N-S striking faults. The frequency of these structures increases towards the Upper Rhine Graben. Moreover, NW-SE striking faults, such as the Trimbach Olten Fault (see Fig. 2-2), occur. The roughly E-W striking Jura Main Thrust forms the transition to the Deformed Tabular Jura in the north.

The Deformed Tabular Jura is less intensely deformed than the Folded Jura. The lower Aare valley separates this tectonic unit into a western and eastern part. The western is separated from the northward adjacent Tabular Jura by the ENE-WSW striking Mandach Thrust. The eastern part of the Deformed Tabular Jura is characterized by blind thrusts, the transition towards the Tabular Jura is ill-defined.

The Tabular Jura is characterized by horizontally layered to slightly SSE dipping Mesozoic sediments that run out at the south-eastern edge of the Black Forest Massif. Compared to the Deformed Tabular Jura, the Tabular Jura is less deformed and does not feature regional-scale compressive structures with the exception of the Mettau Fault (cf. Laubscher 1986). To the east and west, the Tabular Jura is influenced by the Hegau-Bodensee-Graben and the southern Upper Rhine Graben, respectively.

As this report is mostly concerned with the hydrological situation within the area of Nördlich Lägern, only a very broad description of the regionally important lithostratigraphic units in the area of interest (see Fig. 2-2A) is given below. A lithostratigraphic geological profile is given in Fig. 2-2B. The regional and local stratigraphy has recently been revised (see e.g. Bläsi et al. 2013; Deplazes et al. 2013; Bitterli-Dreher 2012 or Reisdorf et al. 2011 for a recent stratigraphy). In this report, the stratigraphy according to the regional geological model of Gmünder et al. (2013a) is used which is mainly based on the stratigraphy as defined in Nagra (2010).

- Molasse: The Molasse usually is divided into the Upper Freshwater Molasse (OSM), the Upper Marine Molasse (OMM), the Lower Freshwater Molasse (USM) and the Lower Marine Molasse (UMM). The OSM is a succession of fine sandstones and silt to clay rich rocks as well as marl and freshwater carbonates intercalated with coarse sandstones and conglomerates – the so called Jura Nagelfluh. A significant part of the OMM is comprised of homogeneous, marine sandstones which locally can be regarded as aquifers. The USM is a heterogeneous succession of mainly fluviatile clays, marls, siltstones and fine sandstones that frequently show channels of coarser sandstones. The UMM is absent in northern Switzerland.
- Malm: The final phase of Jurassic sedimentation in the region is marked by an increased occurrence of calcerous rocks. The lithostratigraphic group of "Malm" in general is divided into Felsenkalke/Massenkalke, Schwarzbach Formation, Villigen Formation and Wildegg Formation. The upper units are comprised of layered, homogenous limestones (Felsenkalke) and more massive limestones (Massenkalke). The Schwarzbach Formation consists of partly fossile-rich, calcareous-rich marls. The Villigen Member consists of mainly limestones with intercalations of clay- and calcareous-rich marls. The Wildegg Formation includes the Effingen Member and the Birmenstorf Member. The Effingen Member is characterized by layered successions of calcareous-rich marls and mostly clay-rich limestones (Deplazes et al. 2013). The often fossile-rich Birmenstorf Member is comprised of limestones and calcareous-rich marls.
- Dogger: The Dogger sediments in the area of interest are comprised of a thick succession of clay-rich rocks with local intercalations of siltstones, marls, sandstones, iron oolites and limestones. At the base of the Dogger, the Opalinus Clay is a regionally homogeneous clay. Above the Opalinus Clay, the Passwang Formation comprises of a number of unconformity-bounded coarsening-upwards successions. The coarsening-upward successions start typically with siliciclastic mudstones grading into micritic limestones. In the west the Passwang Formation incorporates thicker limestone-successions than in the east. On a regional scale shown in Fig. 2-2 two different types of facies were deposited above the Passwang Formation: the Hauptrogenstein Formation and the Klingnau Formation. In the

western part, a broad oolitic belt, the Hauptrogenstein Formation, was deposited on a carbonate platform. In the eastern part, the Hauptrogenstein Formation is replaced by a marl to clay-dominant facies, the so called Klingnau Formation that was deposited in a more distal setting. The Klingnau-Formation is overlain by claystones and iron oolites, which are called "Upper Dogger".

- Lias: The Staffelegg Formation (the stratigraphic unit comprising all Lias sediments) is characterized by heterogenous clay-rich rocks with some limestones and subordinately sandstones. A detailed description of the Stafelegg Formation of northern Switzerland can be found in Reisdorf (2011). A notable calcareous rich layer is formed by the Arietenkalk (Beggingen Member).
- Keuper: The sediments of the Keuper, the upper lithostratigraphic group of the Trias, can be separated into the Upper Middlekeuper and Gipskeuper. The Upper Middlekeuper consist in general of marls and clays with intercalations of sandstones and dolomites (Traber 2013). Sandstone layers occur mostly in the otherwise clay-rich sediments of the Stubensandstein and Schilfsandstein Formations. These fluviatile sediments show a locally varing composition depending on the depostional setting (flood plain, river channel, delta). Another notable unit is the Gansinger Dolomit, which often consists of marly dolomite. The Gipskeuper mainly consists of clays, dolomitic marls and anhydrite.
- Muschelkalk: The Muschelkalk is the middle of three lithostratigraphic groups within the Trias. In the area of interest, the Muschelkalk is divided into the upper Muschelkalk (top), the Anhydritgruppe (middle) and the Wellengebirge (lowermost unit of the Muschelkalk, not specifically part of the model domain). The upper Muschelkalk is mainly comprised of dolomites (Trigonodus Dolomite) and limestonesmicrites, sometimes separated by thin layers of marl. The limestones are often micrites with partly biodetrital banks. The Anhydritgruppe is a layered succession of evaporites (mainly anhydrite) or anhydrite breccia with thin clay and/or dolomite layers. Within the area of interest, thin salt layers are common. Generally, the Muschelkalk shows a remarkable uniformity with only very little variability, though thicknesses of the different lithostratigraphic units may vary on a regional scale.

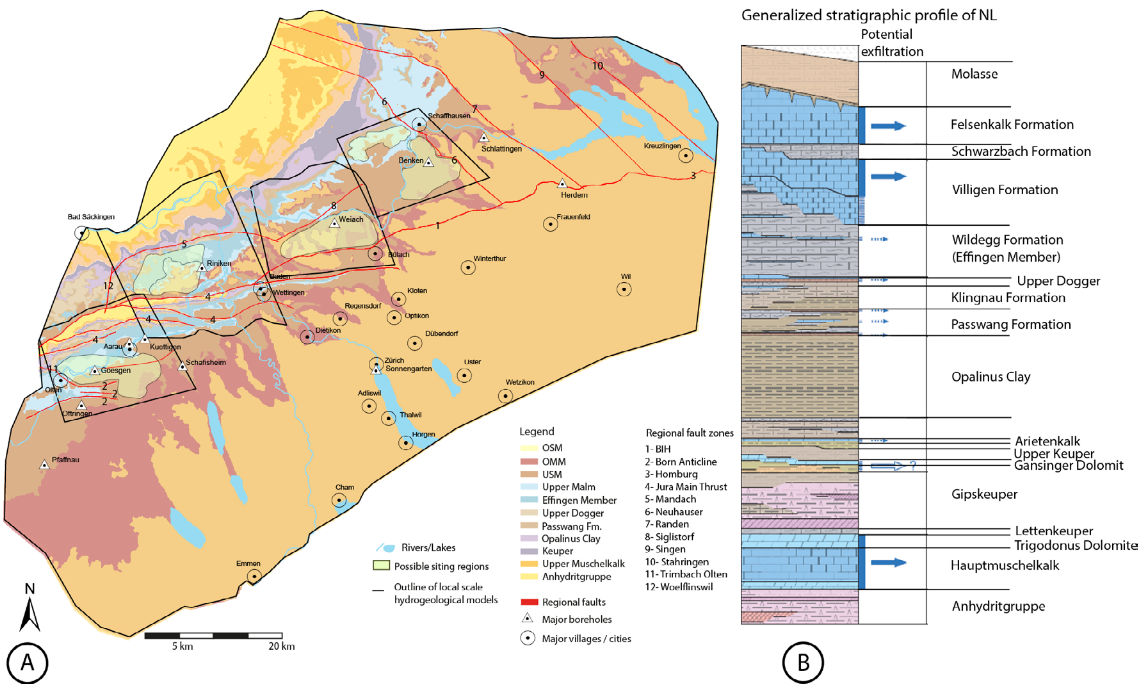


Fig. 2-2: Geological Setting of the Area of Interest.

A) Map of the regionally most important lithostratigraphic units. Note that the Quaternary cover is not shown here. B) Idealized sedimentary sequence of the area in the siting region Nördlich Lägern including possible aquifers and locally transmissive units indicated by blue arrows. Solid blue arrows indicate regionally important aquifers, hollow blue arrows mark possible local aquifers and stippled blue arrows mark potential locally important water conducting units (modified from Nagra 2010).

2.1.2 Regional Hydrogeological Setting

The regional hydrogeological situation is further described in several reports (e.g. Nagra 2002, Nusch et al. 2013) and is currently investigated using a regional hydrogeological model (Gmünder et al. 2013b) based on the sedimentary stack shortly described above and shown in Fig. 2-2B. The hydrology of the area is characterized by the Lake Constance and the rivers Rhine, Aare, Reuss, Limmat, Thur, Töss and Wutach and their respective tributaries. These rivers and the lake constitute the main discharge systems for the aquifers in the area. The area of interest includes parts of the Molasse basin and the most important discharge and recharge locations for the main regional aquifers. These aquifers belong to three main stratigraphic groups, namely the Quaternary deposits, the Tertiary to Permo-Carboniferous bedrock sediments, and the crystalline basement.

- The Quaternary mostly consists of unconsolidated sediments, is present over much of northern Switzerland and contains groundwater. Several activities, including pumping for water supplies, have modified the original groundwater flow systems. The Quaternary aquifer has been included in the model as groundwater from lower aquifers may discharge into, or be recharged from, this aquifer.

- The bedrock Tertiary to Permo-Carboniferous sediments contain several important aquifers. The main aquifer groups are:
  - Tertiary-Malm group with important aquifers in the sandstones of the Upper Marine Molasse and in the limestones of the Malm
  - Upper Muschelkalk (limestones and dolomites)
  - Lower Triassic-Permian group with aquifers consisting of clastic sediments

  These main aquifer groups are generally separated by hydraulic barriers consisting of clays, marls, anhydrites or rock salt. Aquifers within these regional hydraulic barriers include the Hauptrogenstein Formation limestone in the western facies of the Middle Dogger and some limestones, dolomites and sandstones of the Staffelegg Formation and the upper part of the Keuper.
- The first few hundred meters of the crystalline basement may exhibit a high hydraulic conductivity similar to that of some of the sedimentary aquifers. The groundwater of the crystalline presumably circulates along tectonic fracture zones and/or a "weathered" zone at the top. In parts of northern Switzerland, they are connected with the Lower Triassic-Permian aquifer group. In other parts of the region, they are separated from the overlying sedimentary aquifers by a hydraulic barrier of sediments of the Permo-Carboniferous Trough. This group is not included in the present hydrogeological models and will not be discussed here in further detail.

The dominantly horizontal or only slightly dipping bedding of the sediments and the frequent occurrence of hydraulic barriers in the form of clay-rich rocks generally prohibits upflow or downflow of groundwater through the hydrogeological units. Therefore, the deep groundwater of the different aquifer groups exhibit individual characters. However, tectonic faults may represent hydraulic connections between individual aquifers. To estimate the current hydrological situation in the area, hydraulic head and conductivity data for various formations have been gathered in various boreholes throughout the region. These are reported in further detail in Nusch et al. (2013).

2.2 Local Setting

The local scale model Nördlich Lägern (Nördlich Lägern) described here and in subsequent chapters covers an area of 258 km² and mainly lies within the area of the Deformed Tabular Jura (in the south) and Eastern Tabular Jura (in the north) just south of the Black Forest. Several seismic lines, outcrops and one deep borehole (Weiach) within the model domain document its local geological and hydrogeological situation (see Fig. 2-3). The boundaries of the local scale model Nördlich Lägern were chosen so that the model domain includes all relevant outcrops and geologic structures as well as the major borehole relevant for the siting region Nördlich Lägern.

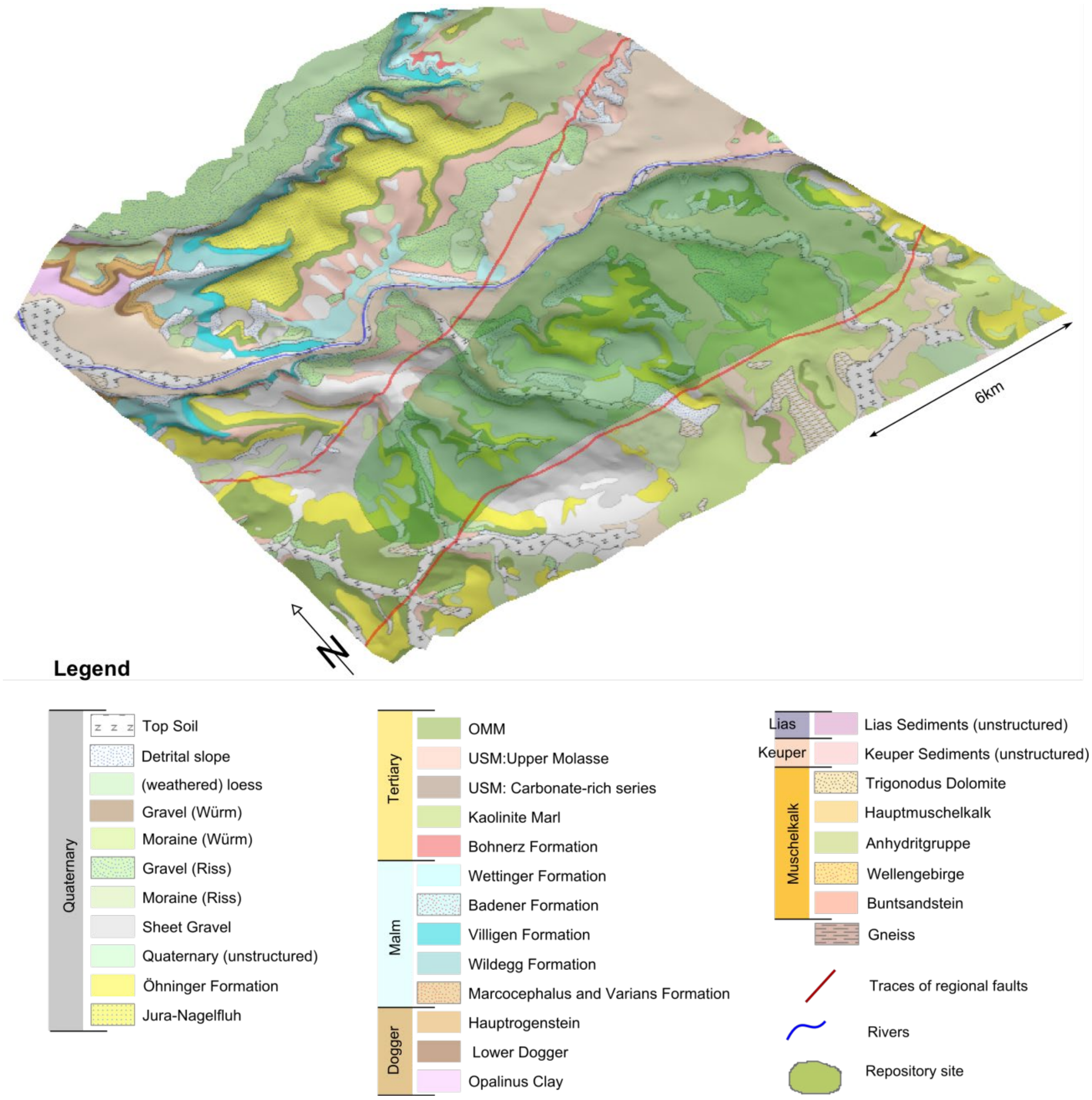


Fig. 2-3: Model Boundaries, Topography and Local Scale Geology of the Local Model Nördlich Lägern (modified from Isler et al. 1984).

2.2.1 Local Scale Geology

The topography of the area is controlled by the south-dipping sedimentary units and the river network (Rhine and its tributaries, see Fig. 2-3). Maximum total relief is around 363 m with the highest point at the Wannenberg (683 m, between the Rhine and Klettgau valley, close to the northern mode boundary) and the lowest point being the Rhine (320 m) where it leaves the model domain to the NW. Disregarding the Quaternary cover, topographic heights are usually covered with Molasse sediments (OSM or OMM) while incision of rivers has eroded valleys in which lower lithostratigraphic units (mostly USM and below) are cut. Within the area, smaller rivers (and valleys incised by them) are oriented roughly N-S with the exception of the Rhine valley. The Rhine, as the locally most important discharge system, runs roughly E-W, has, in most parts, incised into the Molasse sediments and is in direct contact with the Malm aquifer in the central part of the mode domain. Along the northern border of the area, all lithostratigraphic units down to the Opalinus Clay crop out. As mentioned earlier, the model domain includes the transition zone where the Hauptrogenstein Formation, represented by the Spatkalke in the transition zone, in the west is replaced by the Klingnau Formation in the east. Nevertheless, the equivalent hydrogeological unit in the model Nördlich Lägern is called Hauptrogenstein so that terminology is consistent with the regional model though, strictly speaking, it comprises the Spatkalke of the Hauptrogenstein Formation. The local tectonic features include 3 regionally important fault systems that run roughly E-W through the model domain (see Fig. 2-3).

2.2.2 Local Hydrogeological Setting

As mentioned earlier, the main discharge system of the area is the Rhine and potential discharge and recharge locations of interest are the outcrops of the deeper aquifers along the northern border of the model and beneath the Rhine. Depending on the hydrogeological properties of the fault systems, they divide the area into three blocks. However, the fault systems must be viewed in a regional context so that, even if they are impermeable, groundwater may still flow from north to south outside of the model domain. Locally however, the fault zones may effectively prohibit groundwater flow between these blocks and decouple discharge/recharge zones of the lower aquifers in the south from the rest of the area, only allowing an E-W (or vice versa) directed flow.

Measurements of hydraulic heads and/or conductivities in the model domain are sparse. Only one deep borehole, the borehole Weiach, lies within the model domain of the local model Nördlich Lägern (see Fig. 2-3). The tests to characterize the local hydrogeology performed in this borehole include measurements of hydraulic heads at various depths. However, as can be seen in Fig. 2-4, most of the tests have been performed aiming at the permo-carboniferous rocks and the crystalline basement and therefore are of limited use for the modelling described in this report.

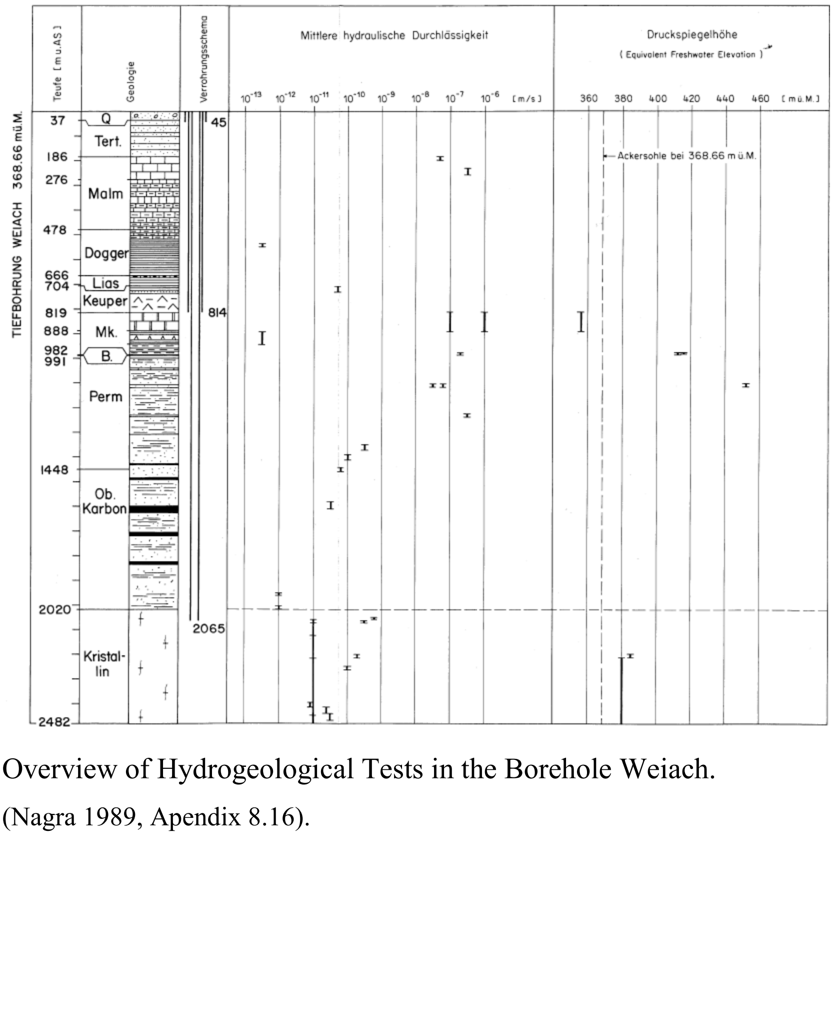


Fig. 2-4: Overview of Hydrogeological Tests in the Borehole Weiach.

(Nagra 1989, Apendix 8.16).

Some of the original test shown in Fig. 2-4 have been reanalysed and transmissivities have been calculated (see Fig. 2-5).

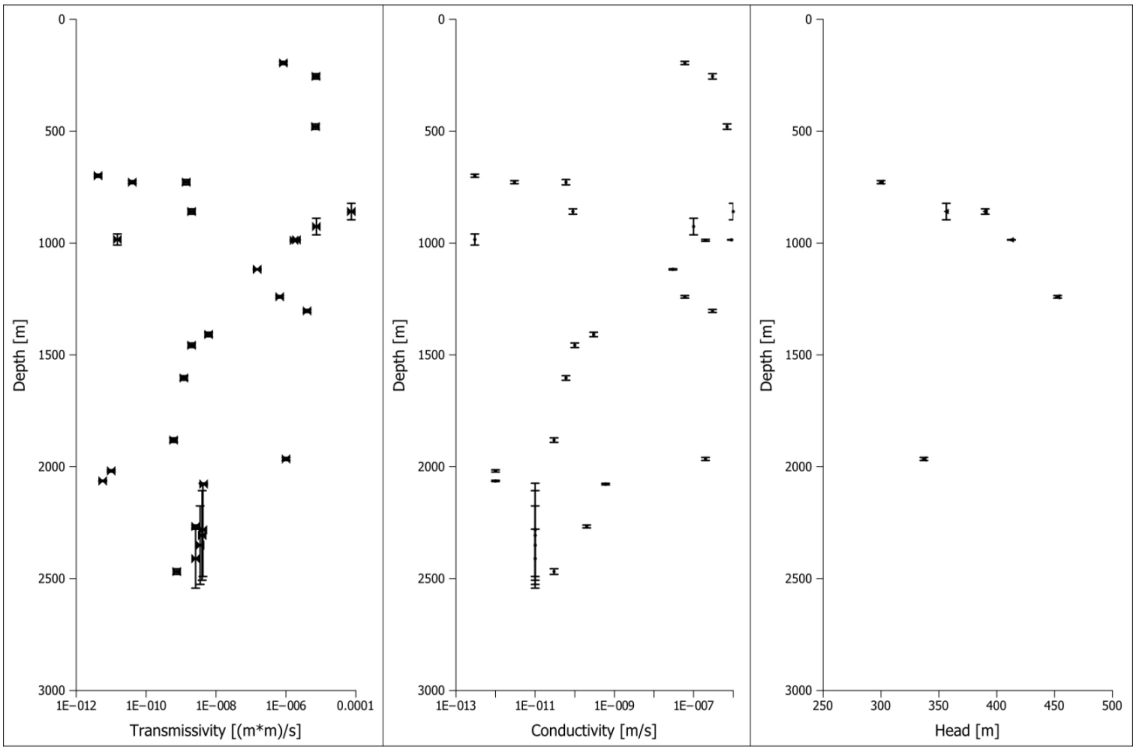


Fig. 2-5: Reanalysed Hydraulic Tests and Calculated Transmissivities from the Borehole Weiach (modified from Butler et al. 1989).

Vertical bars reflect the interval length over which measurements took place.

Other boreholes within the model domain are used for either drinking water (including mineral water) or for the production of geothermal energy. Most of these boreholes use the highly transmissive aquifers of the Molasse and Malm. All available and reliable head measurements (including some of the Muschelkalk and also some from boreholes just outside the model domain) have been used as they may indicate how well the model describes the hydrogeology in the area.

3 Model Implementation

3.1 Overview

3.1.1 Regional Scale Hydrogeological Model

Based on the information shortly summarized in Chapter 2, a geological model (GeoMod 2012, see Gmünder et al. 2013a) using all available sources such as seismic lines, boreholes, outcrops etc. has been compiled (see Fig. 3-1). Based on this geological model, a regional hydrogeological model was established. The layers included in the regional hydrogeological model are (from top to bottom): the Quaternary, OSM, OMM, USM, the Malm aquifer, the Effingen Member, the "upper" Dogger, the Hauptrogenstein aquifer, the "lower" Dogger, the Opalinus Clay, the clay-rich Lias and Keuper, the Keuper aquifer, the Gipskeuper, the Muschelkalk aquifer and the basal Anhydritgruppe. The Keuper aquifer was not part of the geological model but was constructed using simple thickness rules in the hydrogeological model. The regional fault system implemented in the geological model had to be simplified in the regional hydrogeological model to limit the complexity of the mesh generation process and simulations. For this purpose, the faults were rotated vertically with the centre of rotation being at the top surface.

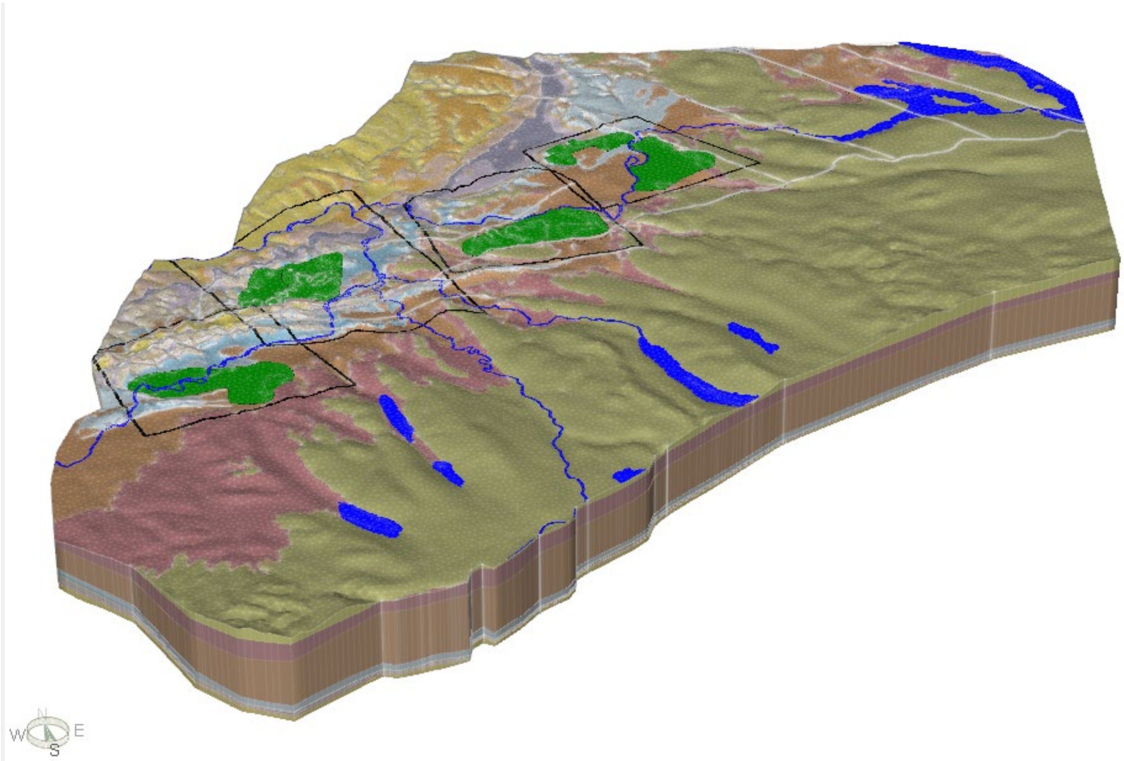


Fig. 3-1: 3D Hydrogeological Model including all relevant Horizons and Layers.

Black lines delineate the area of the local scale models (from west to east: JS, JO, NL and ZNO/SR), green poylgons resemble the siting regions, white lines are trace lines of regional faults implemented in the model. Only the major rivers and lakes (blue) are shown. 2x vertical exaggeration, Quaternary cover not shown.

Local Scale Hydrogeological Model

In order to construct the local-scale hydrogeological models, the different local scale geological models were cut out of the regional geological model (see Fig. 3-1) and the same hydrogeological units as in the regional model were constructed. In addition, based on information from the borehole in Weiach, several hydrogeological units were added to ensure an adequate representation of the local groundwater flow conditions.

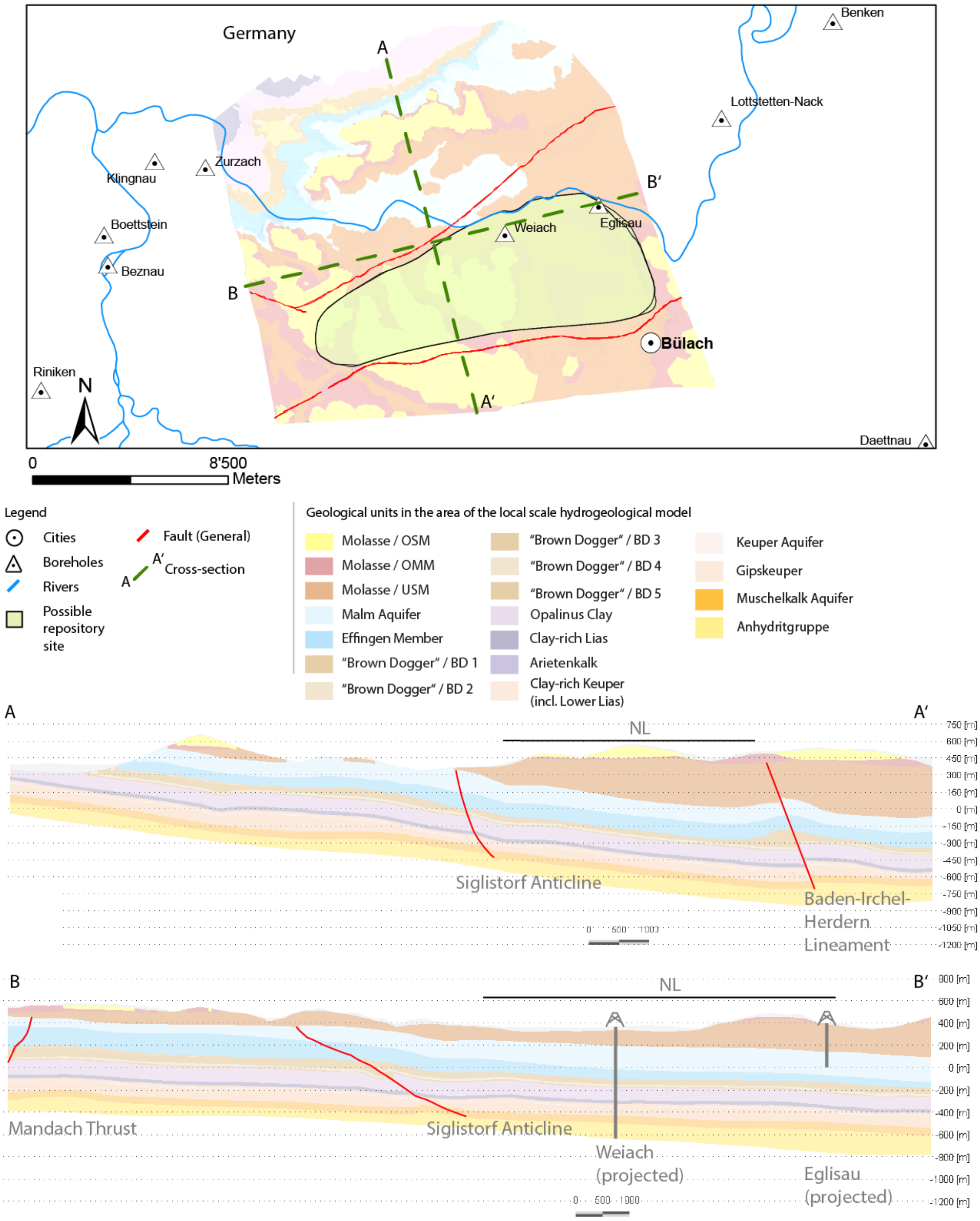


Fig. 3-2: Local Model Nördlich Lägern without Quaternary Cover.

2x vertical exaggeration, black bars in cross section depict location of the siting region.

Thus, potential local aquifer systems/transmissive units were implemented within the Dogger, Lias and Keuper units. These units have all been included using thickness rules (usually the minimum and maximum thickness of the layer and the distance to the next layer already existing in the geological model). The added hydrogeological units in the local model Nördlich Lägern were the Keuper aquifer (constant thickness of 10 m), the Arietenkalk (constant thickness of 3 m) and the Sissach Member (BD5), a thin layer of constant thickness (10 m) just above the Opalinus Clay (see Table 3-1). The resulting model is shown in Fig. 3-2.

Since the spatial resolution of the local model is much higher compared to the regional model, it was possible to represent the faults in greater detail with the actual dip as specified in the geological model (though the geometry of the faults have already been simplified there, see Gmünder et al. 2013a). However, some (additional) simplifications of the Mandach Thrust and the Siglistorf Anticline, have been performed (see Fig. 3-3). In the geological model, these two fault systems are separated from each other (see Fig. 3-3a). In the volumetric hydrogeological model, the faults have been connected (keeping the possibility of treating them separately in terms of parameter assignment if needed, see Fig. 3-3b). This is reasonable since it is quite likely that these two major faults actually are connected even if this cannot be shown from surface outcrops. The Siglistorf Anticline extends from the base of the USM to the bottom of the Muschelkalk. The Baden-Irchel-Herdern Lineament (BIH) extends from the base of the OMM to the base of the model (base Anhydritgruppe). These simplifications respect the general hydrogeological importance of the fault system and decreased the complexity of the model.

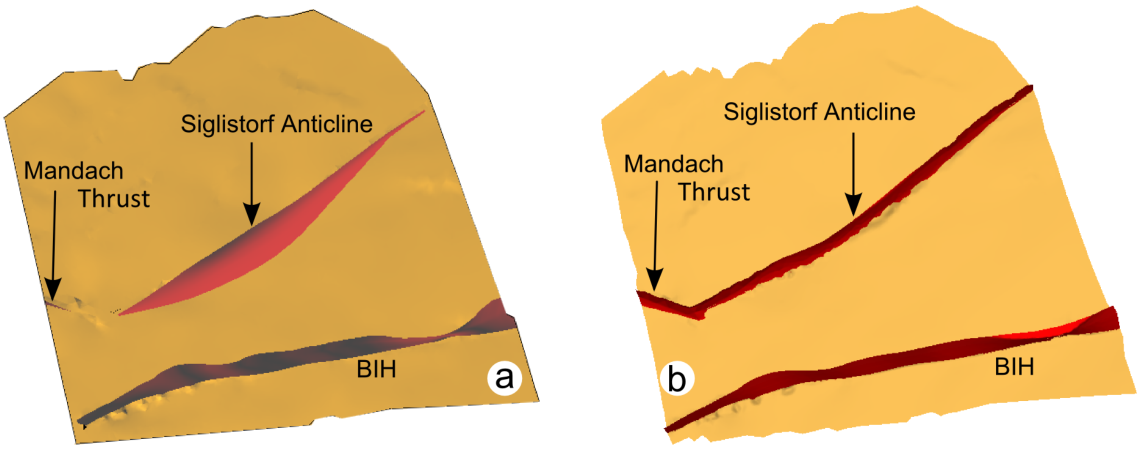


Fig. 3-3: Simplification/Changes of Faults within the Model Area.

a) Original shape of regional faults in the 3D geological model. b) changes of the regional faults in the volumetric model used for hydrogeological simulations. The Mandach Thrust and the Siglistorf Anticline have been connected, the general appearance of the Siglistorf Anticline has been adjusted. Note that almost no changes had to be done for the Baden-Irchel-Herdern Lineament (BIH).

In the subsequent chapters, a detailed overview of the model setup in terms of mesh generation (Chapter 3.2), property assignment (Chapter 3.3) and boundary conditions (Chapter 3.4) is given.

3.1.2 Used Software

For numerical implementations and simulation runs of the hydrogeological local models, the latest FEFLOW® Version 6.1 (DHI-WASY 2012) is used. FEFLOW is a professional software package for modelling fluid flow and transport of dissolved constituents and/or heat transport processes in the subsurface.

FEFLOW is a completely integrated system from simulation engine to graphical user interface, containing pre- and post-processing functionality and an efficient simulation engine, featuring user-friendly modern graphical interface, providing easy access to the extensive modelling options. FEFLOW also includes a public programming interface for user code.

FEFLOW is used by leading consulting firms, research institutes, universities and government organizations all over the world. Its scope of application ranges from simple local-scale to complex large-scale simulations.

3.2 Model Geometry

3.2.1 General Aspects

Based on the finite element method, FEFLOW allows using arbitrary triangulated grids representing the top boundary of the model (e.g. top ground surface). In the vertical direction, however, the mesh must follow the triangulation of the surface grid. This means that all the element layers representing the hydrogeological units must be present throughout the whole model domain. If, for instance, a geological unit reaches the topography (i.e. crops out) then the corresponding numerical layer has to continue to the model boundary even where this formation is not present. A minimal thickness and the conductivity of the underlying geological unit are then allocated to that (dummy) part of the numerical layer.

Other restrictions to shape and size of the elements are mainly dictated by the required numerical accuracy and the available computer capacity. In order to avoid an influence of the element shape on the model results, the form factor of the elements, i.e. the ratio between maximum and minimum dimension of an element should not be too large. Therefore, a ratio lower than 10 was maintained for the model at hand. With respect to the size of the elements, a compromise should be found between numerical accuracy and computational speed. Considering present-day computer capacities it is possible to calculate models with up to 25 million elements in a steady state FEFLOW run. In general, the model setup consists of 3 main stages

- Construction of the horizontal mesh
- 3D gridding according the geological structure
- Allocation of hydrogeological properties and boundary conditions

The different steps are described in more detail in the subsequent chapters.

3.2.2 Horizontal Discretization

The choice of the model area to be discretized was described in Chapter 2 In a first step, a so-called super-element mesh of the top horizon was constructed. This super-mesh honours (1) outcrop lines of hydrogeological units, (2) lateral boundaries of discontinuous layers, and (3) intersections of horizons with fault zones which all could be derived from the geological model. In a similar way, the traces/contours of significant rivers and lakes were incorporated. In the end this super-element mesh consisted of 57 super-polygons illustrated in Fig. 3-4 (top).

Based on the super-element mesh a finite-element mesh was automatically triangulated using the Advancing Front Mesh Generator in FEFLOW. Near outcrops of the geological formations considered or near the faults zones, where high head gradients are expected, mesh refinements are introduced. The final surface mesh consists of 39761 nodes and 79132 elements. The original mesh, resulting from the triangulation of the so called super-polygons (see Fig. 3-4 top), was not sufficient to properly map e.g. outcrops of hydrogeological units on the surface. Therefore, these areas had to be refined (see Fig. 3-4, bottom). In addition, to be able to reproduce the topography, additional areas had to be refined. The resulting finite mesh therefore shows triangle lengths that vary between 80 and 300 m in areas with a smooth topography and no outcrops (of hydrogeological units or faults) and 10 and 25 m in refined regions showing a high topography contrast and/or outcrops of hydrogeological units or faults. The resulting surface mesh is shown in Fig. 3-4 (bottom).

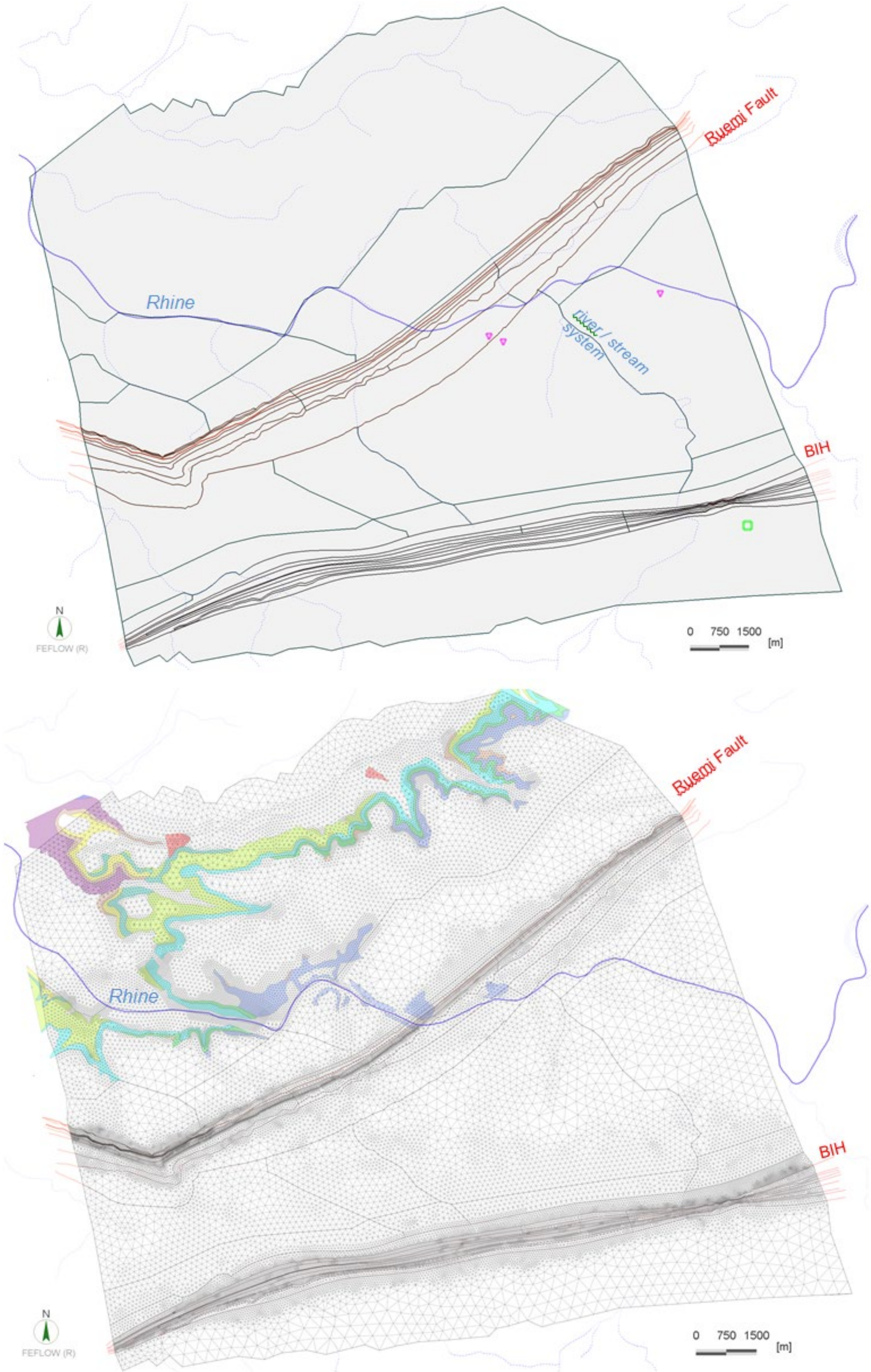


Fig. 3-4: Horizontal Model Discretisation. Top: Black lines represent borders of the super-polygons or trace lines where faults cut the respective surface. Bottom: Finite-Element Mesh generated from meshing the super-polygons. The lengths of the triangles varies between 80 and 300 m in general and 10 and 25 m in zones of mesh refinement, e.g. near outcrops (coloured polygons) or along traces of faults (red lines indicate locations where the faults intersect the geological formations considered).

3.2.3 Vertical Discretization

General Aspects

3D-gridding follows a layered approach (i.e. in-depth repetition of the surface mesh) according to the horizon data as defined by the geological model (see Chapter 3.1). The geological data provided contains the elevations (horizons) of 13 basic geological formations (from top to bottom: Quaternary, OSM, OMM, USM, Villigen, Effingen Member, Oberer Dogger, Hauptrogenstein, Passwang, Opalinus Clay, Lias+Keuper, Oberer Muschelkalk, Anhydritgruppe). As argued above, additional subdivision of the Passwang (3 layers) and the Keuper-Lias (5) formation was introduced due to hydrogeological evidence (see also next chapter).

Furthermore, the model includes 2 regional faults, the Siglistorf Anticline (including a small part of the Mandach Thrust) and the Baden-Irchel-Herdern Lineament (BIH) which separate the model domain into 3 blocks. As each mesh layer has to be present in all the 3 blocks (see also Chapter 3.2.4) the resulting FEFLOW model consists of 55 model layers listed in Table 3-1.

In order to import the geological layer-based data from the geological model into the FEFLOW-model, the plug-in "GOCAD2Elevation" was used which automatically interpolates the elevation (and/or thickness) of FEFLOW nodes along corresponding horizons of the geological model.

Workflow

The general workflow of vertical discretization can be summarized as follows:

- Setup of a primary geometry of the 3D-model according to the layering of the geological model
- Definition of reference data "Geological Units" for the geol. formations and "Regional faults" for the regional faults considered
- Adaption or correction of model layers for smoother representation of the geological formations along the regional faults or outcrops, combined with necessary mesh refinements
- Vertical refinement of the regional geological formations Passwang and Keuper-Lias due to local hydrogeological evidence
- Adaption or correction of the divided layers for smoother representation of the geological formations along the regional faults or outcrops, combined with a second mesh refining.

Tab. 3-1: Implemented Layers of the 3D Model Nördlich Lägern.

Geological Era	Model Layer (geol. units) of regional model	Hydrogeol. units considered in the hydrogeol. regional model	Model Layer (geol. units) of local model Nördlich Lägern	Geological units in Nördlich Lägern (according to geol. regional model)	Hydrogeol. units in Nördlich Lägern	Thicknesses of hydrogeol. units (at location of the borehole Weiach)
Quaternary	1	Quaternary	1	Quaternary	Quaternary	28 m
Tertiary (Molasse)	2	OSM	2	OSM	OSM	-
	3	OMM	3	OMM	OMM	-
	4	USM	4	USM	USM	159 m
Malm (Upper Jurassic)	5	Malm aquifer	5	Villigen Formation	Malm aquifer	210 m
	6	Effingen Member	6	Effingen Member	Effingen Member	90 m
Dogger (Middle Jurassic)	7	"Upper Dogger"	7	"Upper Dogger"	BD1	10 m
	8	"Hauptrogenstein"	8	"Hauptrogenstein"*	BD2	-
	9	"Passwang - Klingnau", not subdivided	9	Klingnau Fm.	BD3	36 m
			10	Passwang Fm.	BD4	20 m
			11	Sissach Member	BD5	10 m
	10	Opalinus Clay	12	Opalinus Clay	Opalinus Clay	112 m
Lias (Lower Jurassic)	11	Lias, not subdivided	13	Upper Lias	Clay-rich Lias	30 m
			14	Arietenkalk	Arietenkalk	3 m
			15	Lias + Upper Mittelkeuper	Clay-rich Keuper (incl. lower Lias)	21 m
Keuper (Triassic)	12	Keuper aquifer	16	Gansinger Dolomit/Schilfsandstein	Keuper aquifer	10 m
	13	Gipskeuper	17	Gipskeuper	Gipskeuper	69 m
Muschelkalk (Triassic)	14	Muschelkalk aquifer	18	Muschelkalk aquifer	Muschelkalk aquifer	69 m
	15	Anhydritgruppe	19	Anhydritgruppe	Anhydritgruppe	130 m

* The hydrogeological unit Hauptrogenstein comprises the Spatkalke of the Hauptrogenstein Fromation. See Chapter 2.2.1 for discussion.

Additional Hydrogeological Classification

As argued in Chapter 3.1 and listed in Table 3-1, the complex unit Lias-Keuper was divided into five sub layers, i.e. from top to bottom: "clay-rich Lias" (30 m thickness), Arietenkalk (3 m), "clay-rich Keuper incl. lower Lias" (21 m), Keuper aquifer (10 m) and "Gipskeuper". Elevations were computed according the layer thicknesses with Bottom Opalinus Clay as the reference. In a similar way, the Passwang Formation was divided into three sub layers, BD3, BD4 (20 m) and BD5 (10 m) referenced to Top Opalinus Clay.

3.2.4 Regional Faults

In the geological dataset generated and provided by SIMULTEC AG for setting up the local models, the relevant regional faults are defined as inclined faults. With respect to the local model at hand, two regional faults, the Baden-Irchel-Herdern Lineament (BIH) and the Siglistorf Anticline, had to be implemented (e.g. Fig. 3-4). The handling of inclined faults in the FEFLOW model is illustrated in Fig. 3-5. Each inclined fault and the adjacent fault surfaces are represented by the inclined parts of three additional one meter thick model layers corresponding to the fault locations. These additional fault layers are numbered as follows:

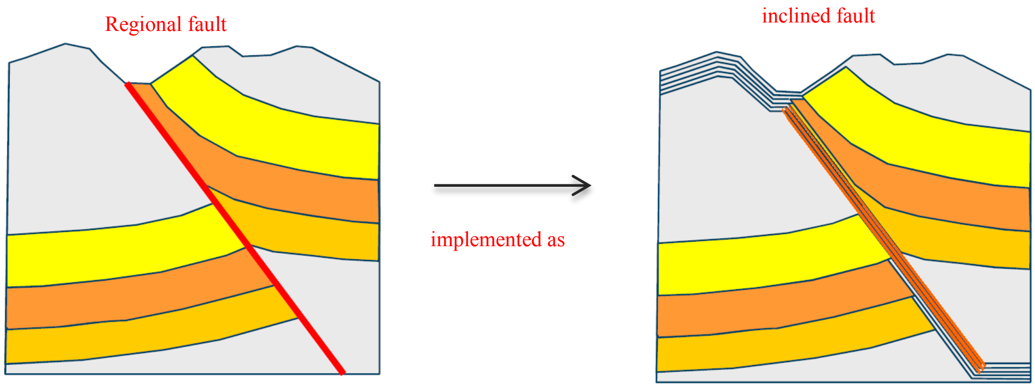


Fig. 3-5: Illustration of Fault Implementation in a FEFLOW-Model.

In order to ensure a correct transition between the fault and the connected geological units, the corresponding intersection lines have to be present in the horizontal surface mesh (see Chapter 3.2.2). The situation is illustrated in Fig. 3-6 and Fig. 3-7. Fig. 3-6 shows parts of polygons of the horizontal super-mesh (black lines). The polygons represent intersection lines (projected onto the surface mesh) between the BIH and the modelled geological horizons. The red line indicates an arbitrary reference line with numbered intersection points. These points refer to the numbered vertical (red) lines in Fig. 3-4 in order to illustrate where the geological horizons connect to the fault and how the layering is handled in this context.

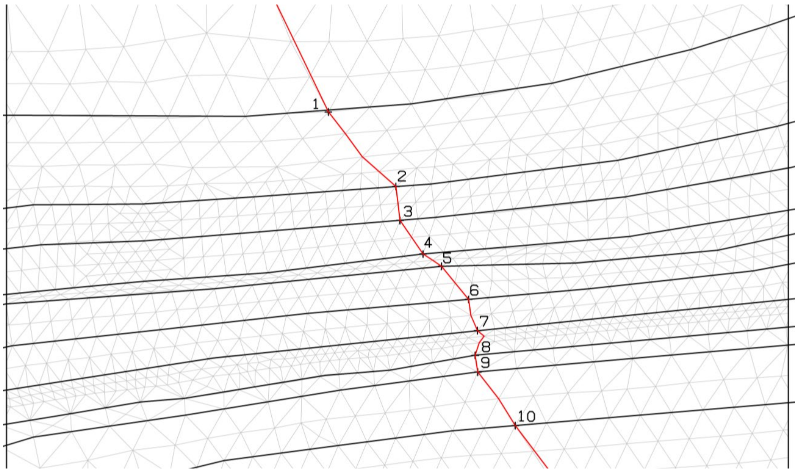


Fig. 3-6: Intersection between BIH and Geological Horizons (Situation/surface Mesh).

Black lines indicate polygons of the super-mesh (i.e. surface projection of intersection lines), red indicates a reference line with numbered intersection points (to be compared with Fig. 3-4).

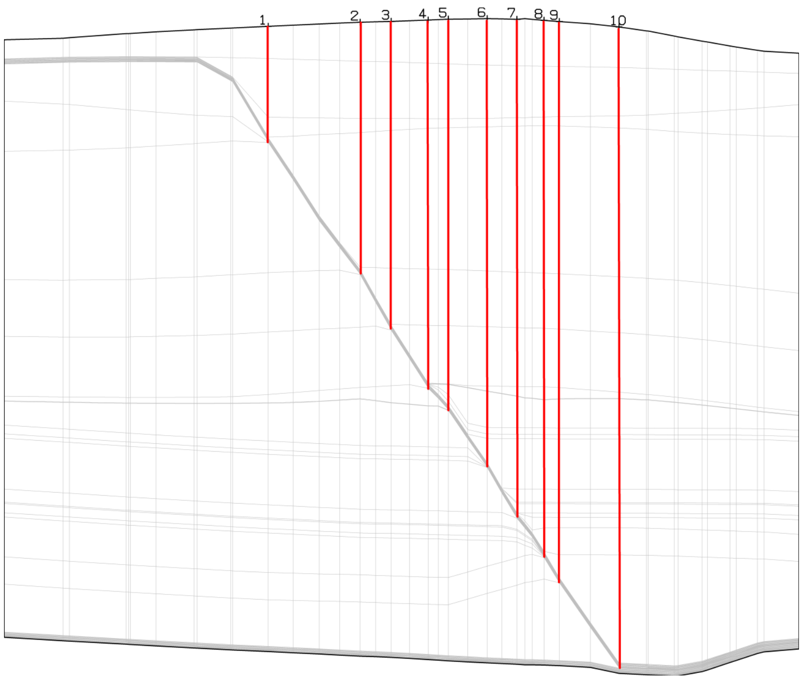


Fig. 3-7: Intersection between BIH-fault and Geological Horizons (Vertical Section through Reference Line with Numbered Intersection Points in Fig. 3-6).

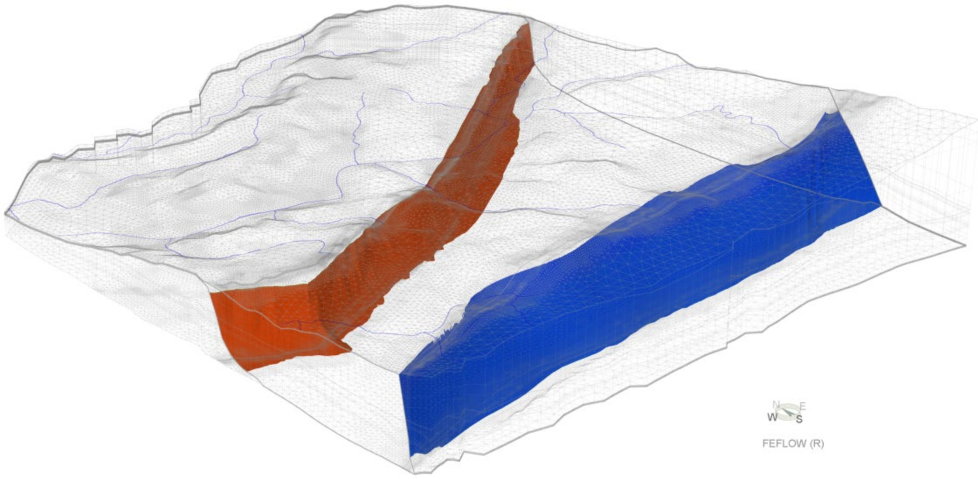


Fig. 3-8: 3D View from SW of the Regional Faults Implemented as Inclined Faults.

2x vertical exaggeration.

3.2.5 Composite Mesh

In spite of all the numerical tools involved to discretize the complex 3D geometry, additional adaptions and corrections are necessary. In particular, the connections of geological layers along faults and outcrops need final (manual) interaction. The resulting 3D FEFLOW-model consists of 4352260 finite elements and 2226616 nodes in total. It contains 55 model layers (56 horizons), representing the 19 geological units listed in Table 3-1 and visualized in Fig. 3-9.

Further 3D-views of the Nördlich Lägern model are presented in Fig. 3-10 to Fig. 3-11. As (partly) shown in Fig. 3-10 the elevation of the model domain varies from 320 to 670 masl on the top and between 28 and -1160 masl at the bottom.

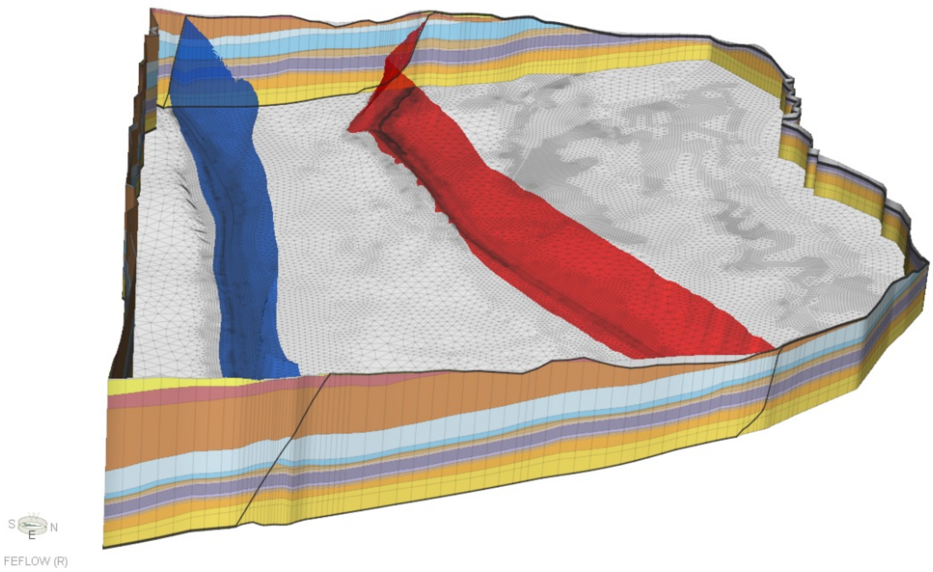


Fig. 3-9: 3D-View of the Nördlich Lägern Model from the E. Lateral Boundaries with Geological Layering, Implemented Faults and Basic 2D-mesh along Bottom of the Domain.

2x vertical exaggeration.

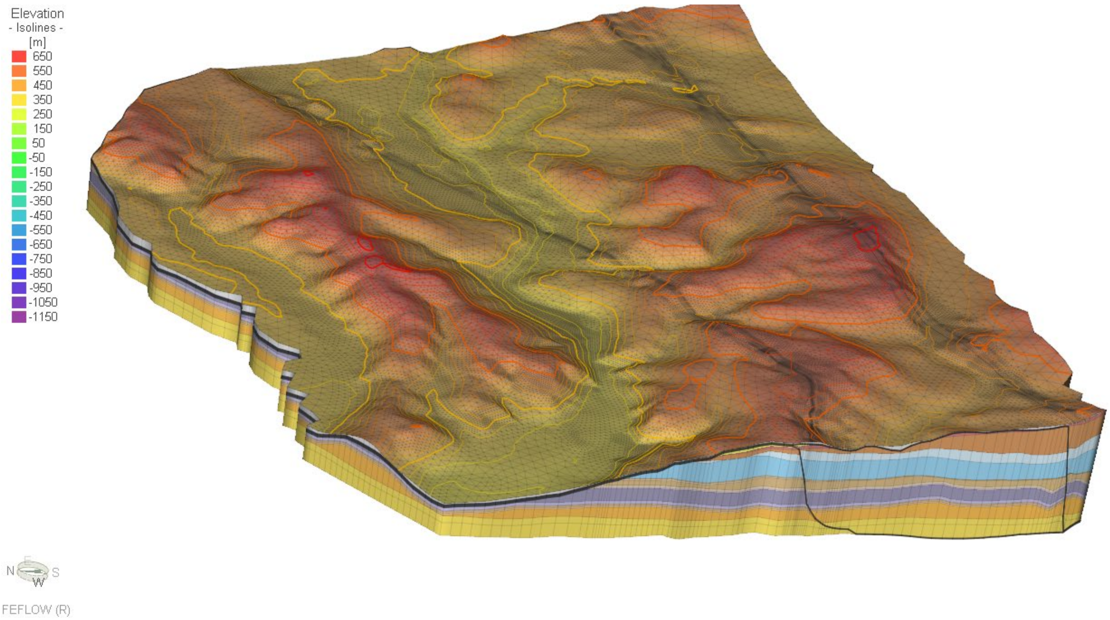


Fig. 3-10: 3D-View of the Nördlich Lägern Model: Lateral Boundaries with Geological Layering, 2D-surface Mesh with Elevations.

2x vertical exaggeration.

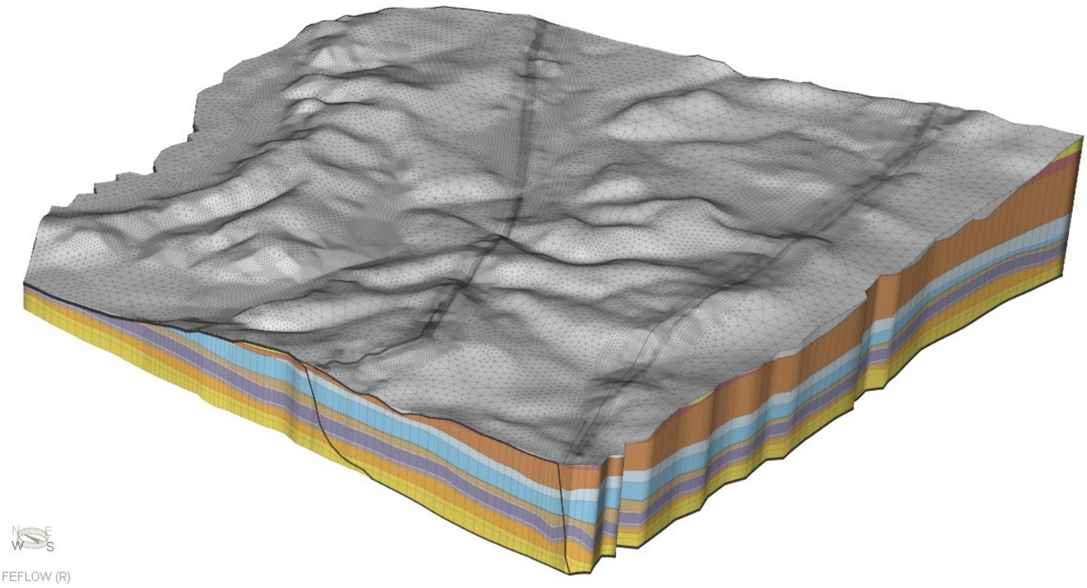


Fig. 3-11: 3D-View of the Nördlich Lägern Model from SW: Lateral Boundaries with Geological Layering, Surface Mesh with Fault Traces.

2x vertical exaggeration.

3.3 Property Assignment

3.3.1 General Aspects

In rock aquifers the groundwater flow takes place in a complex system of pores, fissures, fractures and local and regional scaled fault structures. To model the flow in a scaled model required by the present project, the hydrogeological system has to be simplified. As described earlier, the two relevant regional faults are considered as discrete model elements where different conductivities can be assigned in parallel and/or perpendicular directions. The flow properties of the smaller faults, fractures and fissures enter into a conductivity of a postulated homogeneous equivalent porous media. To consider the layered character of some geological units, they are supposed to have an anisotropic conductivity tensor with a higher conductivity parallel to bedding.

Like commonly applied in the finite element method, FEFLOW uses a cell-based definition of properties such as the hydraulic conductivity. Therefore, K-values have to be assigned to each element of the 3D-mesh.

In order to accommodate the anisotropy of the hydraulic conductivity, the FEFLOW-option "General Anisotropy with computed angles" is applied. This option makes use of the fact that the principal axes of the 3D anisotropy tensor generally correlate with the geological layered structure and, provided that the 3D shape of the layers is known, the spatial rotation of the principal directions can be accomplished by computation. Provided (as assumed in the present case) that the conductivity is orthotropic inasmuch the higher conductivity is parallel to the layering, the lower conductivity is oriented normal to the stratigraphy and the top and bottom faces of the elements fit the stratigraphic layering, the transformation of the principal directions can be derived. Anisotropy is then computed during runtime based on the inclination/slope of the elements. To account for transversal conductivity of the faults, the latter have been represented by regular 3D-elements (see Chapter 3.2) and as such will be treated numerically as common elements with anisotropic features described above.

With respect to handling of layer conductivities in the vicinity of fault intersections, similar issues arise as before during mesh construction. In this context, the hydraulic conductivities of discontinued layers have to be adapted (e.g. based on user-defined minimal thicknesses) and assigned to adjacent geological layers. In this way, a smooth transition of the conductivity along the faults can be obtained (Fig. 3-12).

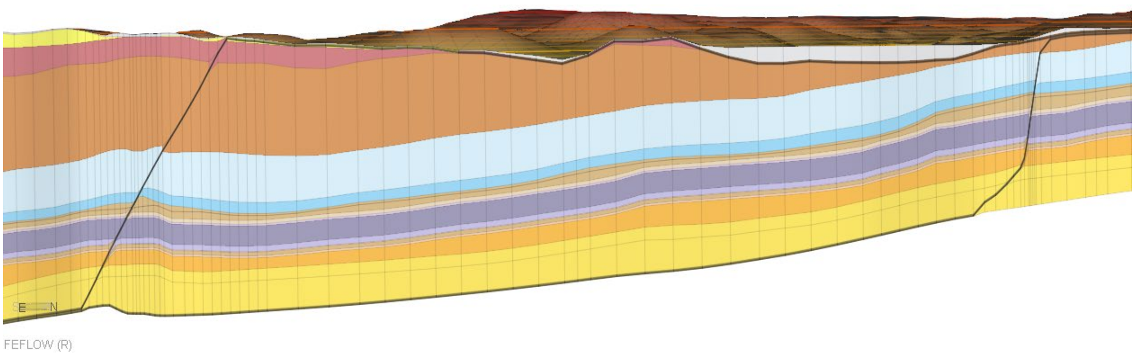


Fig. 3-12: Conductivity Assignment along Faults.

Discontinued layers from geological units are properly adjusted according the hydro-geological layers passed through.

3.3.2 Hydrogeological Units

The Nördlich Lägern model represents one link in the model chain from regional to site scale. Therefore, the regional hydrogeological model (Gmünder et al. 2013b) forms the basis of the conductivities to be assigned. In a first step, the hydrogeological units of the Nördlich Lägern model honour the values of the regional model as listed in Table 3-2 also taking into account regional heterogeneity (zonation) within those formations (see Gmünder et al. 2013b). In some units of the hydrogeological regional model a spatially varying hydraulic conductivity has been assigned to account for different processes influencing the rock permeability (karstification, cementation, fracturing etc.). The assigned values and the arguments for these zonations are detailed in Gmünder et al. (2013b, Chapter 4.5). This spatial variability of the regional model has also been used for the respective units in the local scale model, namely for the Malm aquifer (Fig. 3-13a), the Hauptrogenstein (Fig. 3-13b) and the Muschelkalk (Fig. 3-13c) so that the local scale model is consistent with the regional model (see also Chapter 4.1.1) and boundary conditions necessary for the local scale model can easily be transferred from the regional model.

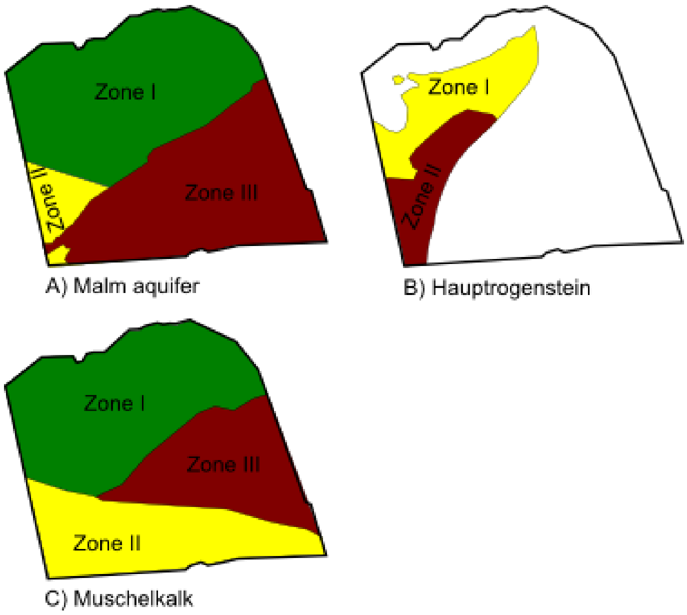


Fig. 3-13: Zones of Different Conductivities Implemented in the Local Model Nördlich Lägern (see Gmünder et al. (2013b) for a detailed discussion).

As described above (Chapter 2.1) additional, locally important, hydrogeological layers have been incorporated into the Passwang and Keuper-Lias units of the Nördlich Lägern model resulting in a higher vertical resolution. The hydraulic conductivity values assigned to these new layers were chosen based on hydrogeological considerations. The conductivities assigned to the regional model have been used to calculate correct conductivities for the newly created layers based on their (average) thicknesses (see Tab. 3-3). Therefore, the overall conductivity in the local model is consistent with the regional scale model.

Tab. 3-2: Hydraulic Conductivities according the Regional Model (Gmünder et al. 2013b).

Note that in case of the Keuper aquifer, the whole local model is located in the same zone.

Layer	Description	Kh [m/s]	Kv [m/s]
1	Top Layer (Quaternary)	variable	variable
2	OSM	2.00E-8	2.00E-11
3	OMM	1.00E-6	1.00E-9
4	USM	Zonation	2.00E-11
5	Malm aquifer	Zonation	Zonation
6	Effingen Member	1.00E-11	1.00E-12
7	'Brown Dogger' / Rest-Dogger 1	1.00E-11	1.00E-12
8	Hauptrogenstein aquifer / Rest-Dogger 2	Zonation	Zonation
9	'Brown Dogger' / Rest-Dogger 3	1.00E-11	1.00E-12
10	Opalinus Clay	1.00E-13	2.00E-14
11	Lias	1.00E-13	2.00E-14
12	Keuper aquifer	Zonation	Zonation
13	Gypsum-Keuper	1.00E-14	1.00E-14
14	Muschelkalk aquifer	Zonation	Zonation
15	Anhydrit Group	1.00E-10	1.00E-10

Tab. 3-3: Hydraulic Conductivities of the Hydrogeologically Refined Units 'Brown Dogger' and Lias.

Geological unit of the regional model	**Local model layer**	**Conductivity [m/s]**	
		Horizontal K_h	**Vertical** K_v
'Brown Dogger' / Rest-Dogger 3	BD3	$5\ 10^{-13}$	$1\ 10^{-13}$
	BD4	$5\ 10^{-12}$	$1\ 10^{-12}$
	BD5	$5\ 10^{-10}$	$5\ 10^{-10}$
Lias	Clay-rich Lias	$1\ 10^{-13}$	$1\ 10^{-13}$
	Arietenkalk	$1\ 10^{-12}$	$1\ 10^{-12}$
	Clay-rich Keuper	$1\ 10^{-12}$	$1\ 10^{-12}$
	Keuper aquifer	$1\ 10^{-9}$	$1\ 10^{-9}$
	Gipskeuper	$1\ 10^{-14}$	$1\ 10^{-14}$

The resulting model layer structure with the considered hydrogeological units (with 2x vertical exaggeration) is given in Fig. 3-14.

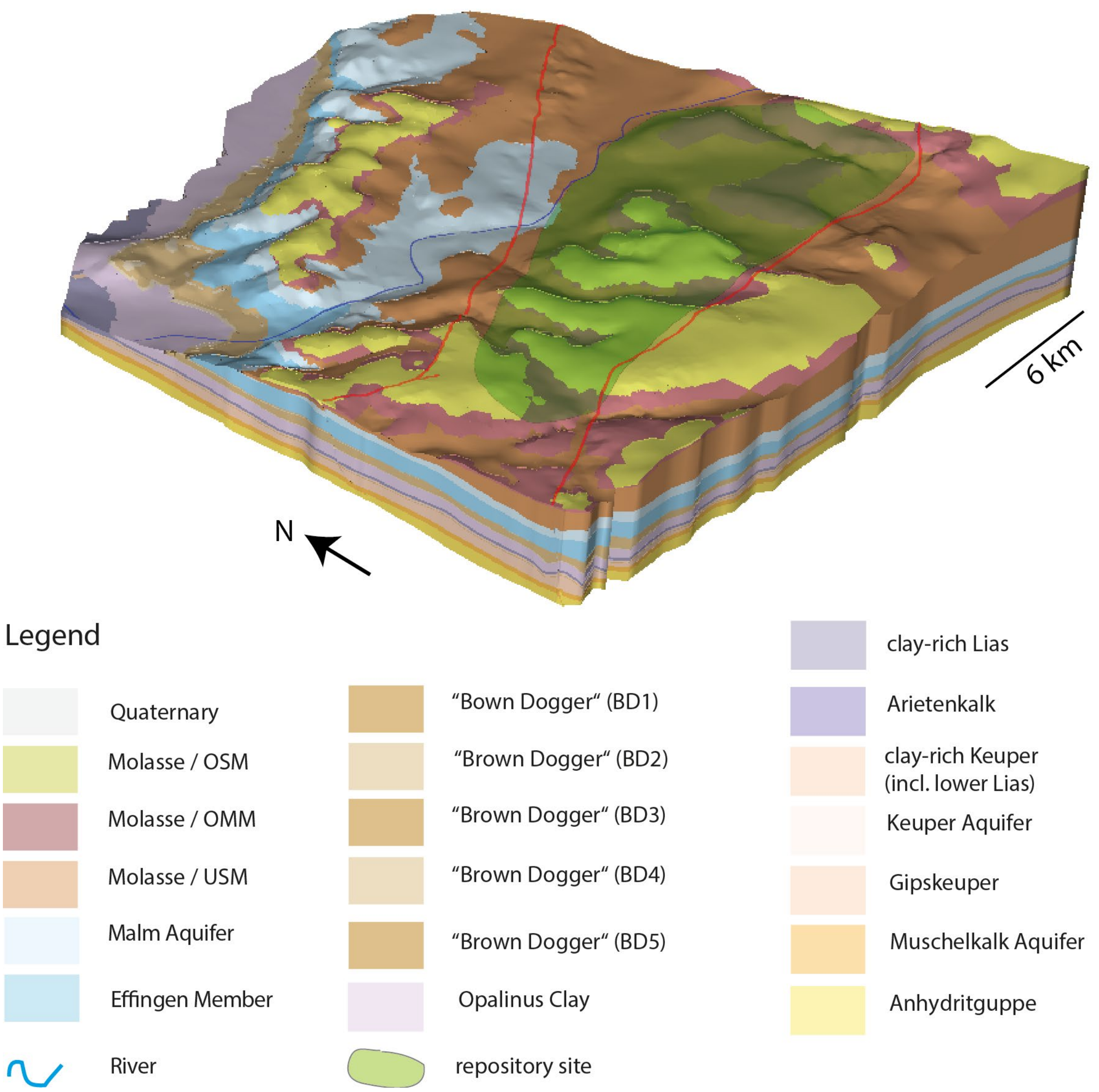


Fig. 3-14: 3D View of the Implemented Hydrogeological Units without Quaternary Cover. 2x vertical exaggeration.

3.3.3 Faults

As stated above, faults are incorporated in the mesh using regular 3D-finite elements (in contrary to frequently used 2D-elements). Therefore, fault elements obtain (anisotropic) properties like other hydrogeological units. This method allows to easily accommodate the inherent uncertainty with respect to the fault behaviour (connecting, sealing, etc.) so that different hypotheses can be investigated by assigning corresponding anisotropy tensors explained in detail in Chapter 3.3.1. The scenarios will be described below in Chap. 4ff.

3.4 Boundary Conditions

Because the local model represents a cut-out of the regional model, the boundary conditions of the local model have to reflect the hydraulic conditions given by corresponding scenarios of the higher-scale model. These include Dirichlet boundaries, i.e. the so-called Fixed/Prescribed-Head Boundary Conditions (FH) along parts of the top and lateral aquifer boundaries as well as spatially distributed recharge (FQ) along the top boundary. The implemented boundary conditions are shortly described in the subsequent chapters.

3.4.1 Top/surface Boundary

FH Boundary Conditions were implemented for the Quaternary aquifer on the top of the model domain along and/or around the rivers or main streams according to Fig. 3-15.

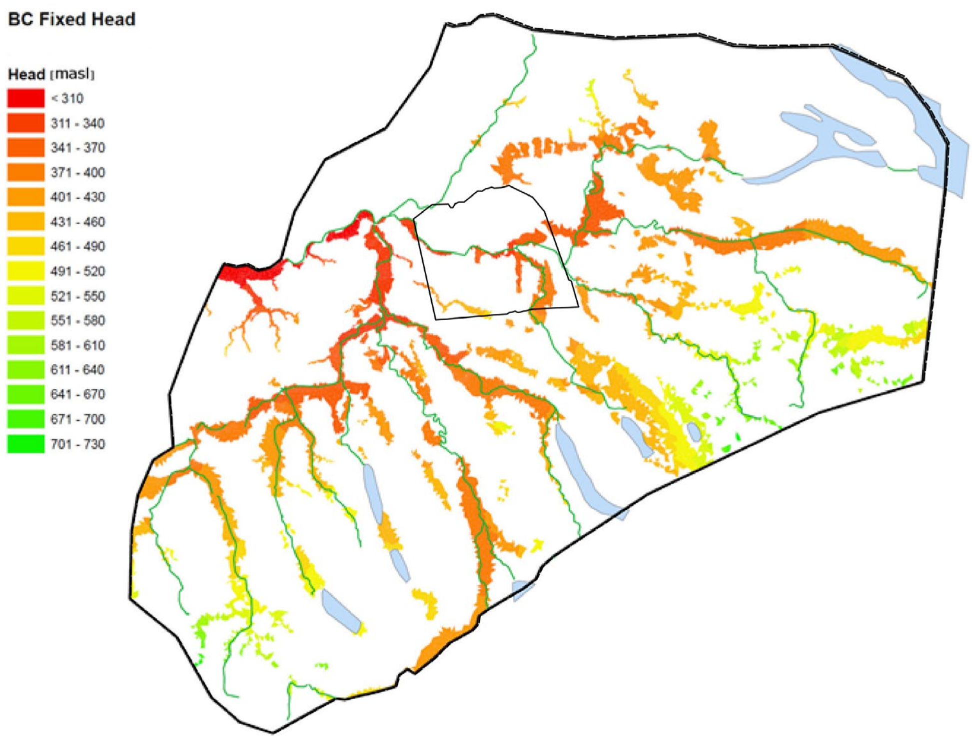


Fig. 3-15: Groundwater Heads Considered as Fixed Head Boundary Conditions at the Top of the Model Domain in the Regional Model (Gmünder et al. 2013b).

Additionally, spatially distributed groundwater recharge is assumed along the top layer of the model. According to the regional model, a constant and spatially homogeneous groundwater recharge rate of 139 [mm/year] has been chosen (see Fig. 3-16). This value was derived from the surface water flow corresponding to the 95th percentile of the annual flow of the main stream/river of the sub-basins (Q347, Sanford 2002).

Along regions where the Quaternary aquifer does not exist or outcrops of other aquifers do not occur, recharge is neglected due to the low conductivity. Furthermore, a seepage BC has been imposed locally as shown in Fig. 3-17, allowing groundwater to discharge in case the groundwater level reaches the topography.

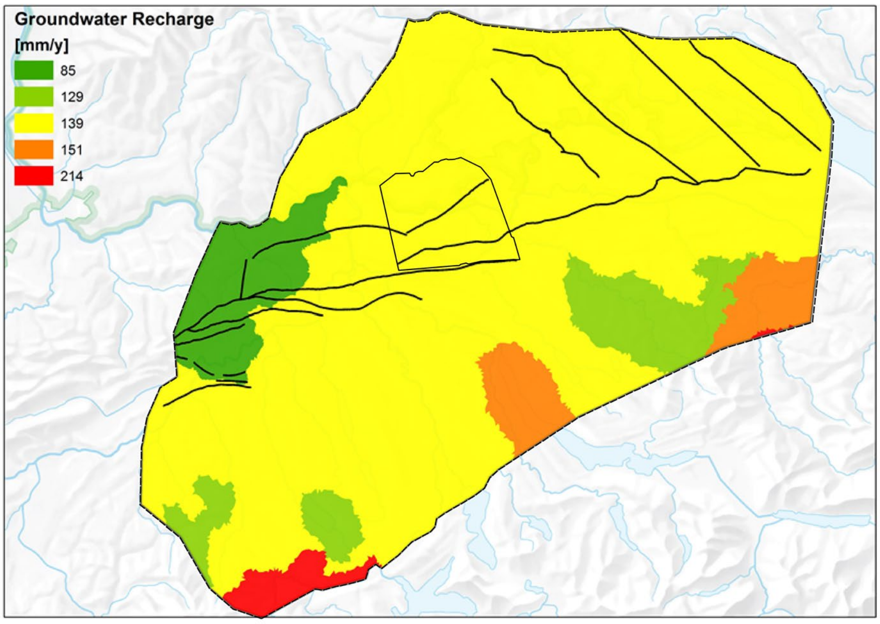


Fig. 3-16: Distribution of the Groundwater Recharge (Precipitation) as Considered in the Regional Model.

(Gmünder et al. 2013b). Zones located in German territory (not covered by the recharge map) obtain the same values as the nearby Swiss regions.

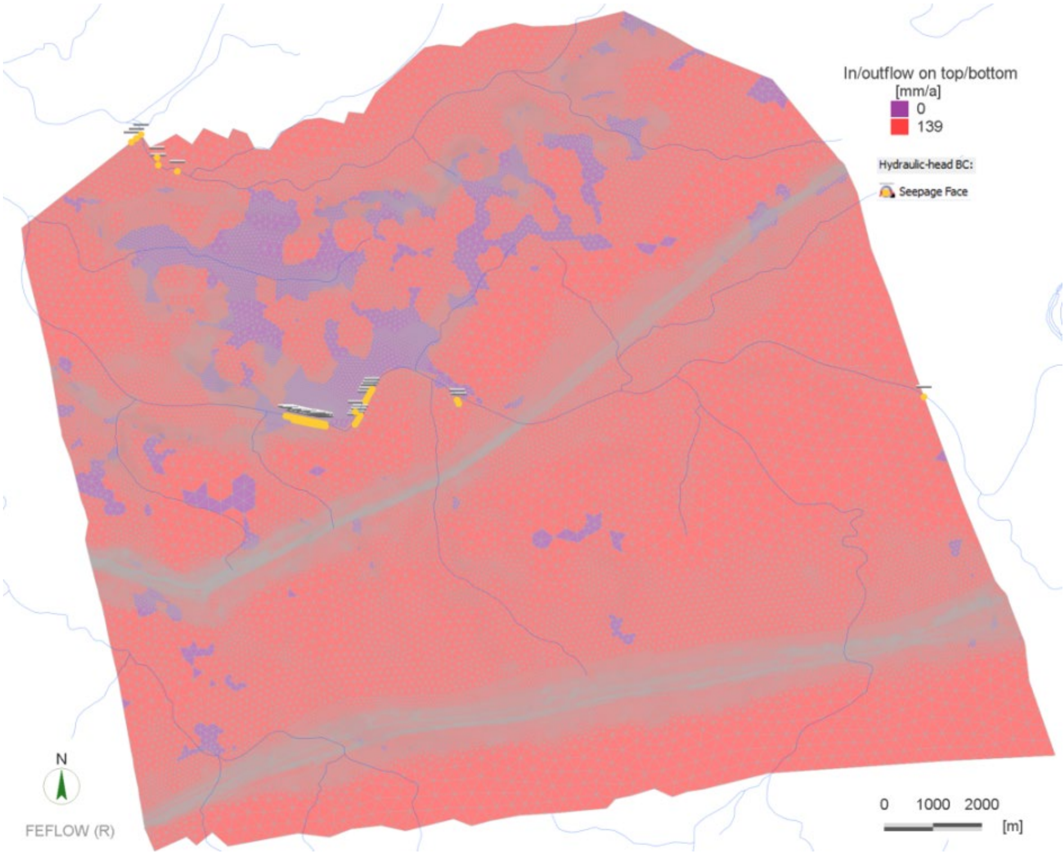


Fig. 3-17: Groundwater Recharge and Seepage Boundaries as Implemented in the Local Nördlich Lägern Model.

To prevent the development of lakes due to e.g. high recharge at the top that can not be discharged fast enough due to low conductivities, seepage boundary conditions had to be implemented for some elements and/or recharge was set to 0 in some areas.

3.4.2 Lateral Boundaries

The deeper regional aquifers (mainly Muschelkalk aquifer and Malm aquifer) obtain FH conditions adopted from the regional model according to their occurrences along the lateral borders. For this purpose, the hydraulic heads of the considered boundary nodes represented by their 2D-coordinates were interpolated from results of the corresponding aquifer layer of the regional model. Boundary nodes along the additional local aquifers/potentially transmissive units, not present in the regional model and incorporated according Chapter 3.2, obtain the head values from the superior (joint) layer of the regional model. In order to properly map the head values along the faults at lateral boundaries, first the corresponding node coordinates of the local model are projected onto the (vertical) fault of the regional model before head interpolation is accomplished.

3.4.3 Bottom

The Anhydritgruppe constitutes the bottom layer. This hydrogeological unit has been assigned with a relatively low conductivity so a theoretical water exchange with deeper formations can be neglected. Thus, no flow conditions have been implemented along the bottom boundary of the model.

4 Modelling Results

4.1 Modelling Strategy

A retraceable modelling strategy was adopted to ensure a balanced assessment of the key features and processes which govern groundwater flow conditions in the siting region Nördlich Lägern. The general workflow comprises the following elements (Figure 4-1):

- A consistent representation of groundwater flow conditions at all relevant scales was achieved by the nested modelling approach
- A set of complementary working hypotheses was specified, covering a wide spectrum of groundwater flow scenarios.
- The consistency of the (regional) simulations with present day conditions was checked by comparison of the modelling results with the available field data. Sensitivity analyses were performed to investigate both conceptual uncertainties and parameter uncertainties.
- The simulation results were analysed and interpreted. The plausibility and consistency of the modelling results were evaluated by comparison with the regional scale simulations.

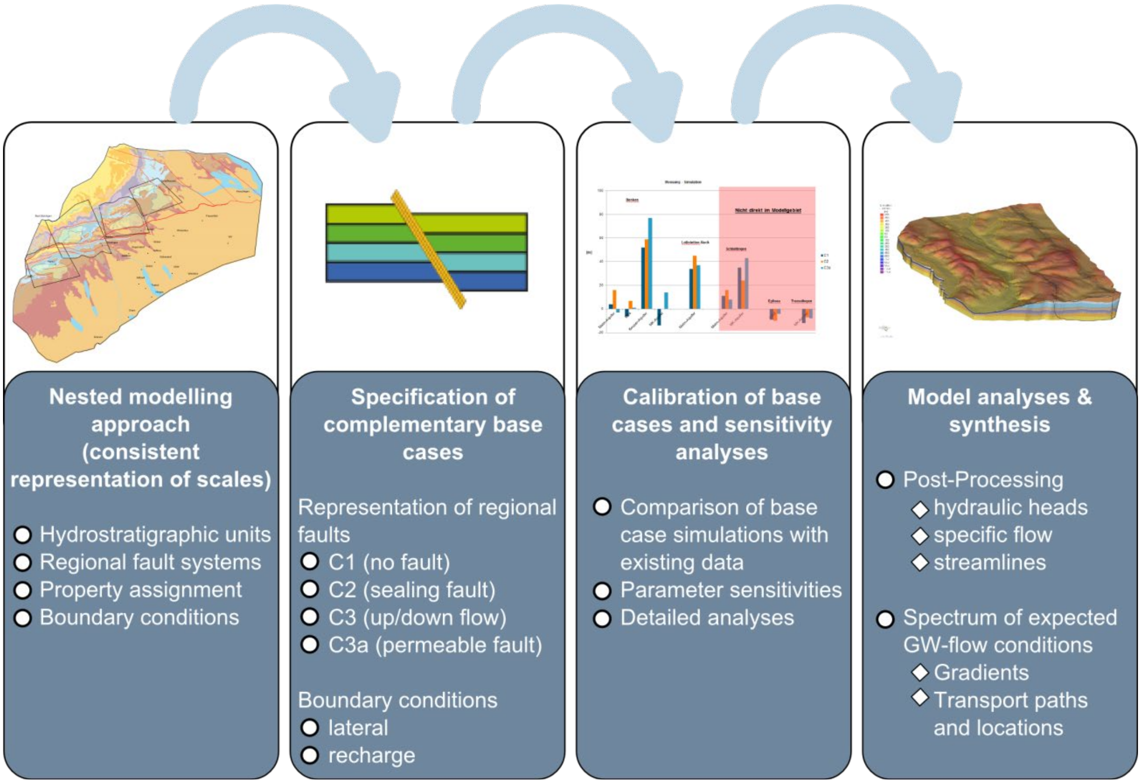


Fig. 4-1: Modelling Strategy Adopted for the Hydrogeological Simulations.

4.1.1 Nested Modelling

As outlined in detail in Chapter 2, the siting region Nördlich Lägern is located in the Vorfaltenzone of the eastern tabular Jura, where local hydrogeological conditions are characterized by the following geological setting:

- Two regional fault systems (BIH, Siglistorf Anticline) divide the siting region in three major subdomains.
- Outcrop lines of the Malm aquifer induce complicated groundwater circulation
- Clear evidence was found for regional scale variability of hydraulic conductivity in several hydrogeological units, such as the Keuper aquifer, sub-units of the 'Brown Dogger' and the Malm aquifer.

Understanding the impact of this geometrical and hydrogeological complexity on the local scale groundwater system requires detailed modelling by means of dense spatial discretisation. However, on the regional scale, minimum element size is restricted due to numerical execution time and memory constraints. In order to ensure a consistent description of groundwater flow in both, the regional and local scale, the solution is to use a nested modelling approach. The principle behind nested modelling is that, consistent with the large-scale groundwater circulation generated by the overall model, detailed local flow fields can be simulated using fine-scale sub-grids as long as lateral boundary conditions are suitably provided from higher scale results. In this context, the present Nördlich Lägern model was implemented as a local sub-grid of the large-scale regional model (Gmünder et al. 2013b) as described in detail in Chapter 3.

4.1.2 Working Hypotheses and Base Cases

The hydrogeological considerations together with its numerical implementation as described in Chapter 2 and Chapter 3, respectively, define reference conditions representing the currently most plausible model configurations with respect to geometry, parameters and boundary conditions. However, general uncertainties exist with respect to the impact of distinct components of the model (e.g. hydrogeological units, faults, etc.) on groundwater flow pattern. In particular, the potential role and significance of the hydraulic behaviour of the fault zones is rather unknown. In this case, it is common practise to model the resultant effects based on different working hypotheses. Using the implementation of faults described in Chapter 3.3.3, it is possible to change their hydraulic behaviour by simply assigning corresponding conductivity parameters. In this context, 4 basic hypotheses have been defined (leading to 4 different Base Cases), each treating the role of the faults in a different manner:

- Hypothesis 1/Base Case 1 ("throw only"): In this case, the fault is assumed non-existent. The controlling factor for flow along or across the (hypothetical) fault plane is the offset of the different hydrogeological units. If an aquifer is offset and abuts onto an aquitard, no flow is possible. In case of an aquifer being offset to abut onto another aquifer, these two aquifers are coupled and flow from one aquifer into the other is possible. The numerical model implements Base Case 1 by assigning the properties of the hydrogeological units to the adjacent elements of the faults.

- Hypothesis 2/Base Case 2 ("sealing fault"): The faults are assumed to exhibit a very low hydraulic conductivity and therefore have a sealing effect. Because flow within the faults was limited to all directions, even cross-flow between aquifers which are coupled through the offset, would not be possible. This effectively divides the model domain into separate blocks. The numerical model implements these conditions assigning a very low conductivity (2e-14 m/s) to the fault elements.
- Hypothesis 3/Base Case 3 ("connecting fault"): In this case, flow along the fault plane (lateral and vertical) is possible while flow across the fault plane is prohibited (or at least only very limited flow is possible). This also divides the model domain into distinct blocks. However, flow along the fault from a deeper aquifer to a higher aquifer (or vice versa) is possible within each block. The numerical model implements Base Case 3 by assigning a relatively high conductivity (1e-6 m/s) to the outer elements of the faults while the central row of elements in the faults only have a very low conductivity (2e-14 m/s).
- Hypothesis 3a/Base Case 3a ("fully connecting fault"): This case assumes that the faults act as fully active connections so that flow along the fault plane (lateral and vertical) as well as flow across the fault plane is possible. The numerical model implements Base Case 3a assigning a relatively high conductivity (1e-6 m/s) to all the elements of the faults (both outer and central row).

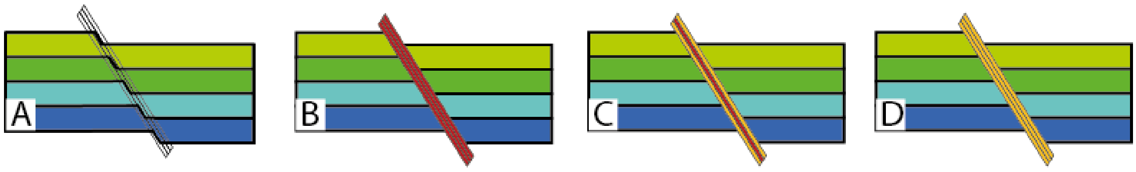


Fig. 4-2: Parameter Assignment of the Different Elements of the Faults for the Different Cases.

Faults in the Base Cases are represented by 3 layers of elements. By assigning different hydraulic properties to the layers, the hydraulic behaviour of the fault can be changed. A) Base Case 1: Fault elements are assigned with the same conductivities as the surrounding rocks. This effectively means that the fault does not exist and flow is governed by offset only. B) Base Case 2: All fault elements are assigned very low conductivities. C) Base Case 3: Fault elements on the outside are permeable, the central row of fault elements are assigned with very low conductivities. D) Base Case 3a: All fault elements are assigned with high conductivities.

4.1.3 Sensitivity Analyses

Uncertainties with respect to the role and significance of individual model components as well as the related parameter uncertainty necessitate the evaluation not only of the Base Cases behaviour but also of variations from the expected system behaviour. The systematic evaluation of this behaviour, including variations, has been performed by means of additional simulation runs as part of a sensitivity analysis (conceptual variations, parameter variations). For instance, the hydrogeological units Arietenkalk and BD5 (Sissach Member) have not been regarded as locally important transmissive units in the Base Cases defined above, but have been assigned higher conductivities in the sensitivity cases, effectively treating them as conductive units while the remaining model was kept unchanged. A complete overview of parameters and boundary conditions used in the simulation runs (base and sensitivity cases) is given in Table 4-1.

Tab. 4-1: Overview on Sensitivity Cases Performed with the Local Nördlich Lägern Model.

Note that the BD5 has been implemented as a higher conductive layer (compared to the Arietenkalk) in the Base Cases already. Therefore, increase of the conductivity of the BD5 in the sensitivity cases is less than the increase of conductivity of the Arietenkalk.

Sensitivity Case	**Base case**	**Hydrogeol. unit**	**Conductivity Sensitivity case** [m/s]	**Conductivity Base case** [m/s]	**Boundary conditions**
C1-BD5	C1	BD5 (Sissach Member)	$1x10^{-9}$	$5x10^{-10}$	C1-from regional model
C2-BD5	C2				C2-from regional model
C3-BD5	C3				C3-from regional model
C1-AKA	C1	Arietenkalk	$1x10^{-8}$	$1x10^{-12}$	C1-Keuper
C2-AKA	C2				C2-Keuper
C3-AKA	C3				C3-Keuper
C1-BD5-AKA	C1	BD5 & Arietenkalk	BD5: $1x10^{-9}$ Arietenkalk: $1x10^{-8}$	BD5: $1x10^{-9}$ Arietenkalk: $1x10^{-8}$	C1-BD5/ C1-Keuper
C2-BD5-AKA	C2				C2-BD5/ C2-Keuper
C3-BD5-AKA	C3				C3-BD5/ C3-Keuper

4.1.4 Modelling Products and Analysis

A thorough and comprehensive analysis of simulation runs involves numerous evaluation tasks yielding a manifold of output in terms of performance measures (i.e., hydraulic heads, groundwater fluxes, hydraulic gradients). In this context, each simulation run is discussed systematically based on a predefined set of so-called modelling products which have been organized as follows:

- Contour plots along selected surfaces (vertical/horizontal sections, geological boundaries, etc.)
- Profiles (tables and charts) along specified lines
- Maps of recharge/discharge areas
- 3D recharge/discharge paths (the limitations of the method used to calculate these paths is detailed in Gmünder et al. (2013b)
- Vertical gradients through the host rock(s)

The above mentioned products are presented in the following chapters. To avoid unnecessary repetition of results such as exact recharge or discharge locations etc., Chapter 4 is mostly descriptive while Chapter 5 summarizes and explains the results.

The position and orientation of the cross-sections shown in subsequent chapters and the appendices is given in Fig. 4-3 and is the same for all cross-sections in this report.

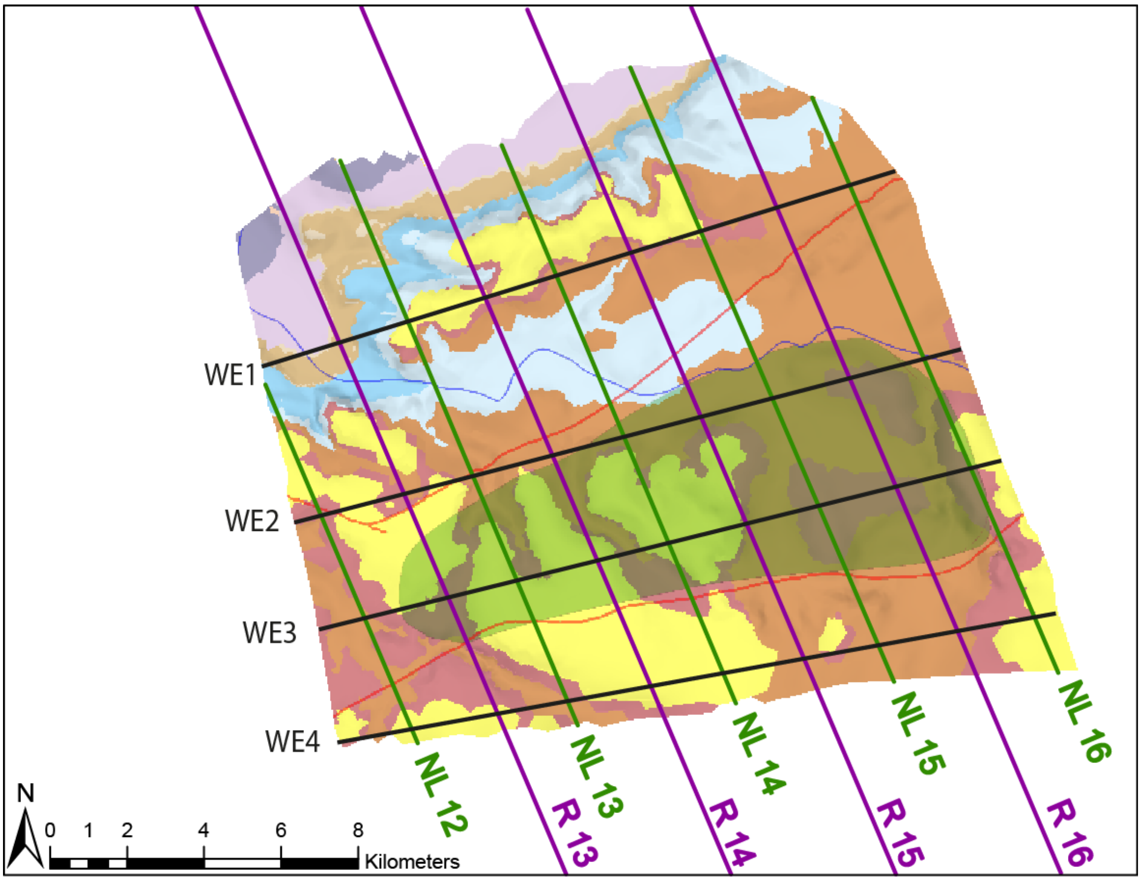


Fig. 4-3: Location of Cross-sections in the Model Area.

4.1.5 Model Calibration and Consistency Checks

In broad terms, model calibration refers to the process of gathering information about the model from measurements of what is being modelled. This includes the identification of model structure (e.g. the role of faults and aquifers) and the inherent heterogeneities defining hydraulic properties. For the Nördlich Lägern model domain at hand, a formal model calibration cannot be performed because hydraulic observation data from boreholes are not available. However, the larger scale regional hydrogeological model has been intensively checked against all available hydraulic measurements and provides a reliable picture of the regional flow pattern (Gmünder et al. 2013b). Thus, an acceptable agreement between the models at both scales will verify the local results to some extent.

Because a substantial model calibration cannot be carried out it is important to accomplish further checks in order to ensure plausibility and consistency of the modelling results. First, a comparison with results of the hydrogeological regional model is important to ensure the correct adoption of boundary conditions and hydrogeological parameters. This comparison is part of the modelling report for the hydrogeological regional model (Gmünder et al. 2013b).

4.2 Base Case C1 ("Throw Only")

4.2.1 Hydraulic Heads

As argued above run C1 refers to a best guess parameter set and boundary conditions described in Chapter 3.3 and 3.4 assuming that the faults only affect the flow system by the offset of the geological units (s. Chapter 4.1). The model calculates hydraulic heads in a range of 460 to 330 masl southern surface boundary and the exit-boundary of the Rhine (Fig 4-4).

Disregarding the Quaternary (surface) aquifers, the deeper flow system is mainly represented by 5 aquifer layers/transmissive units. As illustrated by their flow fields in Fig. 4-5 and 4-6, they reflect two virtually independent flow systems separated by the Opalinus Clay: Malm aquifer, BD2 (Hauptrogenstein) and BD5 (Sissach Member) above and the Keuper aquifer and Muschelkalk aquifer below the potential host rock Opalinus Clay. Vertical sections through flow system are shown in Fig. 4-7.

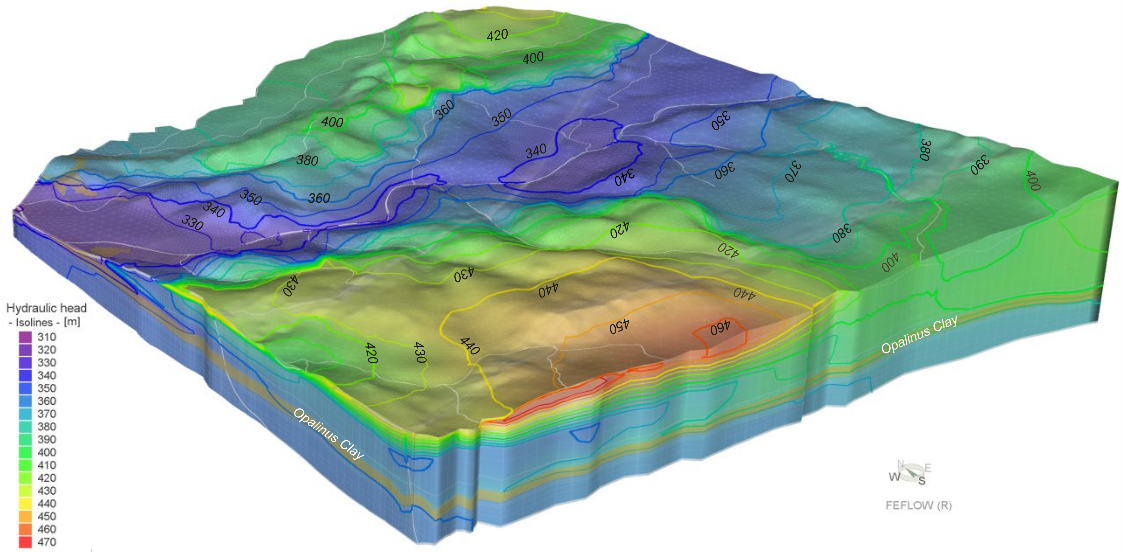


Fig. 4-4: Base Case C1 - Overall 3D View of the Simulated Groundwater Flow System.

Simulated hydraulic heads in the ***Malm aquifer*** vary between 330 and 450 masl (Fig. 4-5a). The head distribution is mainly influenced by the topography, no impact from the two implemented faults is visible because the vertical offset at the faults is smaller than the layer thickness and hence flow across the faults is still possible. The considerable bent of the isolines is caused by the interacting recharge areas at the NE and SE model boundary and along the western part of the BIH. These are explained in more details in Chapter 4.2.2. The main flow direction is towards the Rhine valley.

The unit BD2 (related to the ***Hauptrogenstein***) covers the model domain only to a limited extent (Fig. 4-5b). Here, the main flow direction is from the outcrops in the NE towards the Rhine valley with hydraulic heads between 400 and 320 masl. Due to a complete offset of the layer along the Siglistorf Anticline, the parts north and south of the fault form a separate flow system.

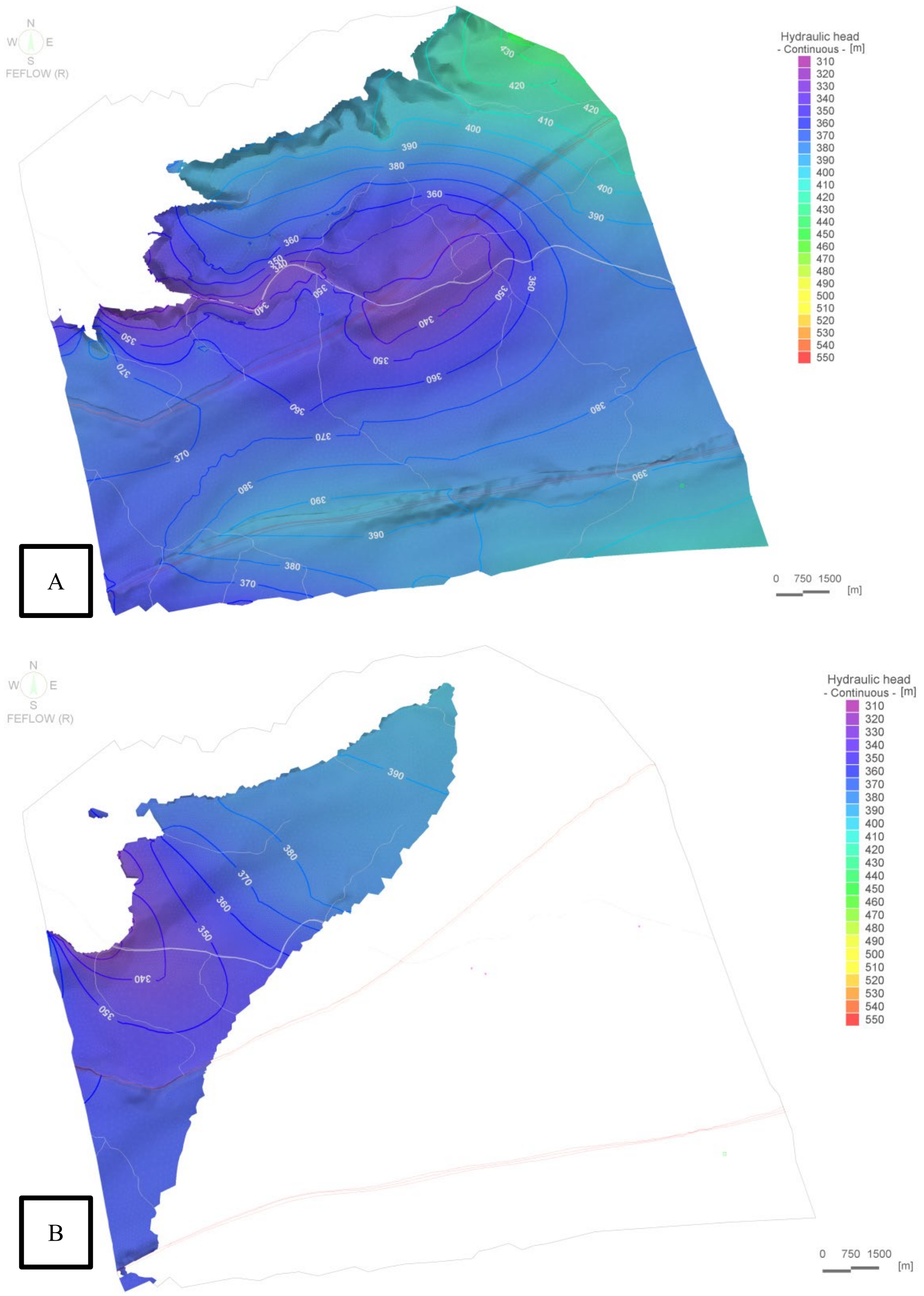


Fig. 4-5: Base Case C1 - Simulated head fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

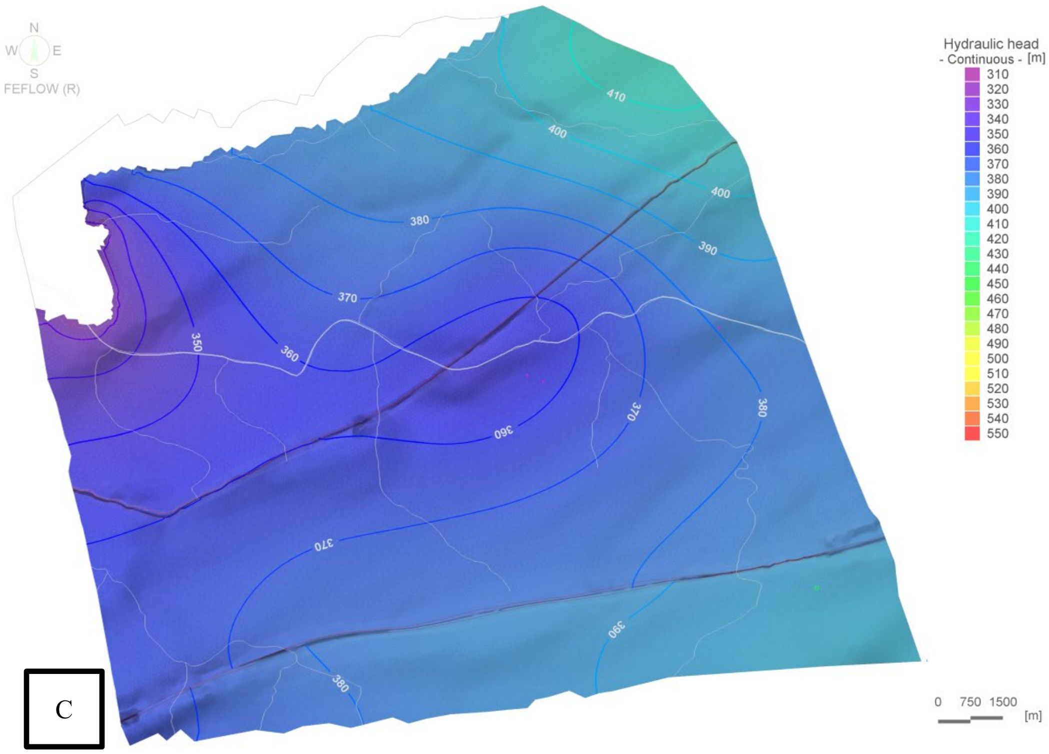


Fig. 4-5: (continued) Base Case C1 - Simulated head fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

The hydrogeological unit BD5 (***Sissach Member***) is modelled as a locally transmissive unit with an average thickness of 10 m directly on top of the Opalinus Clay and is present almost throughout the entire model domain. Simulated hydraulic heads vary between 430 und 320 masl (Fig. 4-5c). A slight head discontinuity can be observed along the southern BIH because the vertical offset along the fault is larger than the layer thickness. The influence of the topography is still visible, though much subdued compared the Malm aquifer. The main flow direction is towards the SW boundary of the model where the BD5 crops out.

The ***Keuper aquifer*** is modelled as an aquifer system of 10 m thickness located below the Opalinus Clay (Fig. 4-6a). As mentioned earlier, its flow system is different from those of the upper aquifers. Sealed off by the low conductive clays above, discrete inflow only occurs from the north-eastern boundary where the recharge area along the high outcrops in the upper Wutach valley (modelled by the regional model, see Gmünder et al. 2013b) have created artesian conditions with hydraulic heads of about 450 masl. Along the western boundary, the water flows out of the modelled domain where heads amount to approximately 350 masl. Due to a significant vertical offset, the Keuper aquifer is separated by the BIH.

The ***Muschelkalk aquifer*** is a significant regional aquifer located below the Keuper aquifer (Fig. 4-6b). Between the two aquifers, the low conductive Gipskeuper acts as an aquitard. The simulated hydraulic heads in the Muschelkalk aquifer vary between 410 und 350 masl. The three regions of different conductivity (s. Chapter 3.3) with a more conductive part near the southern boundary can clearly be identified because the different conductivities cause a change of direction of the isolines (though this effect is less pronounced between the northern two zones). A hydraulic separation of the flow field along the BIH does not occur because the vertical offset along the fault is much smaller than the layer thickness.

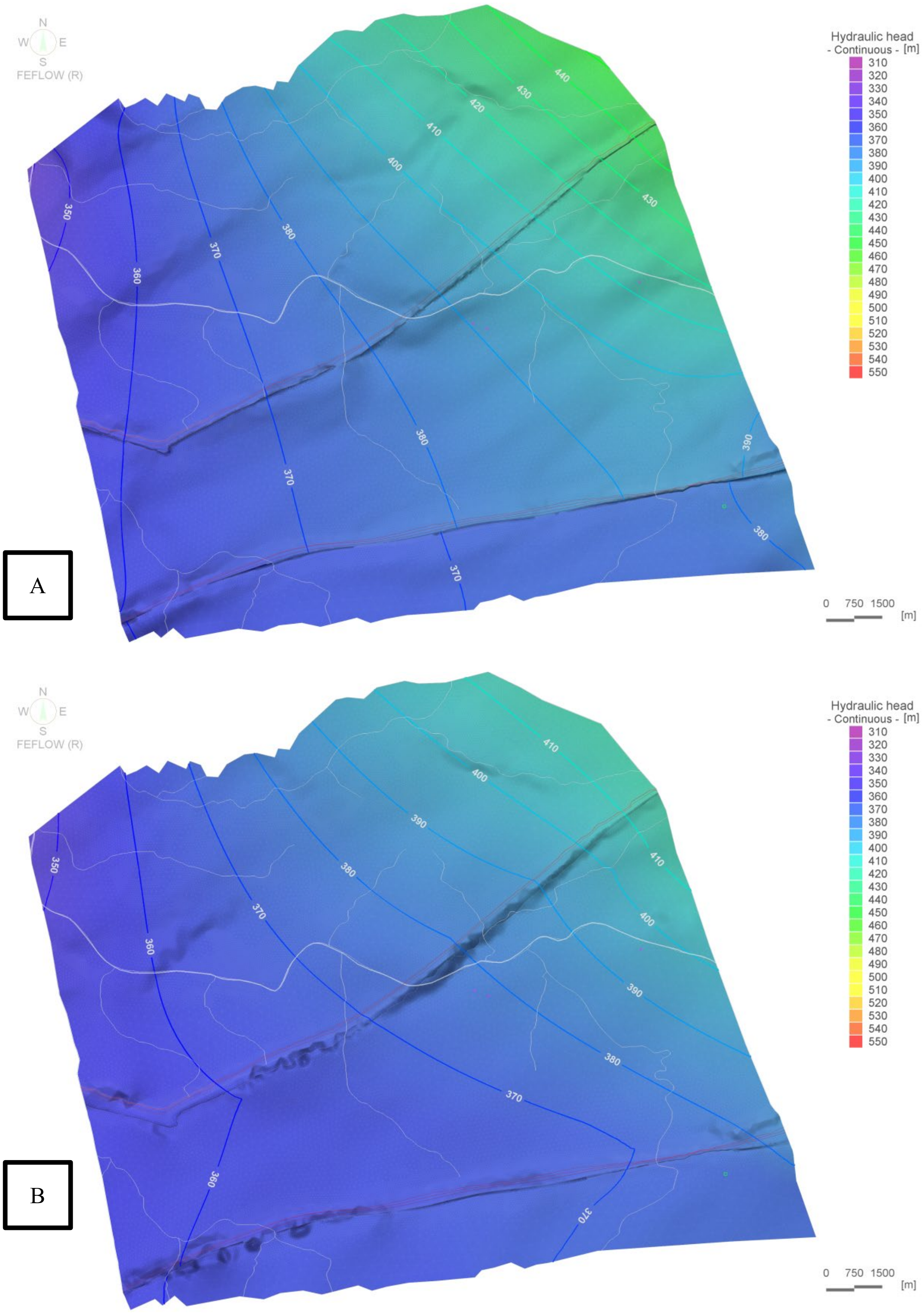
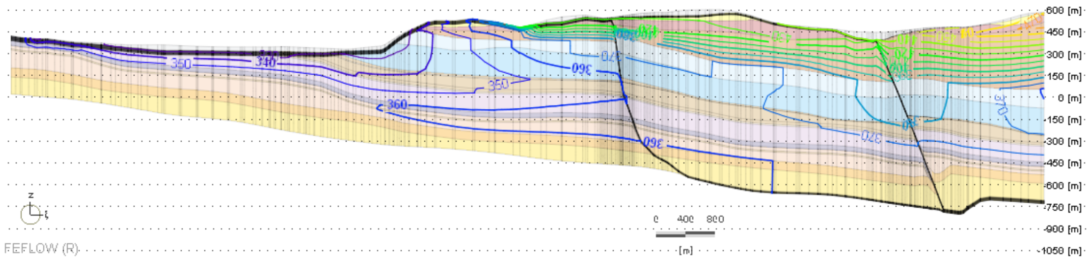
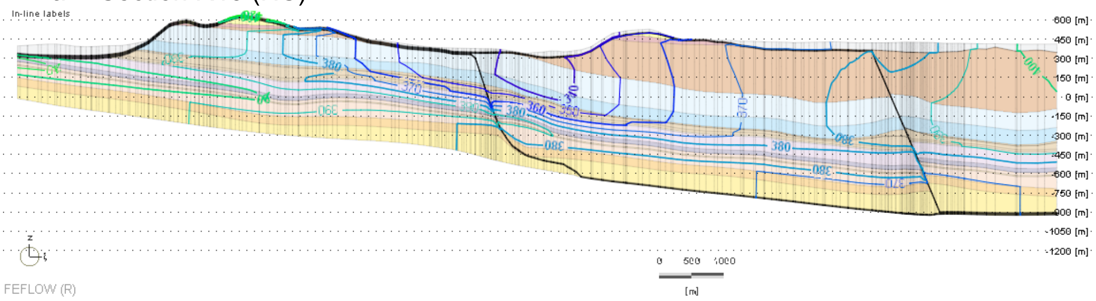


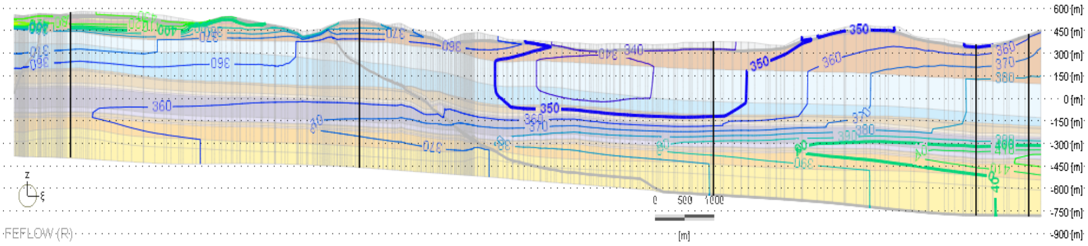
Fig. 4-6: Base Case C1 - Simulated Head Fields along aquifers below the Opalinus Clay. A – Keuper aquifer, B – Muschelkalk aquifer.



a. Section R13 (NS)



b. Section R15 (NS)



c. Section W2 (WE)

Fig. 4-7: Base Case C1 - Simulated Head Fields along Vertical Sections.
(Location see Fig. 4-3, 2x vertical exaggeration).

As mentioned earlier, an upper and a lower flow system developed, separated by the low conductive Opalinus Clay. In order to assess vertical flow through the host rocks, head differences of the BD5 above the Opalinus Clay minus the Keuper aquifer below the Opalinus Clay were evaluated (Fig. 4-8).

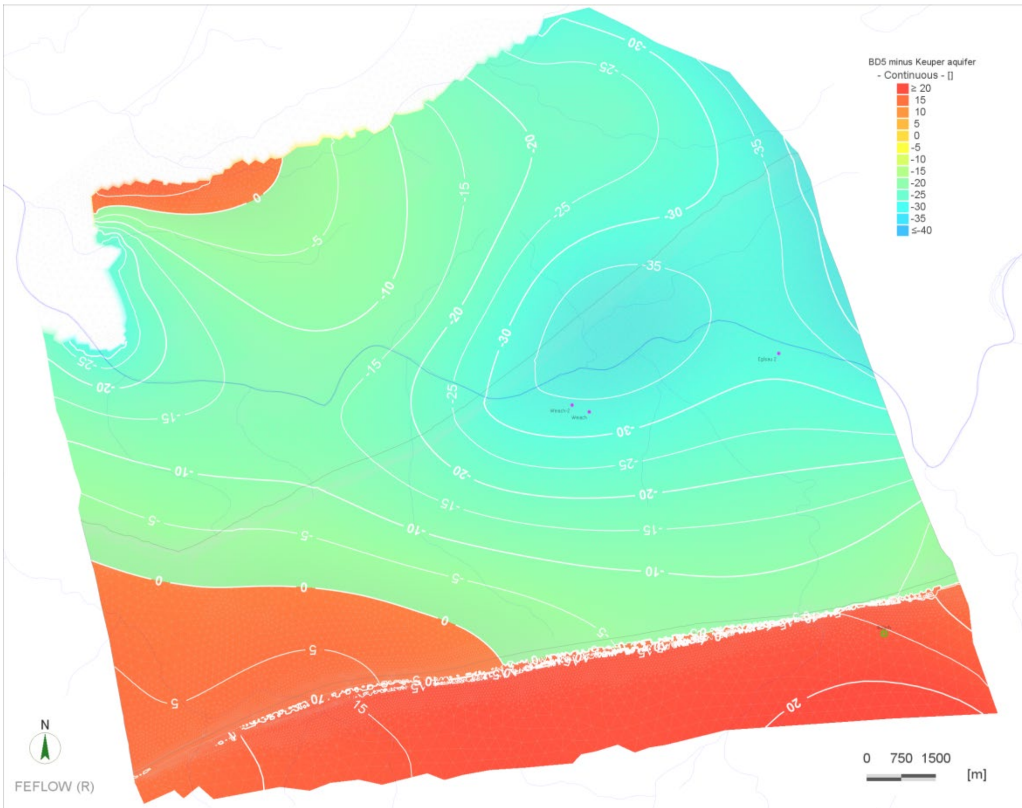


Fig. 4-8: Base Case C1 - Evaluation of Head Differences between the Sissach Member (BD5) and Keuper aquifer.

The reddish coloured regions indicate a positive head difference meaning that vertical groundwater flow is directed downwards. The vertical component of groundwater flow points upwards in regions coloured from light green to blue.

4.2.2 Recharge and Discharge Paths

In order to assess discharge paths of groundwater from the main aquifers Malm and Muschelkalk, particle tracking has been carried out. The particles were started from given points in the aquifers considered. While tracking along the direction of flow (i.e. forward tracking), the paths run to discharge points at the model boundary. Tracking in the opposite direction (i.e. backward tracking), the particles follow the recharge paths until a model boundary is reached indicating where groundwater originates. Fig. 4-9 shows the used starting points in the area of the siting region Nördlich Lägern. The starting points are always located at the shown xy-position, their vertical position is adjusted so that the points lie in the centre of the aquifer.

Fig. 4-10 shows calculated discharge paths (forward tracking) starting from the Malm aquifer as well as recharge paths obtained by backward tracking. The resulting path lines show that the discharge areas of the Malm aquifer are mainly located along the Rhine valley, only a few path lines leave the model domain at the south-western boundary. Along the eastern, southern and, to a lesser extend also the western boundary, recharge mainly occurs outside the model domain. In addition, groundwater recharges south of the BIH domain through the Molasse. The path lines indicate a flow crossing the BIH in the Molasse and, N of the BIH, flow downwards into the Malm aquifer.

The forward path lines starting in the Muschelkalk aquifer (Fig. 4-11) show that groundwater generally flows from the east (recharge) to the west (discharge) in the aquifer. Because of the overlying aquitards, the path lines only show lateral flow, no traces arrive at, or come from, the model surface. The sharp change of directions is caused by the interacting recharge from the NE and SE and by the fact that the Muschelkalk was separated into three regions with different conductivities.

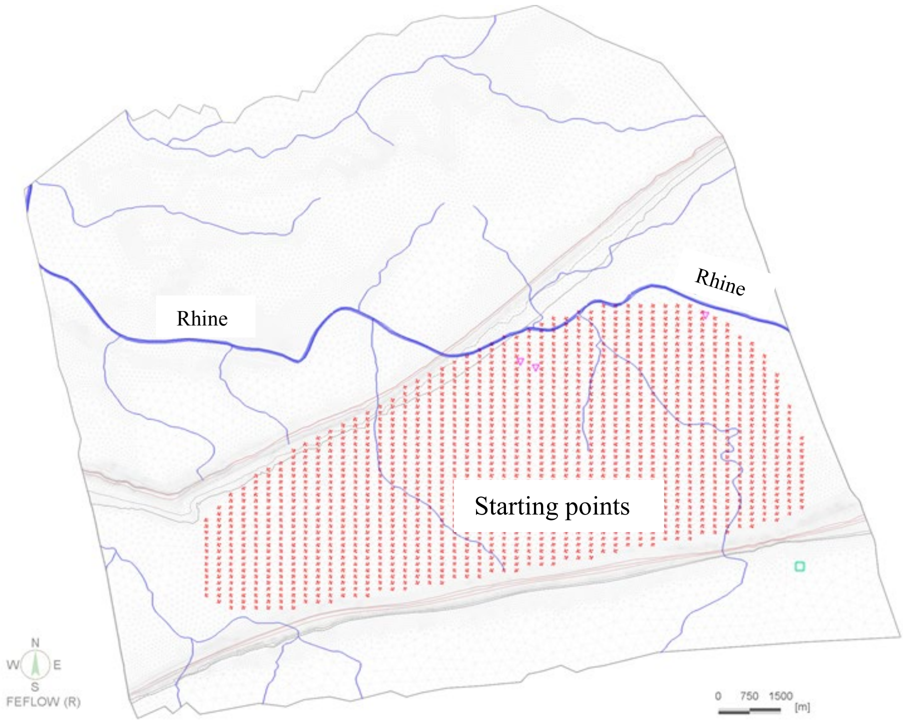


Fig. 4-9: Base Case C1 - Location of Starting Points for the Path Line Computation.

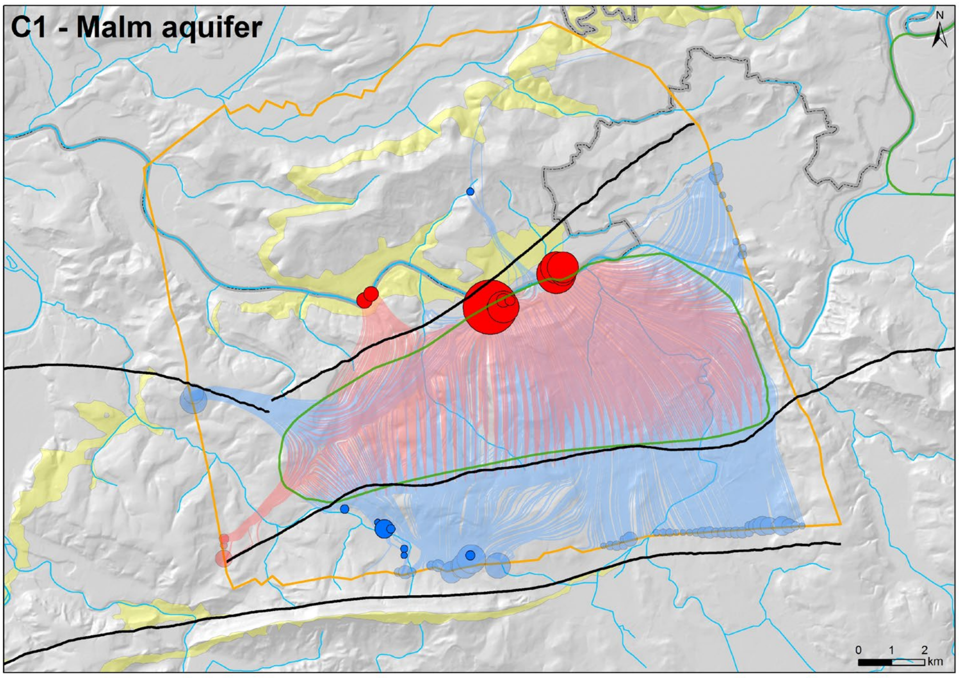


Fig. 4-10: Base Case C1 - Calculated Path lines Starting from the Malm aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

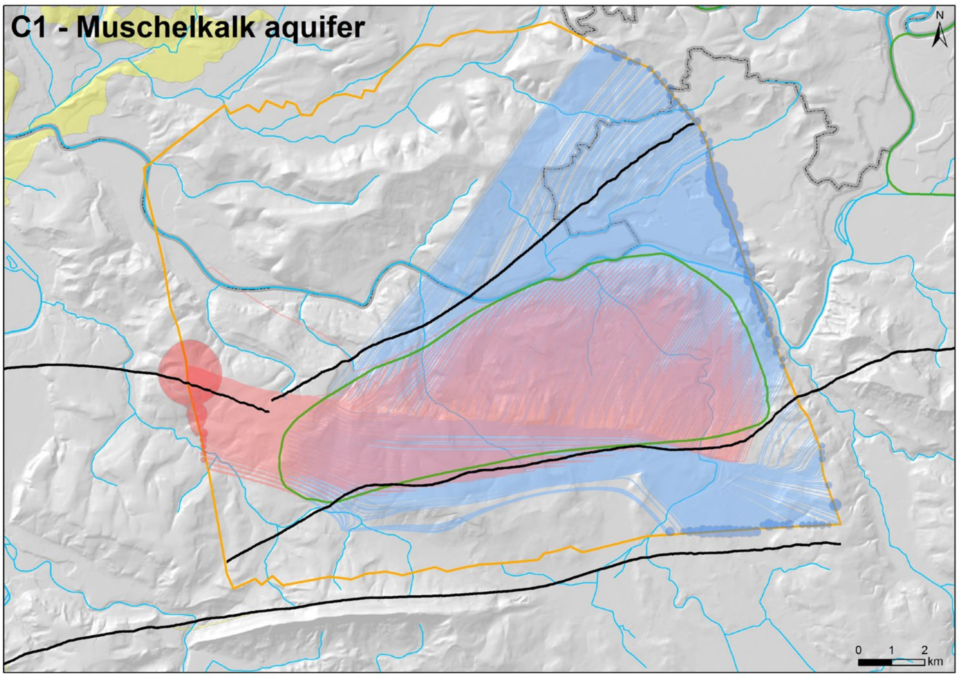


Fig. 4-11: Base Case C1 - Calculated Path lines Starting from the Muschelkalk aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model.)

4.2.3 Sensitivity Runs

The sensitivity runs performed based on Base Case C1 refer to the hypotheses that the two layers BD5 (Sissach Member) and Arietenkalk located above and below the Opalinus Clay, respectively, are considered to be more conductive (i.e. water conducting layers). Two of the 3 simulations only consider one of the layers to be conductive, the third simulations refers to an increased conductivity in both, the BD5 and the Arietenkalk.

In Case **C1-BD5**, the conductivity of the BD5 was increased by a factor of 2 (see Table 4-1). The computed head differences in this layer, compared to the Base Case, are shown in Fig. 4-12. Maximum differences occur along the southern boundary and near the Rhine. A slight increase of hydraulic heads is computed in the centre of the model below the Rhine valley, as well. Within the siting region and also in other layers, the head differences are negligible.

In Case **C1-AKA,** the conductivity of the Arietenkalk-layer was increased by 4 orders of magnitude, i.e. from 1×10^{-12} m/s to 1×10^{-8} m/s (Table 4-1). The increased conductivity causes only a minor increase of observed hydraulic heads below the siting region (~ +5 m within the Arietenkalk) causing the vertical flux through the host rock to be slightly increased. Slightly higher hydraulic heads have also been observed in the north-western area close to the model border. In the south-east, lower hydraulic heads (up to -10 m) occur (Fig. 4-13).

Sensitivity Case **C1-BD5-AKA** represents the combination of sensitivity runs **C1-BD5** and **C1-AKA** (Table 4-1). Computed head differences in the BD5 are almost the same as in Case C1-BD5 (Fig. 4.12) and in the Arietenkalk (Fig. 4-15) almost the same as in Case **C1-AKA** (Fig. 4-12). Therefore, vertical flux between the layers (i.e. through the potential host rock) is the same as in the sensitivity cases described above.

The computed heads in BD5 and Arietenkalk of Case **C1-BD5-AKA** compared to the corresponding Base Case C1 are shown in Fig. 4-14 and Fig. 4-15, respectively. The increased conductivities in the aquifers considered result in minor changes in hydraulic heads but do not change groundwater flow direction.

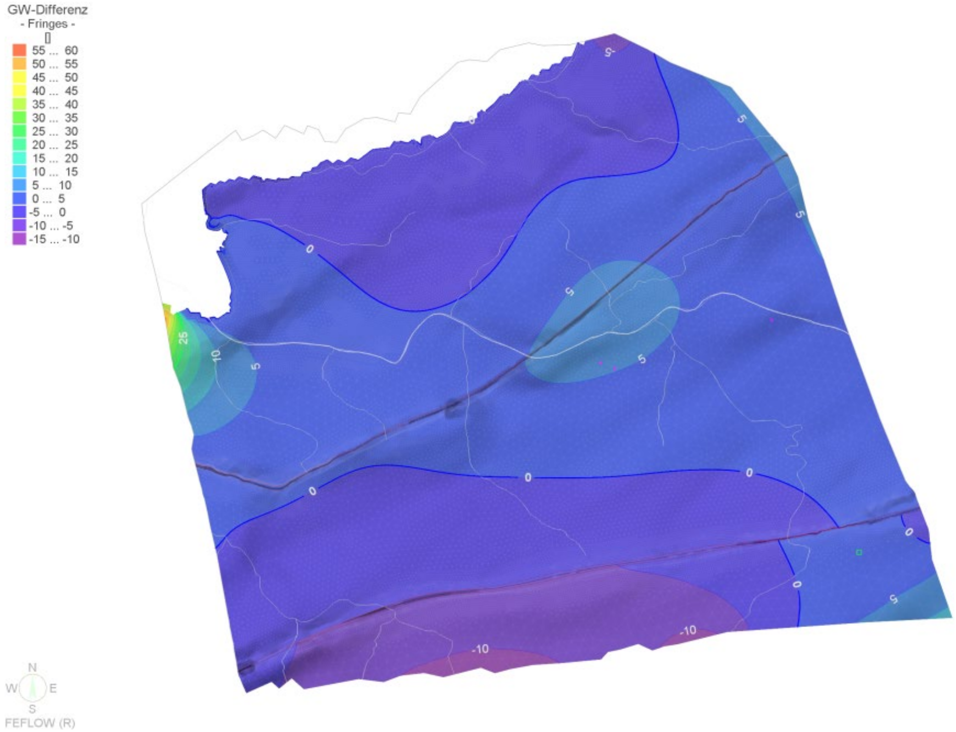


Fig. 4-12: Sensitivity Case C1-BD5 - Head Differences in the Sissach Member (BD5) compared to Base Case C1.

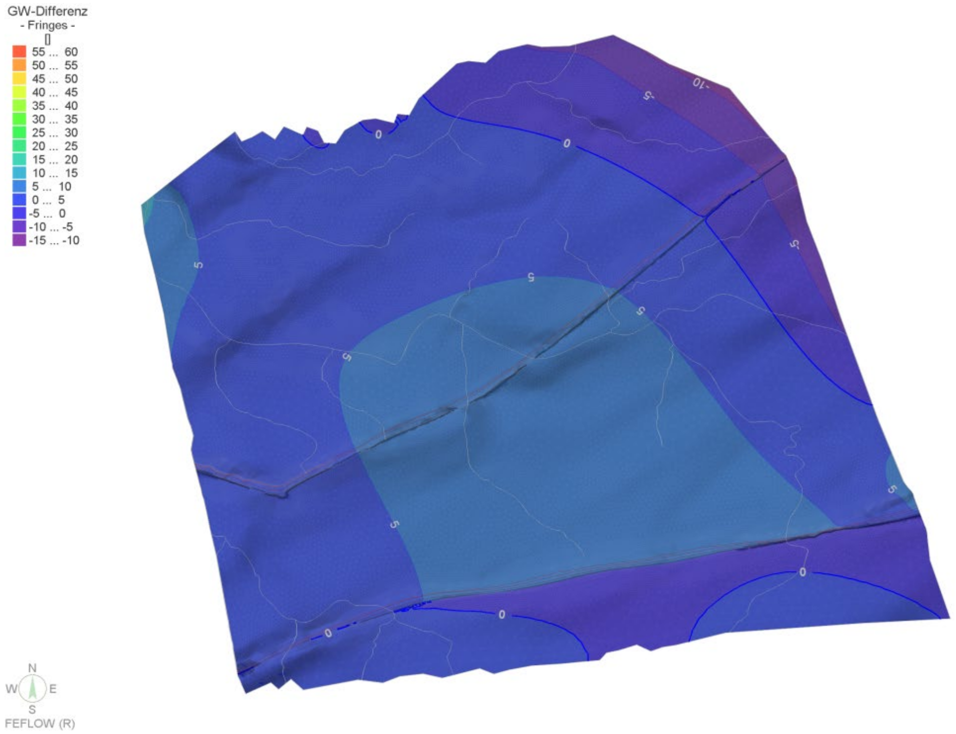


Fig. 4-13: Sensitivity Case C1-AKA - Head Differences in the Arietenkalk compared to Base Case C1.

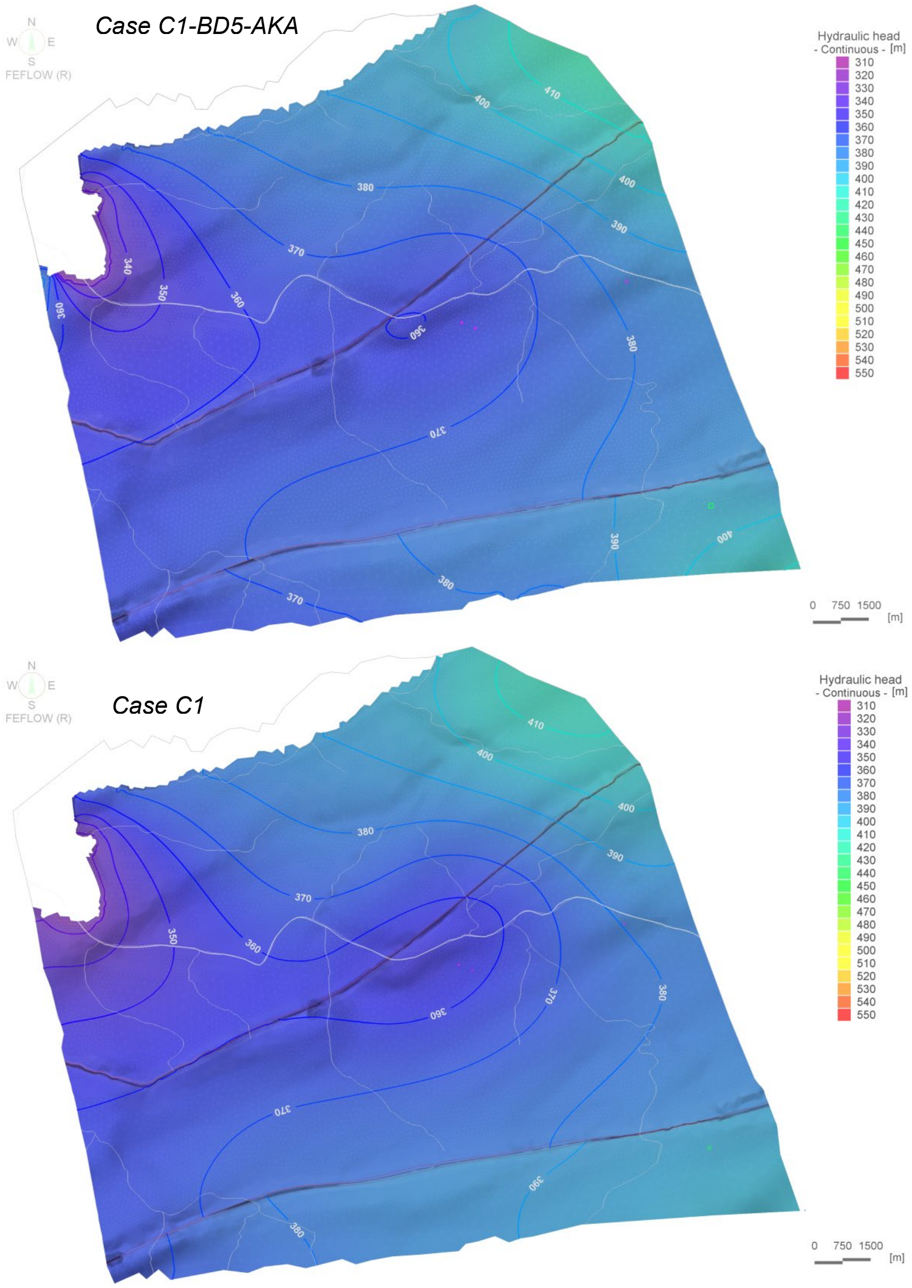


Fig. 4-14: Sensitivity Case C1-BD5-AKA - Head in BD5 compared to Base Case C1.

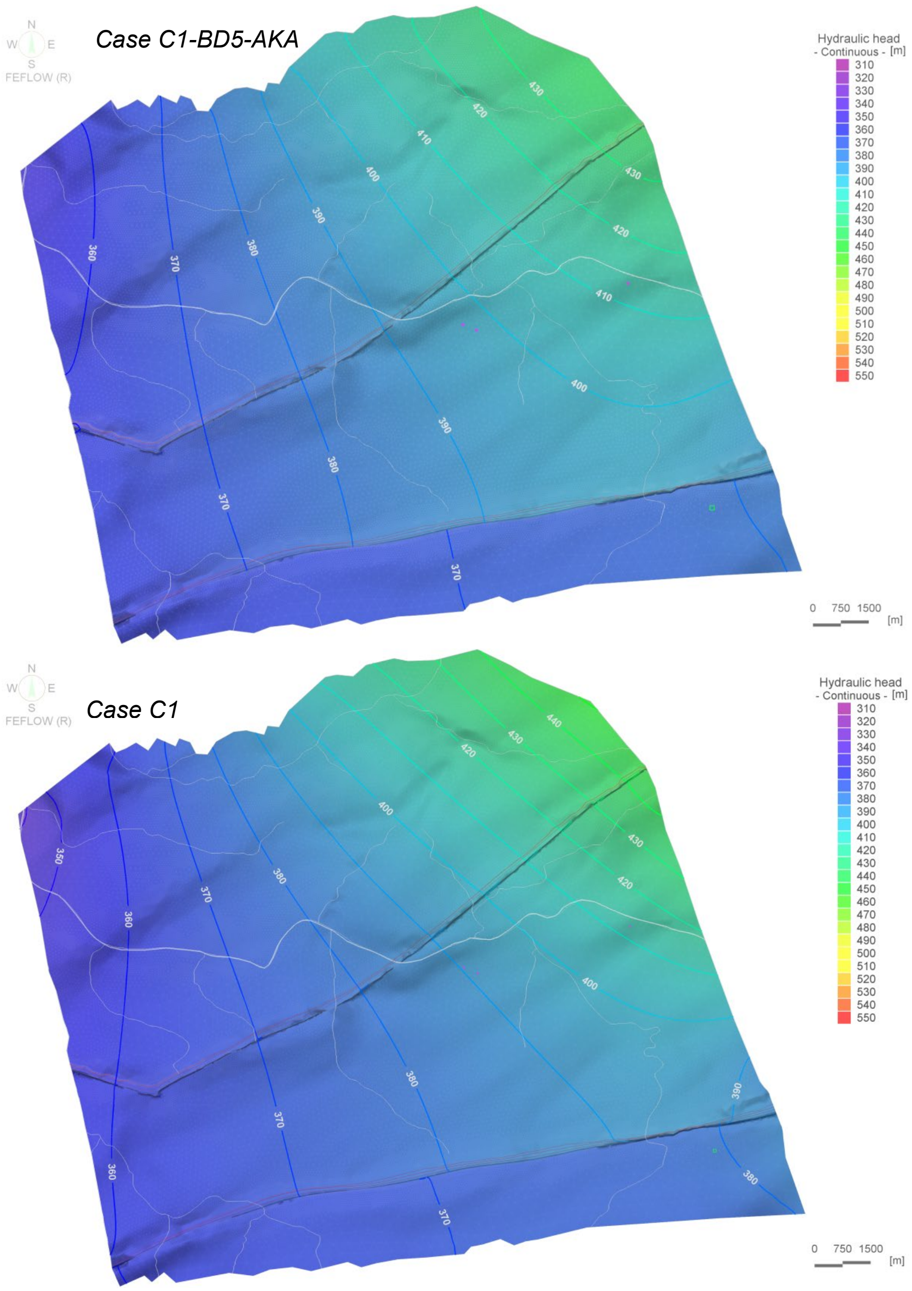


Fig. 4-15: Sensitivity Case C1-BD5-AKA - Head in the Arietenkalk compared to Base Case C1.

4.3 Base Case C2 ("Sealing Fault")

4.3.1 Hydraulic Heads

Run C2 refers to a best guess parameter set and boundary conditions described in Chapter 3.3 and 3.4 assuming that the faults are of very low conductivity (hypothesis "sealing fault", s. Chapter 4.1). The computed flow fields are shown in Fig. 4-16 and 4-17. They reflect two independent flow systems separated by the Opalinus Clay: Malm aquifer, BD2 (Hauptrogenstein) and BD5 (Sissach Member) above and Keuper aquifer and Muschelkalk aquifer below the potential host rock Opalinus Clay. Vertical sections through the flow system are shown in Fig. 4-18.

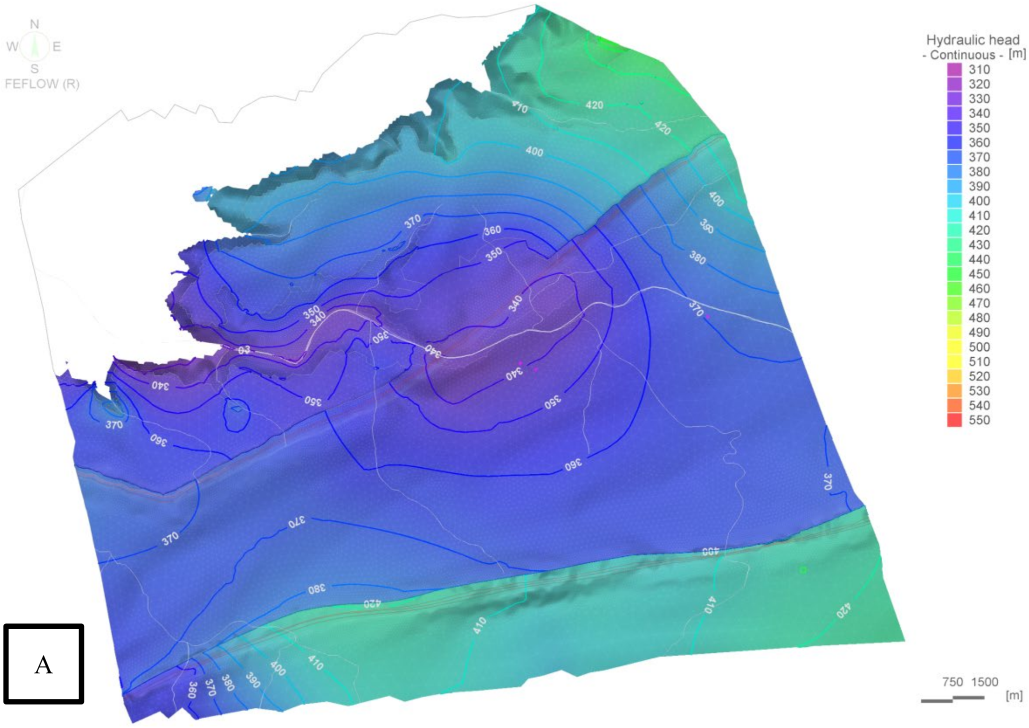
Simulated hydraulic heads in the ***Malm aquifer*** vary between 330 and 450 masl (Fig. 4-16a). The two sealing faults divide the aquifer into three independent blocks. However, in the northern part the head distribution still is influenced more by the topography though offsets along the faults are clearly visible. The lowest head values occur in the Rhine valley while the highest head values occur at the southern and north-eastern model boundary. North of the BIH, flow is directed towards the Rhine valley while south of the BIH, flow is directed from E to W.

The aquifer related to the BD2 (***Hauptrogenstein)*** covers the model domain only to a limited extent (Fig. 4-16b). Here, flow is directed towards the outcrops in the NW (in the Rhine valley) with hydraulic heads between 400 and 320 masl.

The BD5 (***Sissach Member***) is modelled as a locally transmissive unit with an average thickness of 10 m directly on top of the Opalinus Clay and is present almost throughout the entire model domain. Simulated hydraulic heads vary between 435 und 320 masl (Fig. 4-16c). Even though the "sealing faults" separate the flow system into independent blocks, the flow pattern is very similar to that of Base Case C1. Flow north of the BIH is directed towards the Rhine valley and the outcrops in the NW while flow south of the BIH is directed E to W.

The ***Keuper aquifer*** is modelled as an aquifer system of 10 m thickness located below the Opalinus Clay and confining layers (Fig. 4-17a). As mentioned earlier, its flow system is different from those of the upper aquifers. Sealed off by the low conductive clays, discrete inflow only occurs from the north-eastern boundary where the hydrogeological regional model simulated relatively high heads of up to 540 masl. Along the western boundary, the water flows out of the model domain where heads range from 360 masl at the SW-corner and 320 near the discharge area in the Rhine valley.

The ***Muschelkalk aquifer*** is a significant regional aquifer located below the Keuper aquifer (Fig. 4-17b). Between the two aquifers, the low conductive Gipskeuper acts as an aquitard. The simulated hydraulic heads in the Muschelkalk aquifer vary between 430 und 350 masl. Due to the sealing faults, three independent flow systems develop. The flow field is further complicated by the different conductivities assigned to the three zones. As in the previous Base Case, the change of conductivities causes a sharp bend of the head isolines. However, groundwater flow generally is directed from NE to W.



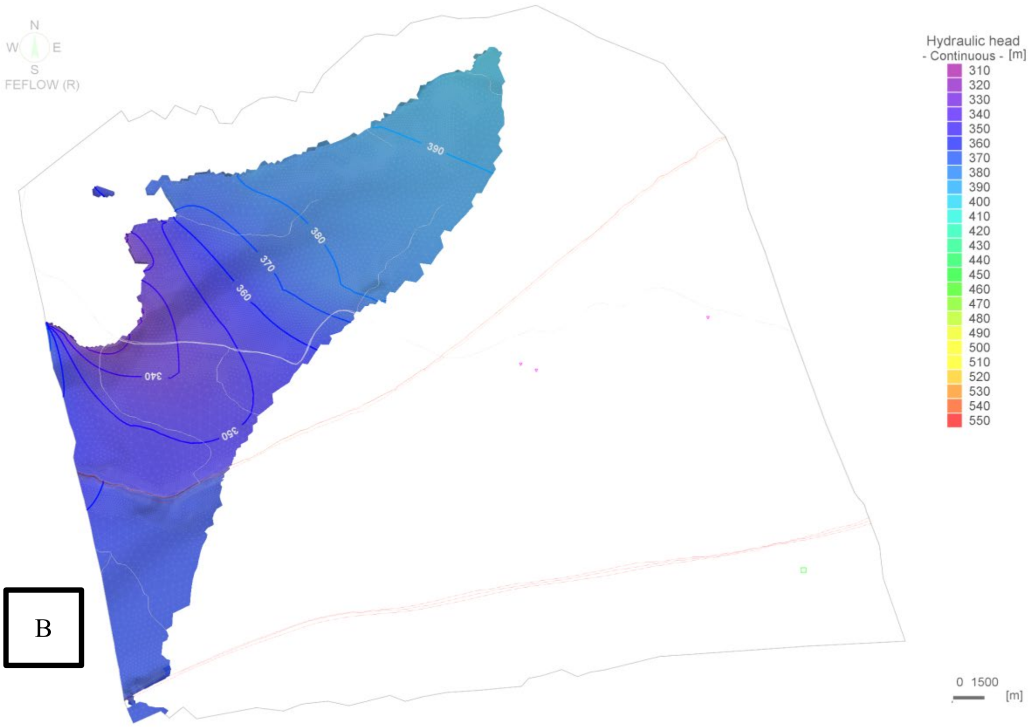


Fig. 4-16: Base Case C2 - Simulated Head Fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

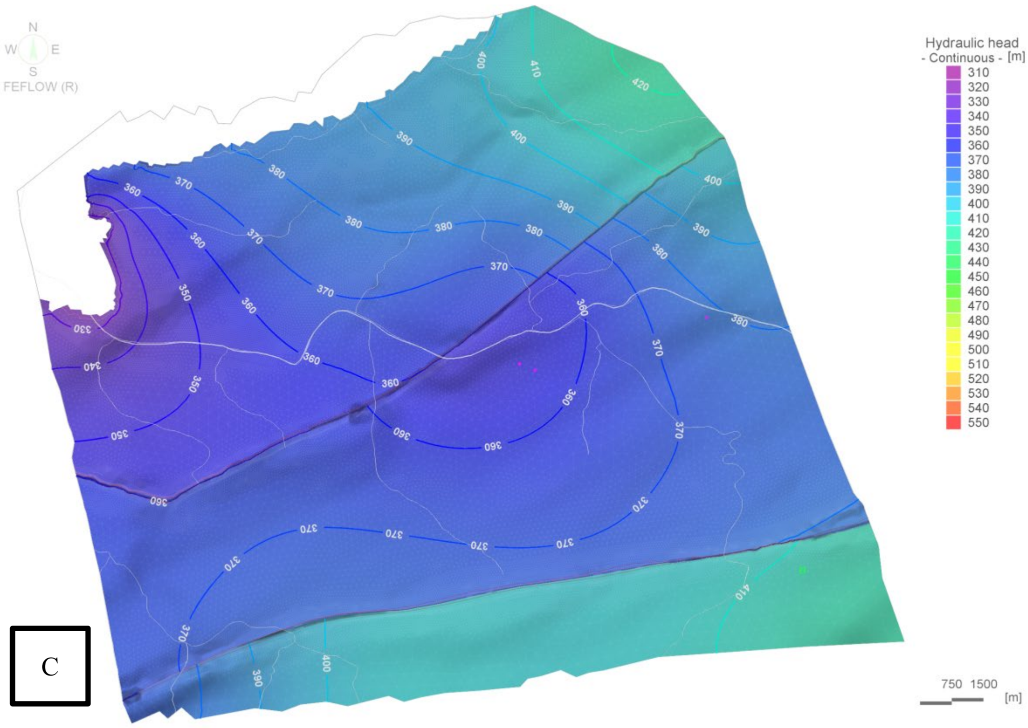


Fig. 4-16: (continued) Base Case C2 - Simulated Head Fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

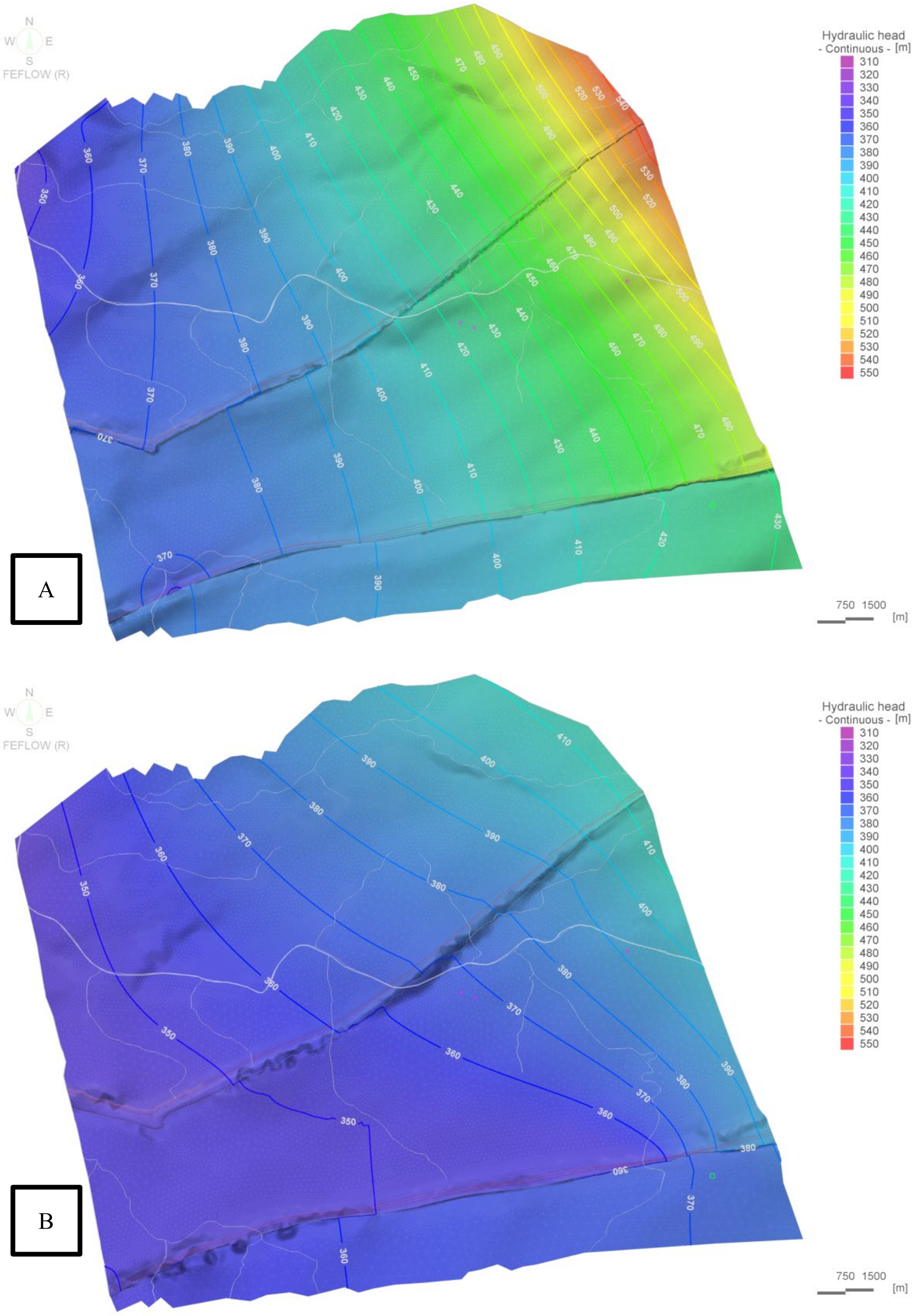
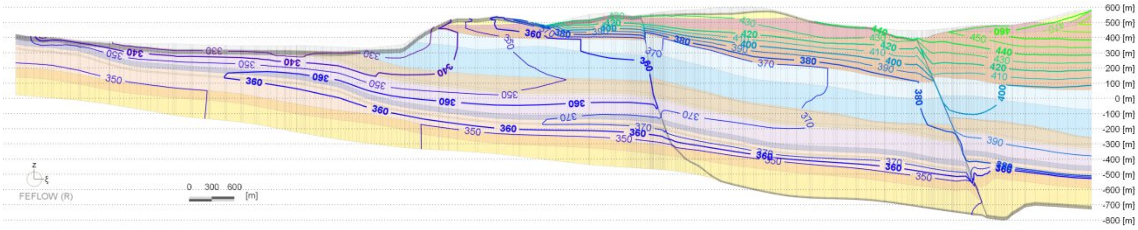
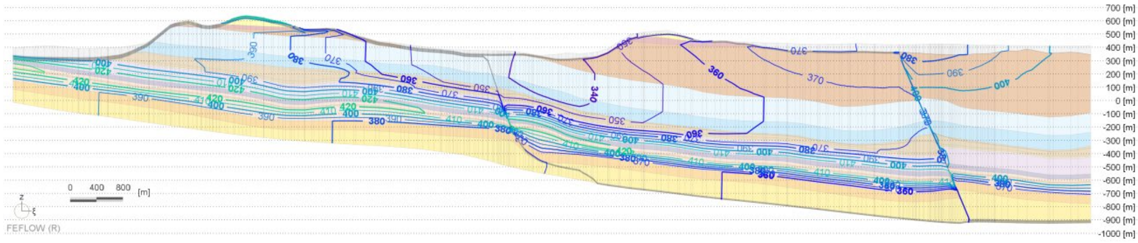


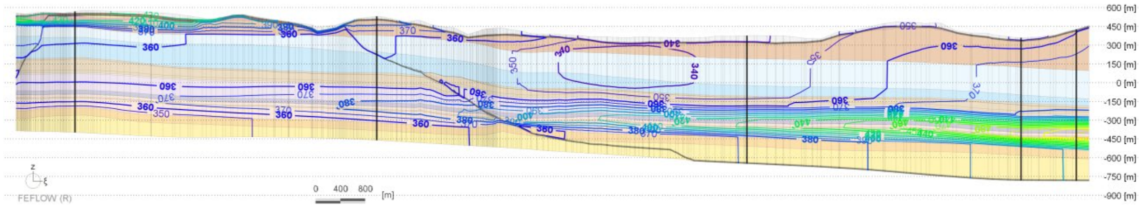
Fig. 4-17: Base Case C2 - Simulated Head Fields along aquifers below the Opalinus Clay. A – Keuper aquifer, B – Muschelkalk aquifer.



a. Section R13 (NS)



b. Section R15 (NS)



c. Section W2 (WE)

Fig. 4-18: Base Case C2 - Simulated Head Fields along Vertical Sections.

(Location see Fig. 4-3, 2x vertical exaggeration).

As mentioned earlier, an upper and a lower flow system develops, separated by the low conductive Opalinus Clay. In order to assess vertical flow through the host rocks, head differences of the BD5 above minus the Keuper aquifer below the Opalinus Clay were evaluated as shown in Fig. 4-19. Due to the sealing faults, which produce higher heads in the Keuper aquifer (Fig. 4-17a, Fig. 4-18), upward flux along the siting region has increased by approximately a factor 4 (in average) compared to Base Case C1 with head differences between 10 and 100 m.

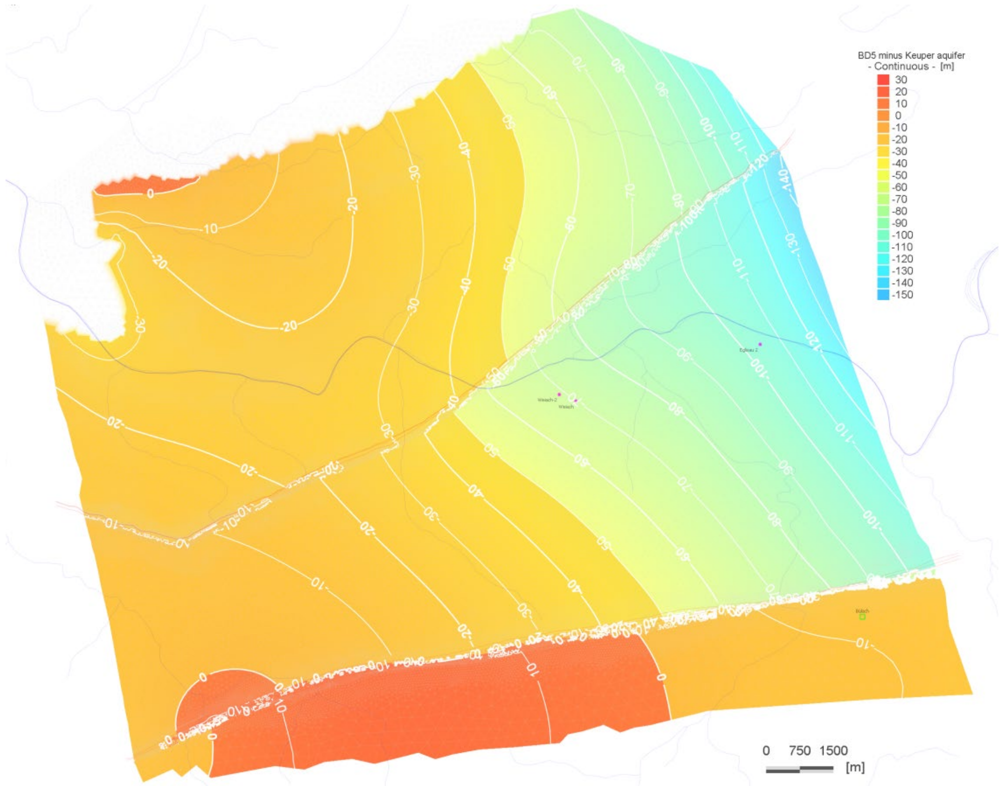


Fig. 4-19: Base Case C2 - Evaluation of Head Differences between the Sissach Member (BD5) and Keuper aquifer.

The reddish coloured regions indicate a positive head difference meaning that vertical groundwater flow is directed downwards. The vertical component of groundwater flow points upwards in regions coloured from orange to light blue.

4.3.2 Recharge and Discharge Paths

Forward and backward particle tracking was also performed for Base Case C2 using the starting points shown in Fig. 4-9.

Fig. 4-20 shows calculated discharge paths (forward tracking) starting from the Malm aquifer as well as recharge paths obtained by backward tracking. Comparable to Base Case C1, the resulting path lines show a recharge from the S through the Molasse (which is in direct contact with the Malm aquifer) into the Malm aquifer. Backward path lines start in the south of the model domain (along the southern limb of the Lägern, see Gmünder et al. 2013b), flow through the conductive Molasse and then into the Malm aquifer (as the BIH does not extend to the surface, flow across the fault in the Molasse is possible). Other recharge paths also originate along the eastern and western boundary. Forward path lines show discharge close to the Siglistorf Anticline along the Rhine valley and at the western boundary.

The forward path lines starting in the Muschelkalk aquifer (Fig. 4-21) show that groundwater basically flows from the north-east to the west in the aquifer. No discharge to the surface is expected because of overlying aquitards. Interestingly, some of the path lines at the western margin show that groundwater flows in the Anhydritgruppe below the Siglistorf Anticline, which was implemented ending just below the Muschelkalk. The backward tracks show recharge paths originating from the lateral boundaries only. Clearly, the region south of the (sealing) BIH fault is blocked off the siting region.

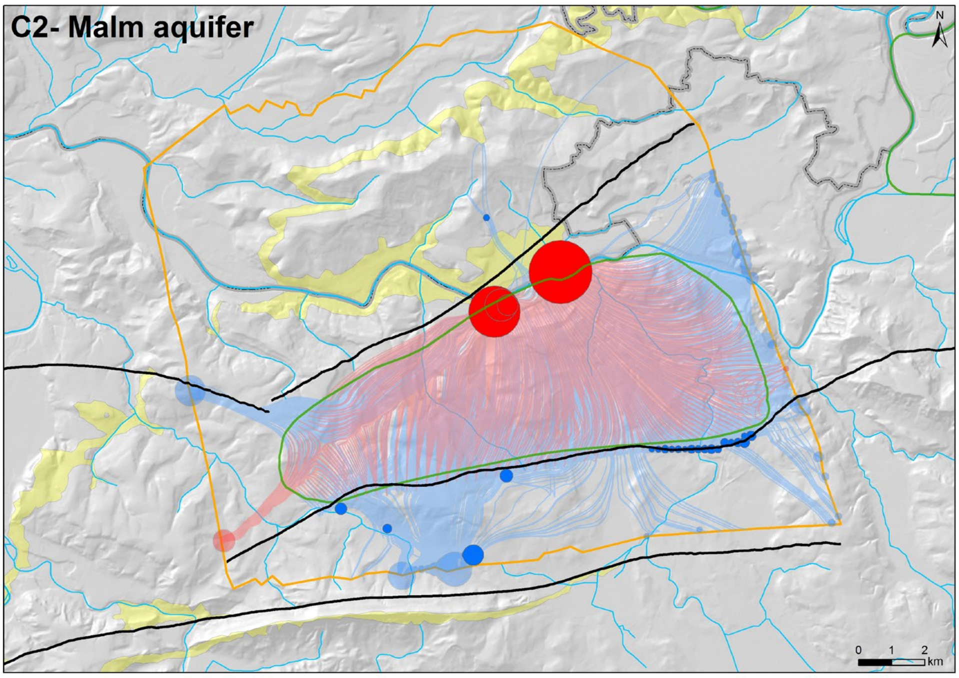


Fig. 4-20: Base Case C2 - Calculated Path Lines Starting from the Malm aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

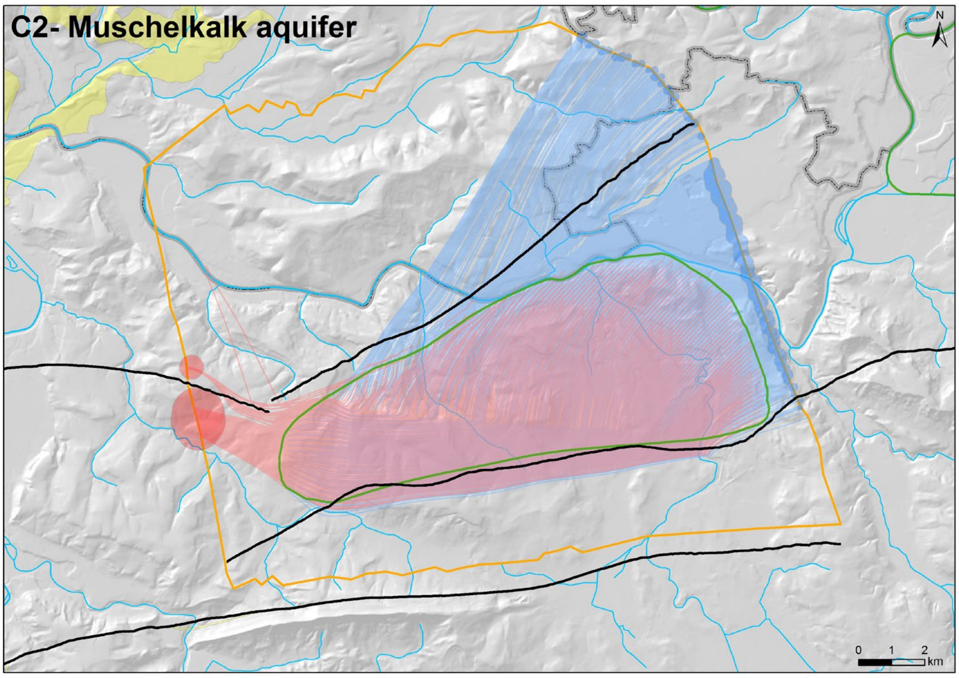


Fig. 4-21: Base Case C2 - Calculated Path Lines Starting from the Muschelkalk aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model.)

4.3.3 Sensitivity Runs

The sensitivity runs performed based on Base Case C2 refer to hypotheses where the two layers BD5 (Sissach Member) and Arietenkalk (see Chapter 3.3) located above and below the Opalinus Clay, respectively, are considered to be more conductive (i.e. water conducting layers) than in the Base Case C2.

In Case **C2-BD5**, the conductivity of BD5 was increased by a factor of 2 (see Table 4-1). The computed head differences in this layer, compared to Base Case C2, are shown in Fig. 4-22. In general, the head differences in most part of the model domain, especially within the siting region, are smaller than 5 m and hence are negligible. A slight increase of hydraulic heads is computed in the centre of the model below the Rhine valley at the northern side of Siglistorf Anticline. The contour of the head differences shows obvious discontinuities and indicates the sealing of the Siglistorf Anticline and BIH Lineament. Maximum differences occur along parts of the western and eastern border because of the different head values given by the hydrogeological regional model for the boundary conditions specified there. The region above the siting region or other layers is almost not affected so that vertical flux through the host rock does not change.

In Case **C2-AKA** (Fig. 4-23)**,** the conductivity of the Arietenkalk was increased by 4 orders of magnitude, i.e. from 1×10^{-12} m/s to 1×10^{-8} m/s (Table 4-1). Due to the increased conductivity, the Arietenkalk has a higher transmissivity. Consequently, higher hydraulic heads (up to 25 m) occur below the siting region (in the Arietenkalk) and to the north of the Siglistorf Anticline causing the vertical flux through the host rock in these areas to increase by about 50% compared to the Base Case.

Because of the different head values defined by the hydrogeological regional model, lower hydraulic heads (up to -20 m) in the north-eastern border area occur.

Sensitivity Case **C2-BD5-AKA** represents the combination of sensitivity runs **C2-BD5** and **C2-AKA** (Table 4-1), computed head differences in BD5 are almost the same as in Case **C2-BD5** (Fig.4-22). Higher hydraulic heads (~25 m) occur below the siting region (Arietenkalk and Keuper aquifer) causing the vertical flux upwards through the host rock being slightly increased (Fig. 4-23). The computed heads in BD5 and Arietenkalk of Case **C2-BD5-AKA** compared to the heads of the Base Case C2 are shown in Fig. 4-24 and Fig. 4-25, respectively. As in the single-layer sensitivity runs, due to the higher hydraulic heads the vertical flux upwards through the host rock increases by about 50%.

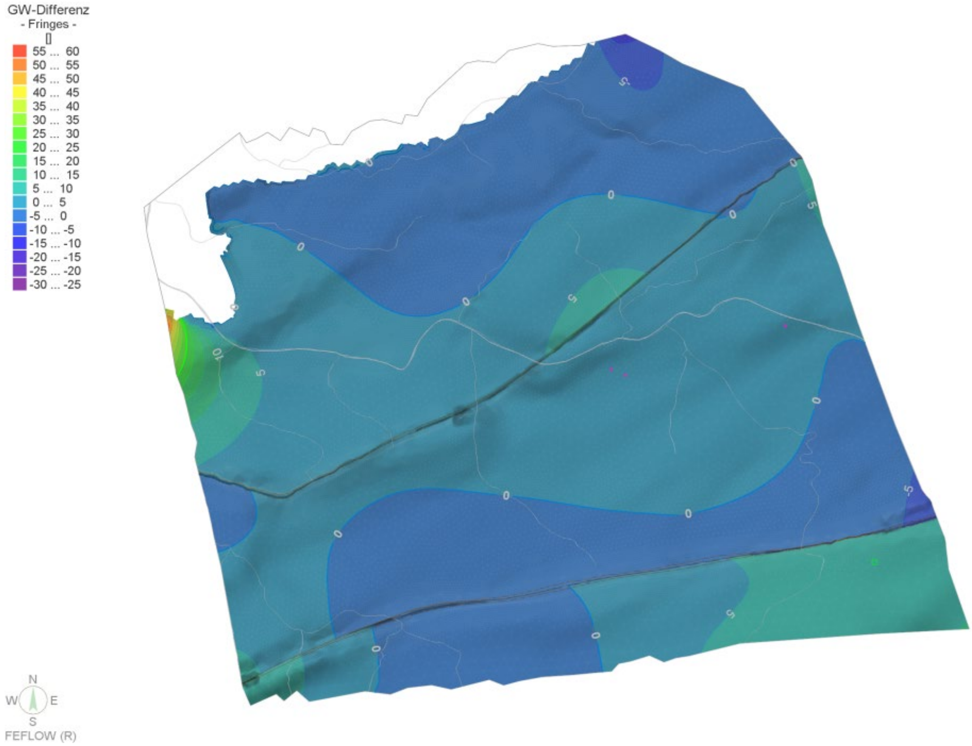


Fig. 4-22: Sensitivity Case C2-BD5 - Head Differences in the Sissach Member (BD5) compared to Base Case C2.

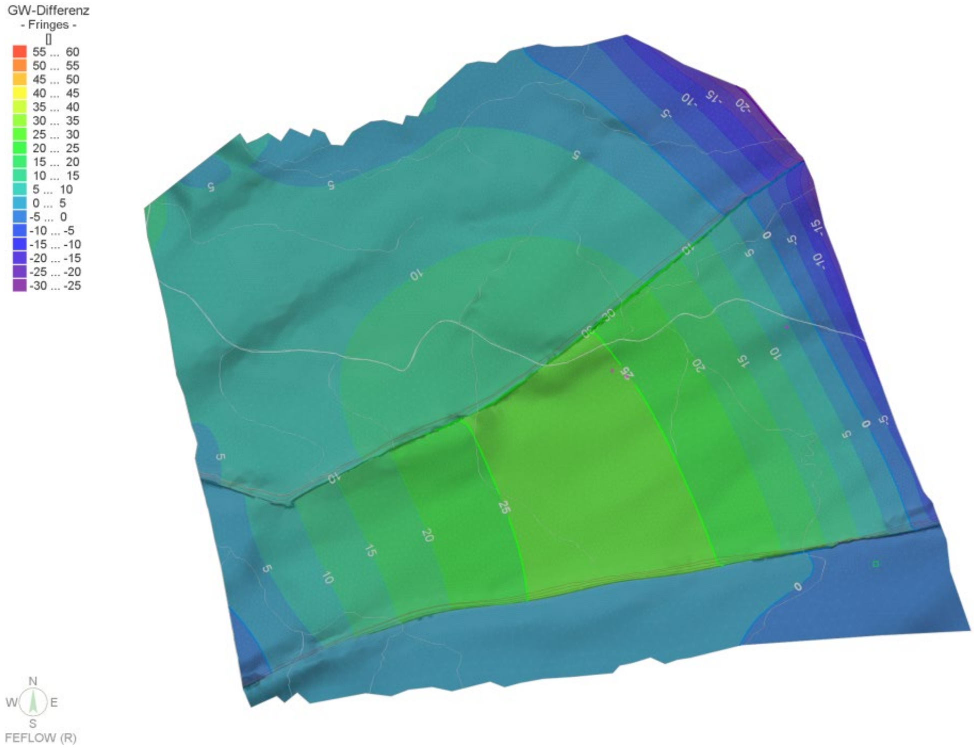


Fig. 4-23: Sensitivity Case C2-AKA - Head Differences in the Arietenkalk compared to Base Case C2.

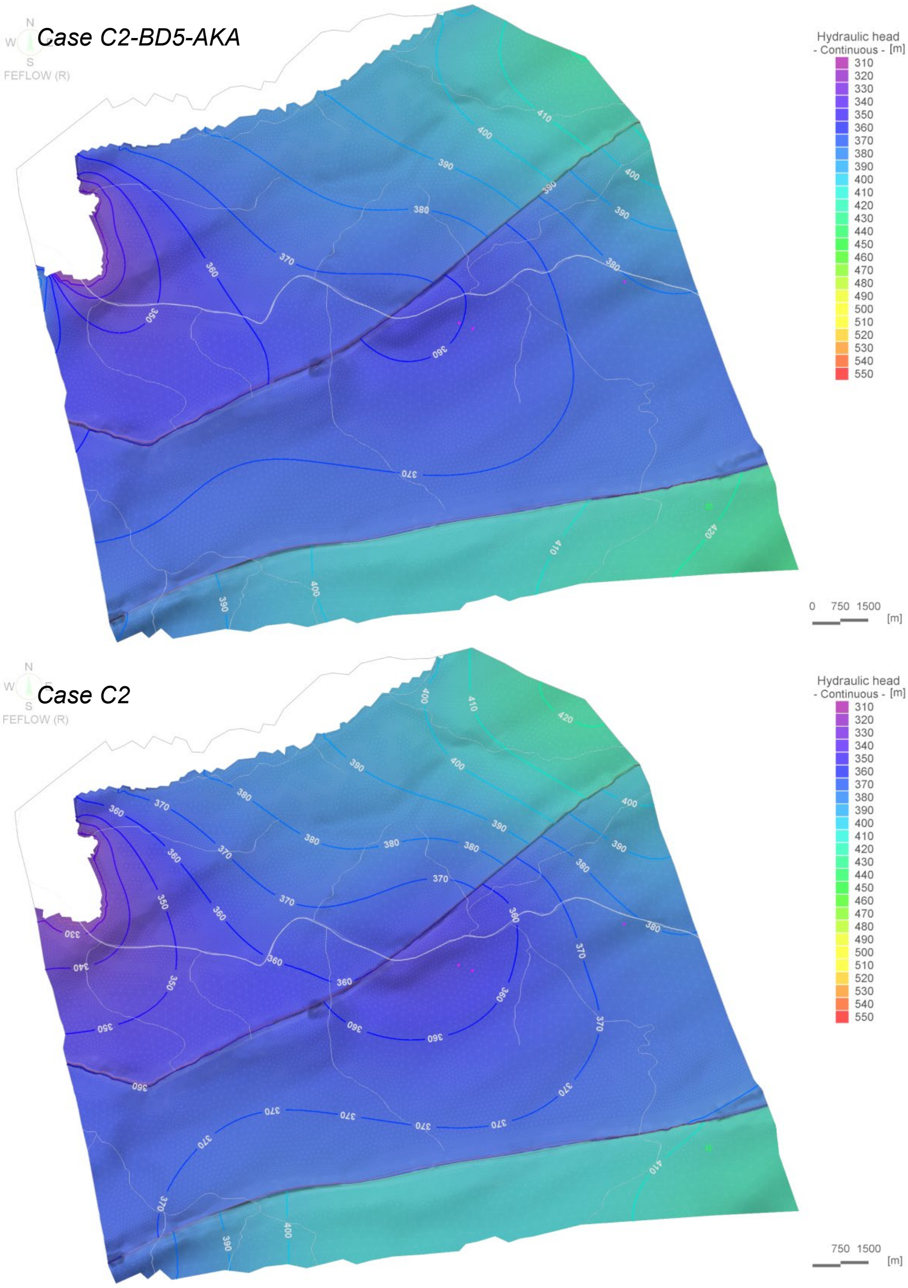


Fig. 4-24: Sensitivity Case C2-BD5-AKA - Head in BD5 compared to Base Case C2.

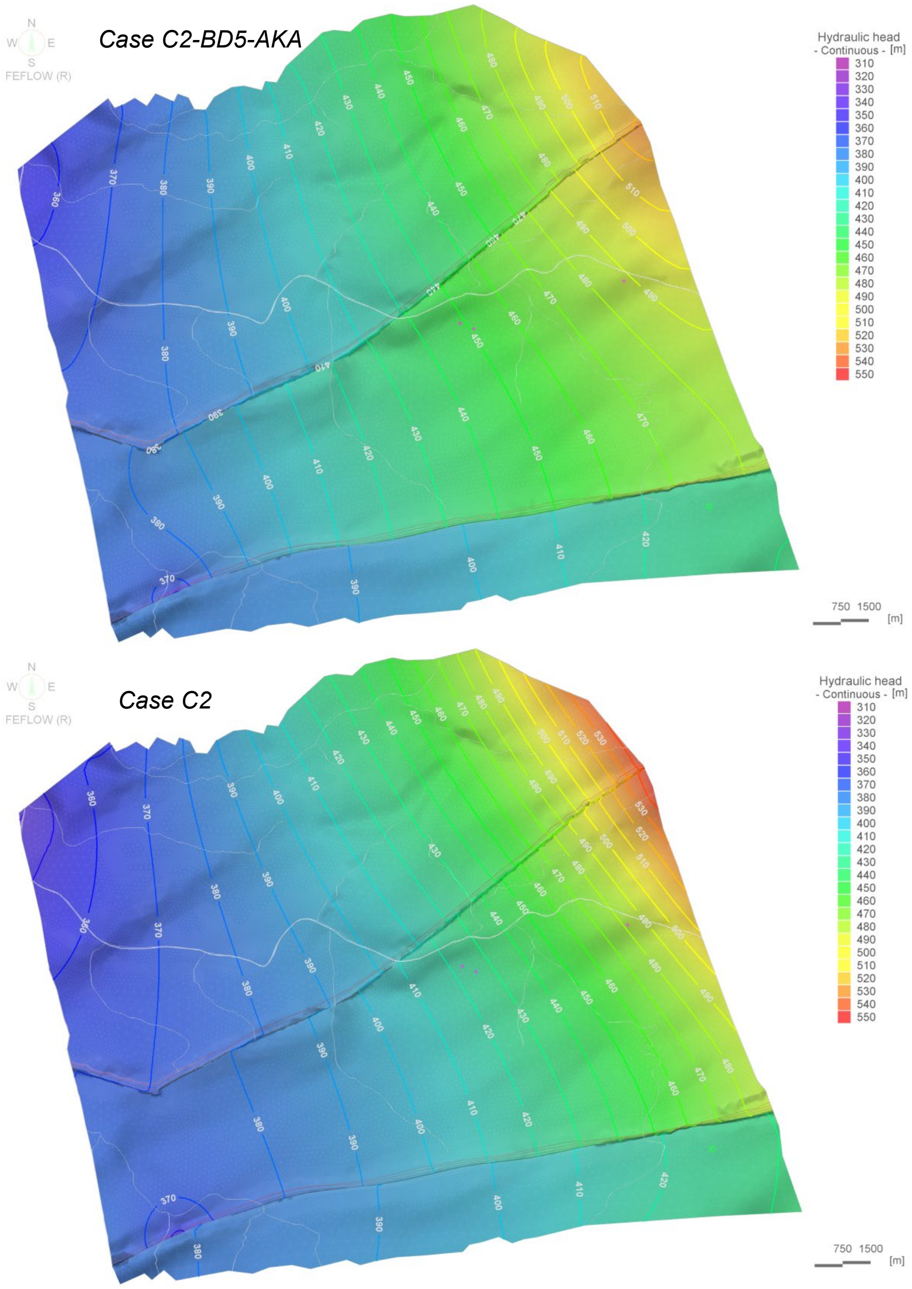


Fig. 4-25: Sensitivity Case C2-BD5-AKA - Head in the Arietenkalk compared to Base Case C2.

4.4 Base Case C3 ("Connecting Fault")

4.4.1 Hydraulic Heads

Run C3 refers to a best guess parameter set and boundary conditions described in Chapter 3.3 and 3.4 under the hypothesis of "connecting faults", meaning that groundwater flow across the faults is disabled. However, because flow along the faults (vertical and lateral) is possible, water exchange between the layers of the multi aquifer system is possible. The computed flow fields are shown in Fig. 4-26 and 4.-27. Vertical sections through flow system are shown in Fig. 4-28.

Unlike the other Base Cases C1 and C2, this case shows no more independent flow systems above and below the low conductive Opalinus Clay which is caused by vertical flow along the faults.

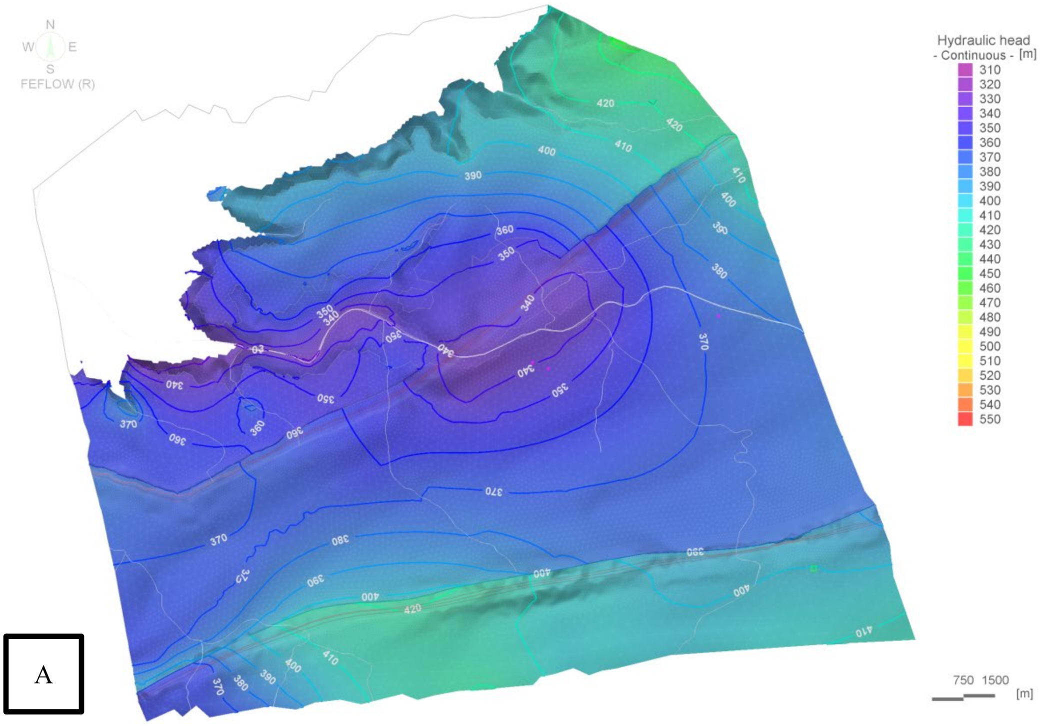
Simulated hydraulic heads in the ***Malm aquifer*** vary between 330 and 440 masl (Fig. 4-26a). Though the head distribution is still mainly influenced by the topography, a significant impact from the sealing faults is visible because horizontal water exchange is suppressed. Flow north of the BIH is directed towards the Rhine valley. South of the BIH, highest head values occur along the BIH, therefore flow is directed away from this area of high heads (towards the E and W).

The aquifer related to the BD2 (***Hauptrogenstein***) covers the model domain only to a limited extent (Fig. 4-26b). Here, the main flow direction is from the outcrops in NE towards the Rhine valley with hydraulic heads between 390 and 330 masl. Compared to the other Base Cases some inflow from the Keuper aquifer is observed at the SW-corner of the BIH.

The BD5 (***Sissach Member***) is modelled as a locally transmissive unit with an average thickness of 10 m directly on top of the Opalinus Clay and is present almost throughout the entire model domain. Simulated hydraulic heads vary between 430 und 320 masl (Fig. 4-26c). The flow pattern is similar to that of the Malm aquifer where water flows from the north-eastern model boundary towards the Rhine valley. Along the BIH, a significant head discontinuity has evolved because water cannot flow across the fault. Comparable to the Malm aquifer, high hydraulic heads were simulated along the BIH and hence flow is directed away from this area towards the E and W.

The ***Keuper aquifer*** is modelled as an aquifer system of 10 m thickness located below the Opalinus Clay and its confining units (Fig. 4-27a). Since flow along the fault (but not across) is possible in this Base Case, the artesian conditions created by high heads along the NE-boundary relieve through the Siglistorf Anticline along the Rhine valley. South of the BIH, head values of 400 masl were simulated. Flow here is mainly directed towards the E and W of the model but gradients in most of the model domain here are very small.

The ***Muschelkalk aquifer*** is a significant regional aquifer located below the Keuper aquifer (Fig. 4-27b). Between the two aquifers the low conductive Gipskeuper acts as an aquitard. The simulated hydraulic heads in the Muschelkalk aquifer vary between 410 und 350 masl. Similar to the Keuper aquifer, north of the BIH recharge into the model mainly occurs through the NE-boundary. Artesian conditions are relieved through the Siglistorf Anticline or the NW-model boundary. South of the BIH, a relatively homogeneous head distribution has developed leading to a low-gradient flow towards the E and W.



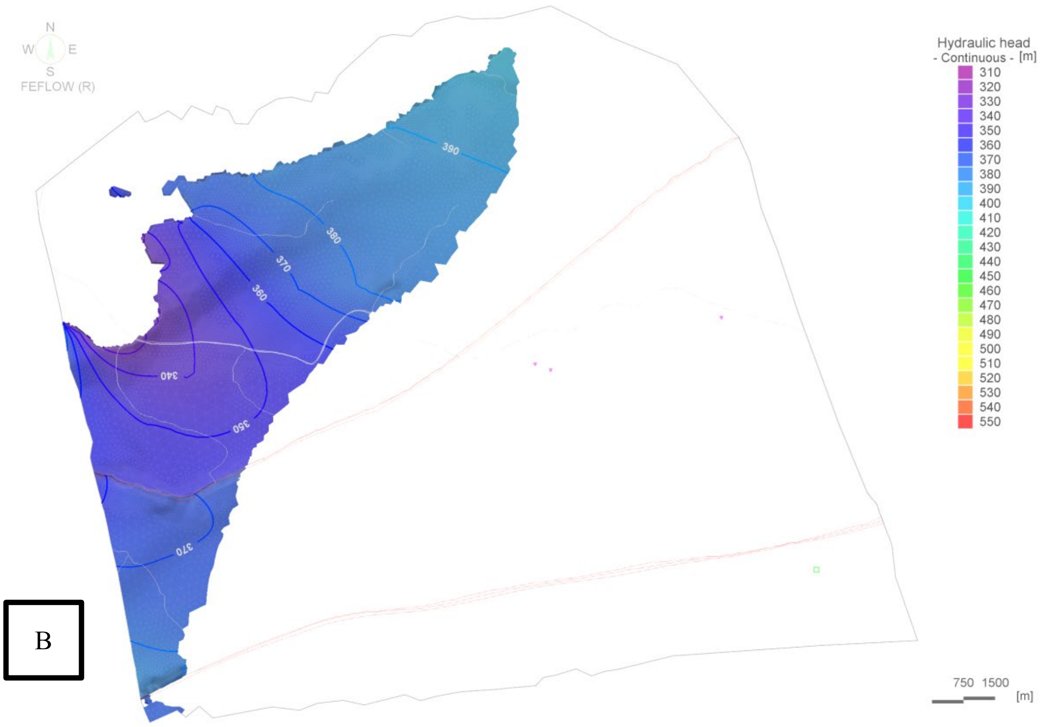


Fig. 4-26: Base Case C3 - Simulated Head Fields along aquifers above Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

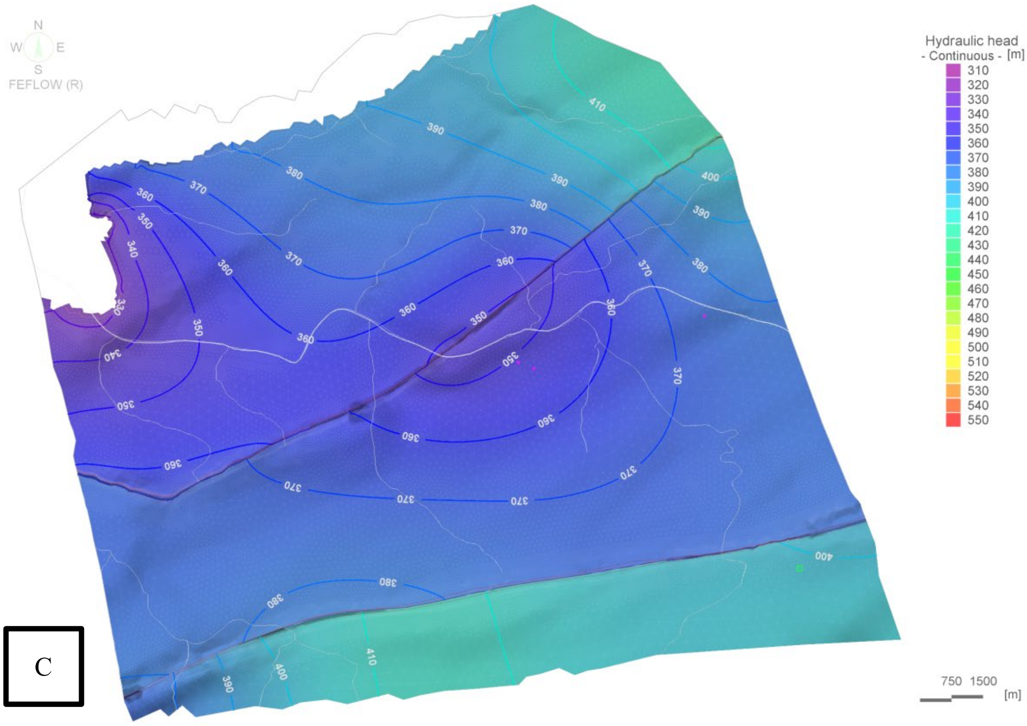


Fig. 4-26: (cont.) Base Case C3 - Simulated Head Fields along aquifers above Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

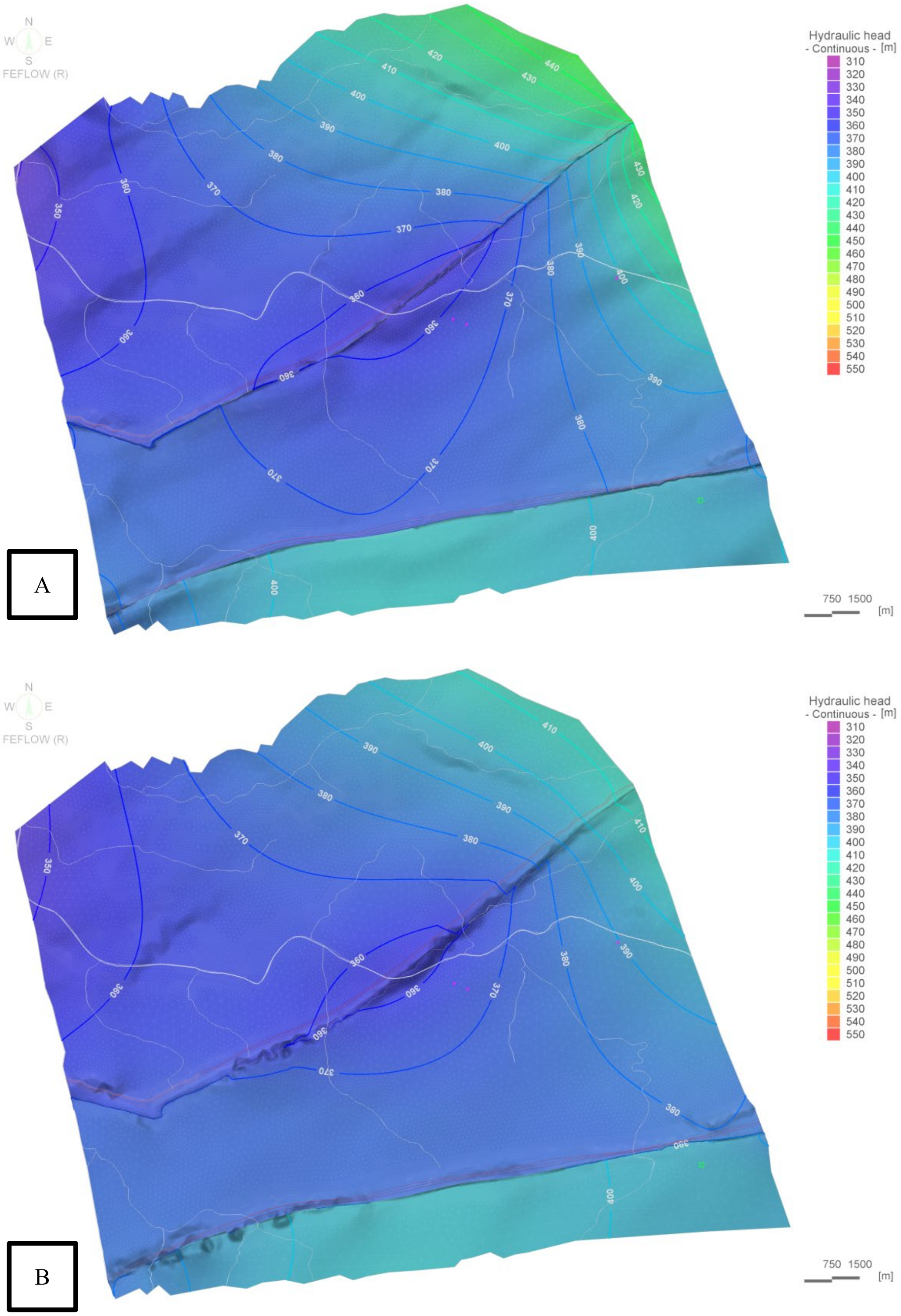
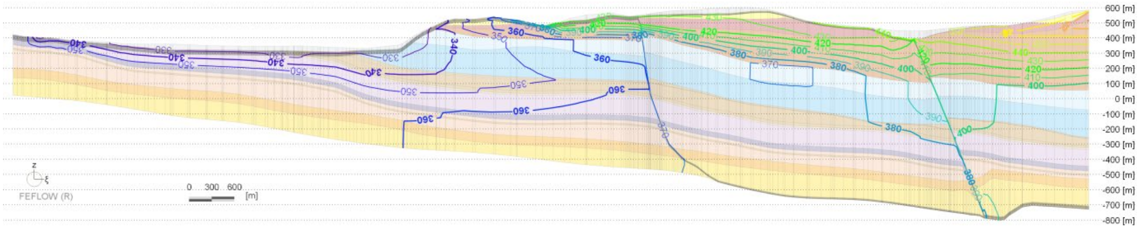
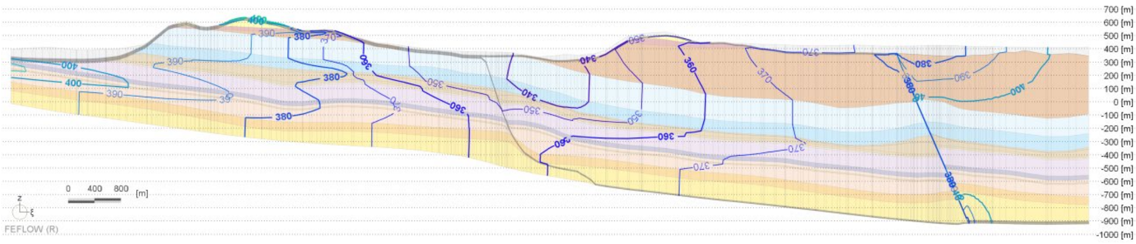


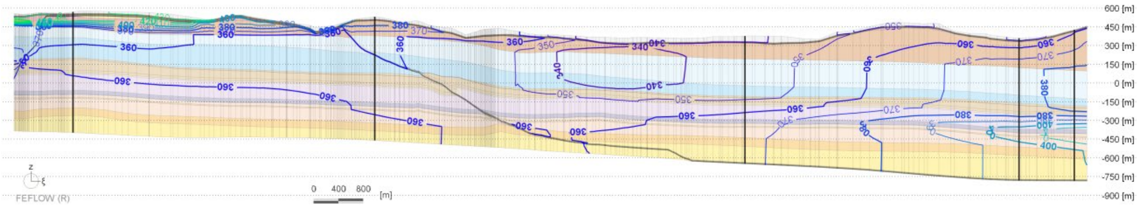
Fig. 4-27: Base Case C3 - Simulated Head Fields along aquifers below the Opalinus Clay. A – Keuper aquifer, B – Muschelkalk aquifer.



a. Section R13 (NS)



b. Section R15 (NS)



c. Section W2 (WE)

Fig. 4-28: Base Case C3 - Simulated Head Fields along Vertical Sections.

(Location see Fig. 4-3, 2x vertical exaggeration).

In this case, the upper and lower groundwater flow system do not develop separately because the low conductive Opalinus Clay is by-passed by the highly conductive outer layers of the fault systems. In order to assess vertical flow through the host rocks, head differences of the BD5 above minus the Keuper aquifer below the Opalinus Clay were evaluated as shown in Fig. 4-29. In contrast to the other Base Cases, vertical head gradients largely disappear within the siting region - a consequence of the relief of the former artesian conditions (Keuper, Muschelkalk) by vertical flow along the "connecting" faults.

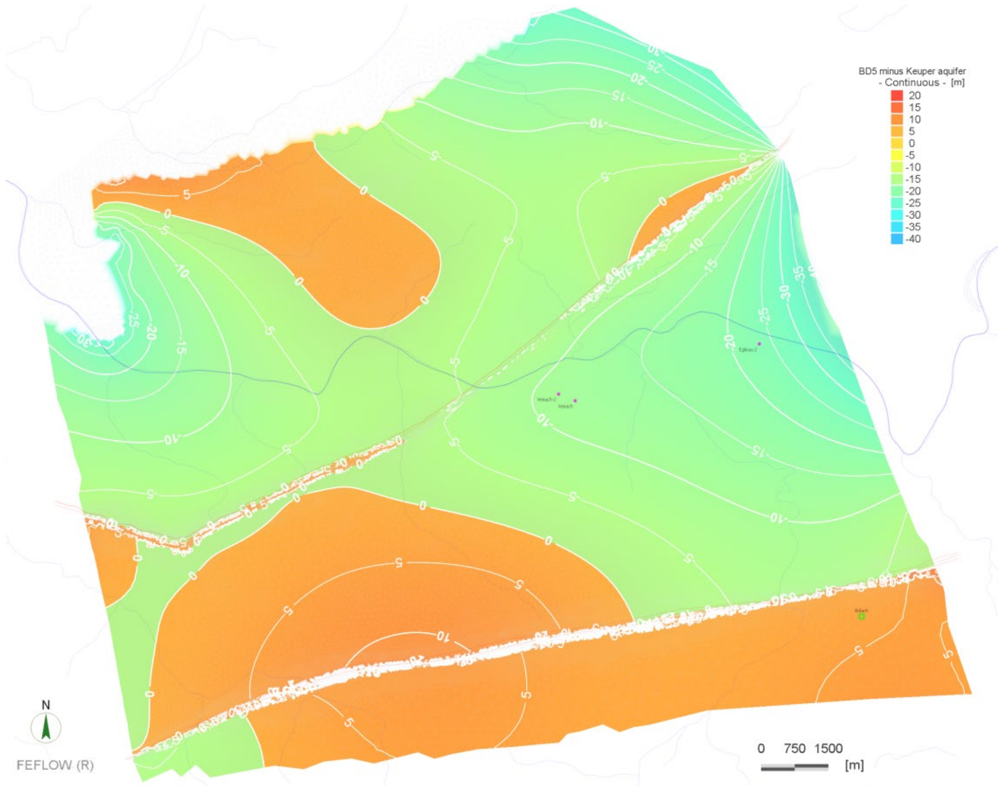


Fig. 4-29: Base Case C3 - Evaluation of Head Differences between the Sissach Member (BD5) and Keuper aquifer.

The orange coloured regions indicate a positive head difference meaning that vertical groundwater flow is directed downwards. The vertical component of groundwater flow points upwards in regions coloured light green to blue.

4.4.2 Recharge and Discharge Paths

Forward and backward particle tracking also was performed for Base Case C3 using the starting points shown in Fig. 4-9.

Fig. 4-30 shows calculated discharge paths (forward tracking) starting from the Malm aquifer as well as recharge paths obtained by backward tracking are shown. The resulting path lines show that the discharge area of the Malm aquifer is located in the Rhine valley. Another discharge area of minor importance seems to be situated to WSW of the model domain. Comparable to Base Case 2, recharge in the south is from the northern limb of the Lägern (see Gmünder et al. 2013b) through the Molasse and down along the BIH. Again, there seem to be additional recharge areas outside of the model domain in the W and towards the E.

The forward path lines starting in the Muschelkalk aquifer show that some of the path lines reach the top of the Molasse in the Rhine valley close to the Siglistorf Anticline which is considerably different from the Base Cases described earlier. Recharge paths of the eastern part below the siting region show that groundwater mainly comes from the eastern lateral boundary while groundwater in the western, higher conductive part below the siting region originates from south of the BIH, flowing through the Molasse and down along the conductive outer layer of the BIH (Fig. 4-31). Also, some of the forward path lines close to the western boundary seem to "jump" across the sealing Siglistorf Anticline by flowing down (and then up again) the outer conductive layers of the fault.

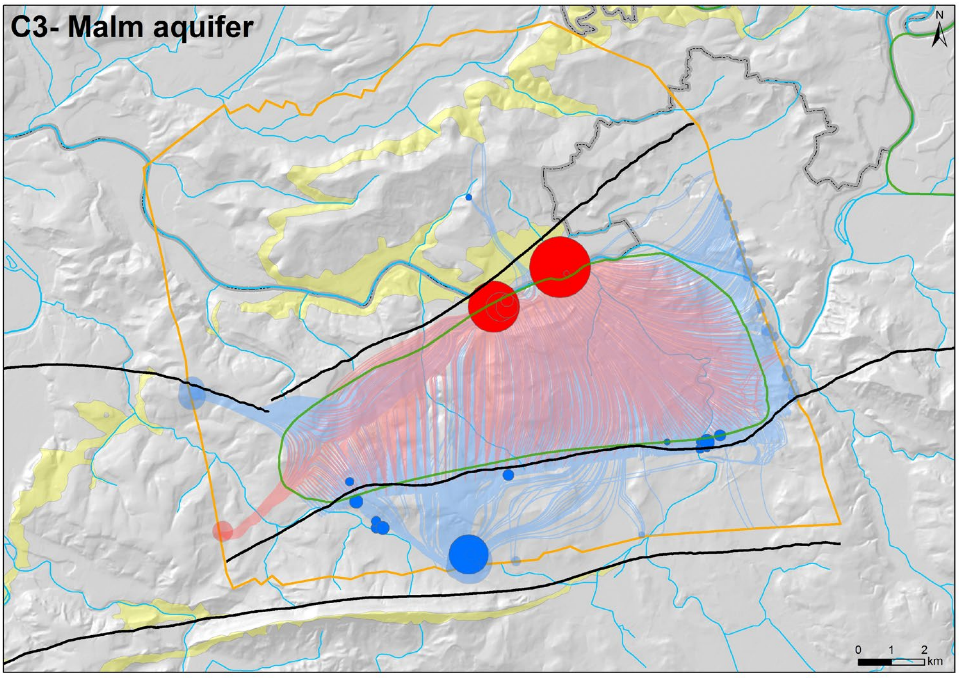


Fig. 4-30: Base Case C3 - Calculated Path lines Starting from the Malm aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

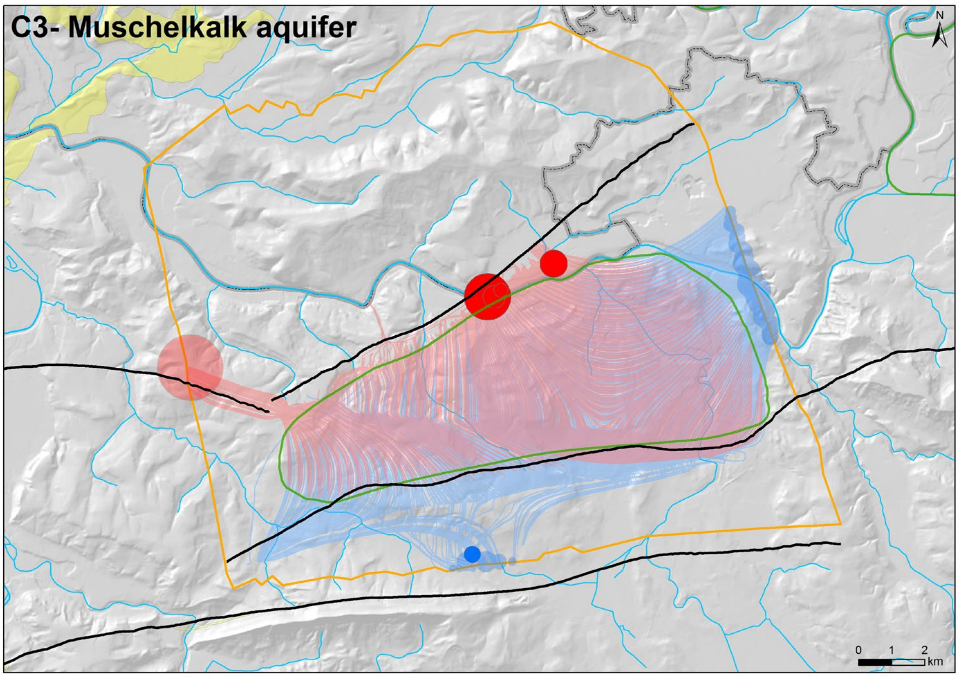


Fig. 4-31: Base Case C3 - Calculated Path Lines Starting from the Muschelkalk aquifer. (Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

4.4.3 Sensitivity Runs

The sensitivity runs performed for Base Case C3 refer to the hypotheses where the two layers BD5 (Sissach Member) and Arietenkalk (see Chapter 3.3) located above and below the Opalinus Clay are considered to be more conductive (i.e. water conducting layers).

In general, head differences compared to Base Case C3 are very low (compare Fig. 4-32, 4-33, 4-34 and 4-35). Due to the significant vertical flow along the faults (here assumed by hypothesis), the impact of the "minor" aquifers has decreased considerably. Because of the different head values given by the hydrogeological regional model for the boundary conditions specified there (see Gmünder et al. 2013b), maximum differences occur along parts of the western and eastern border.

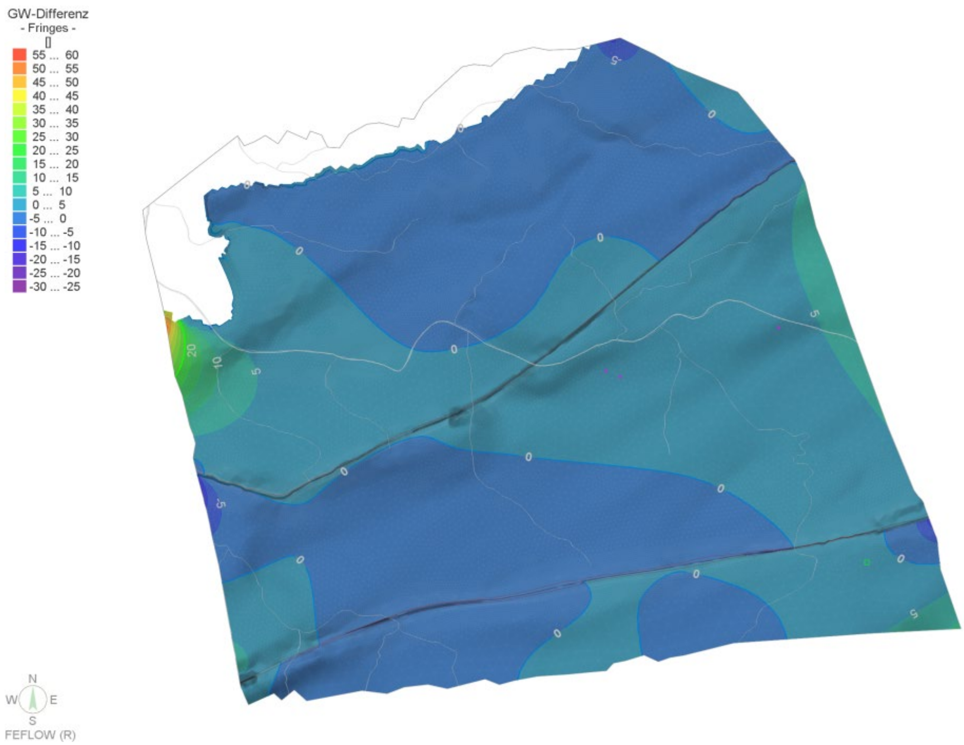


Fig. 4-32: Sensitivity Case C3-BD5 - Head Differences in the Sissach Member (BD5) compared to Base Case C3.

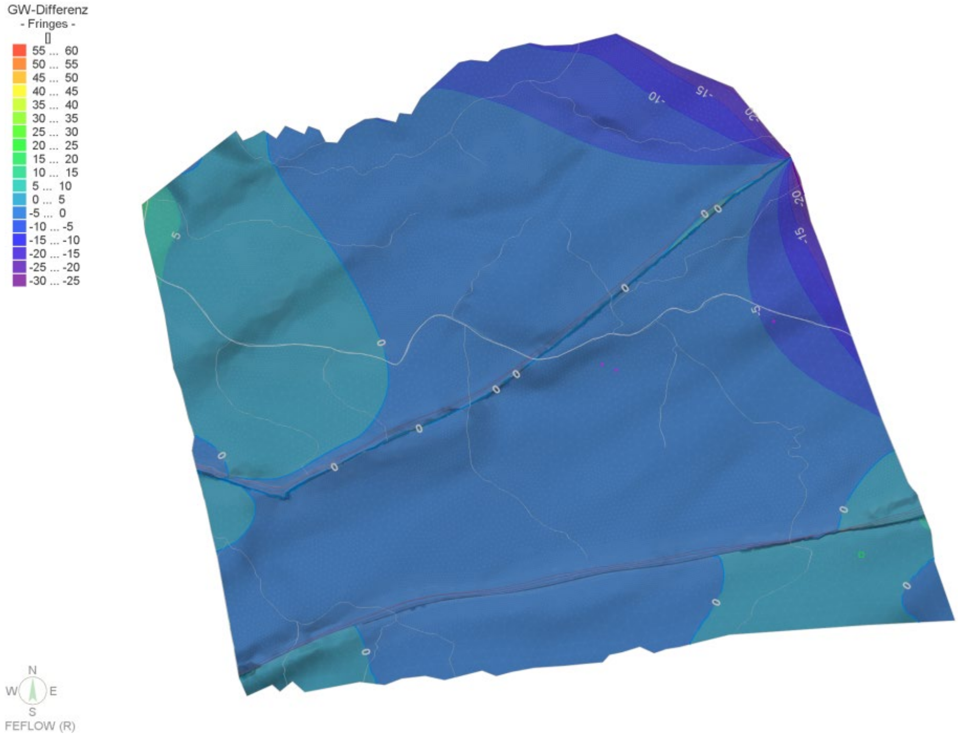


Fig. 4-33: Sensitivity Case C3-AKA - Head Differences in the Arietenkalk compared to Base Case C3.

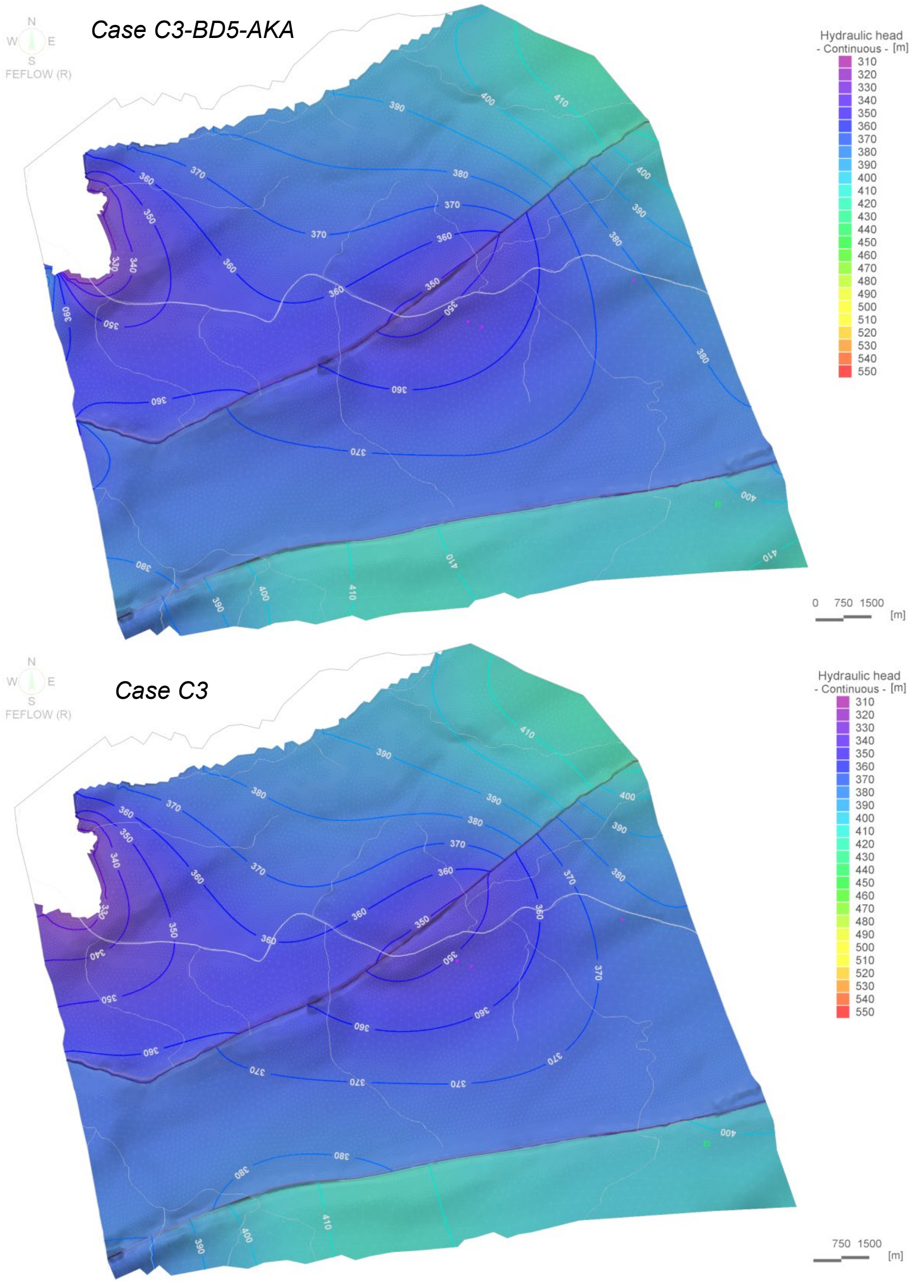


Fig. 4-34: Sensitivity Case C3-BD5-AKA - Head in BD5 compared to Base Case C3.

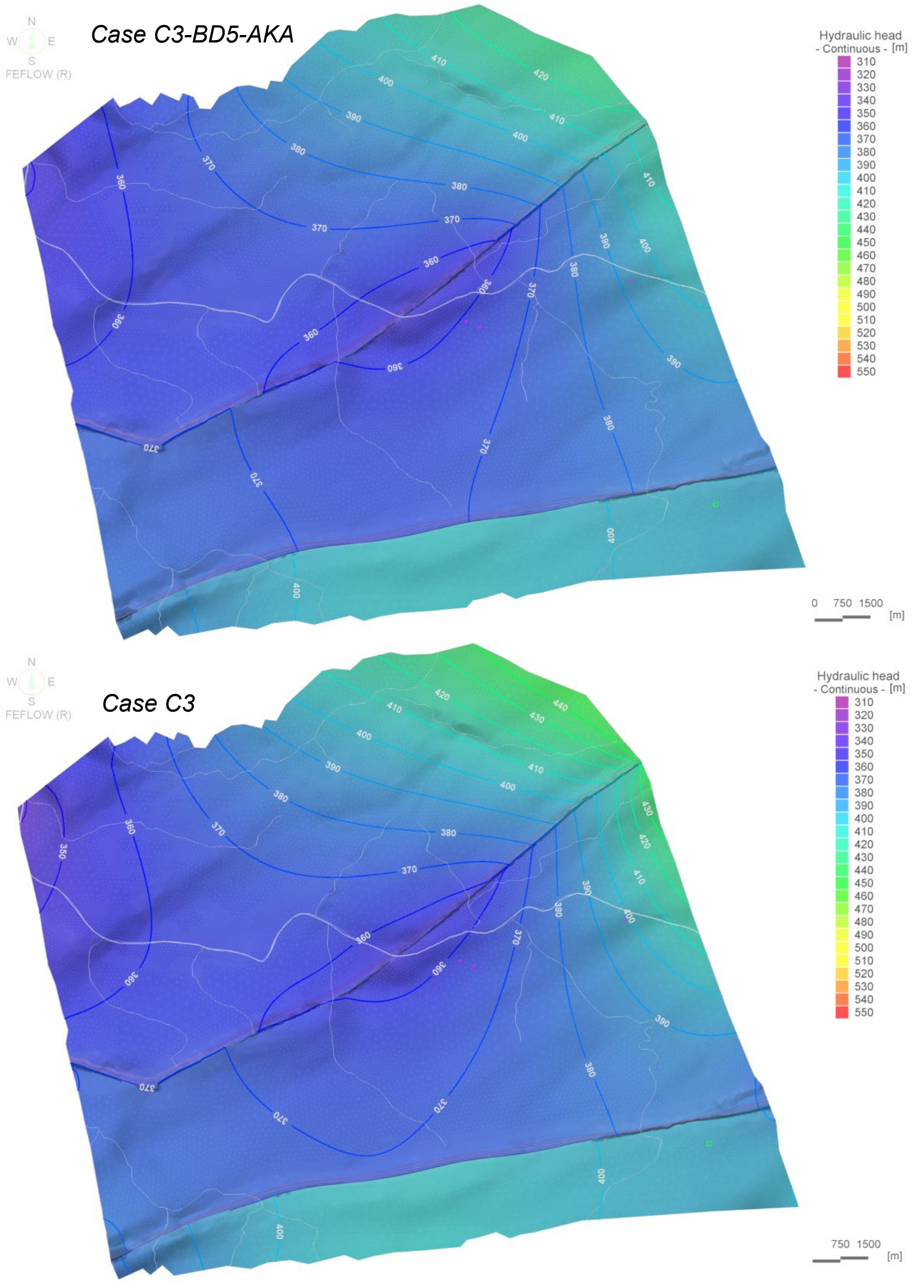


Fig. 4-35: Sensitivity Case C3-BD5-AKA - Head in the Arietenkalk compared to Base Case C3.

4.5 Base Case C3a ("Fully Connecting Fault")

4.5.1 Hydraulic Heads

Run C3a refers to a best guess parameter set and boundary conditions described in Chapter 3.3 and 3.4 under the hypothesis "fully connecting faults", meaning that groundwater flow across and along the faults is possible. Consequently, water exchange across the faults as well as between the layers of the multi aquifer system can evolve. The computed flow fields are shown in Fig. 4-36 and 4-37. Vertical sections through flow system are shown in Fig. 4-38.

Because C3a differs from C3 merely by allowing flow crossing through the fault plane, the flow fields of C3a are comparable to those of C3. However, caused by additional cross flow through the fault plane, groundwater contours of all the aquifers become continuous and smooth along the faults (comp. Fig. 4-36 and 4-37). Since the influence of these changes on the general flow field and respective gradients are negligible compared to Base Case C3, no sensitivity cases have been performed for Base Case 3a.

Simulated hydraulic heads in the ***Malm aquifer*** vary between 330 and 440 masl (Fig. 4-36a). The head distribution is still mainly influenced by the topography though offsets of the isolines along the (permeable) faults do exist. Main flow directions are towards the Rhine valley and, south of the BIH, towards the E and W.

The unit BD2 (***Hauptrogenstein***) covers the model domain only to a limited extent (Fig. 4-36b). Here, the main flow direction is from the outcrops in NE towards the Rhine valley with hydraulic heads between 390 and 330 masl.

The BD5 (***Sissach Member***) is modelled as a locally transmissive unit with an average thickness of 10 m directly on top of the Opalinus Clay and is present almost throughout the entire model domain. Simulated hydraulic heads vary between 410 und 330 masl (Fig. 4-36c). The flow pattern is similar to that of the Malm aquifer where water flows from the recharge areas outside of the model domain towards the Rhine valley. Along the BIH, a significant head discontinuity has evolved due to the offset caused by the fault. Flow here is mainly directed E and W.

The ***Keuper aquifer*** is modelled as an aquifer system of 10 m thickness located below the Opalinus Clay and its confining units (Fig. 4-37a). Similar to the Case C3, the artesian conditions created by high heads along the NE-boundary relieve through the Siglistorf Anticline into parts of the Rhine valley. Consequently, flow is directed towards this area of relieve and/or towards the NW model boundary.

The ***Muschelkalk aquifer*** is a significant regional aquifer located below the Keuper aquifer (Fig. 4-37b). Between the two aquifers the lower conductive Gipskeuper acts as an aquitard. The simulated hydraulic heads in the Muschelkalk aquifer vary between 410 und 350 masl. Similar to the Keuper aquifer, recharge occurs at the NE model boundary and leaves vertically through the Siglistorf Anticline or laterally towards the NW model boundary.

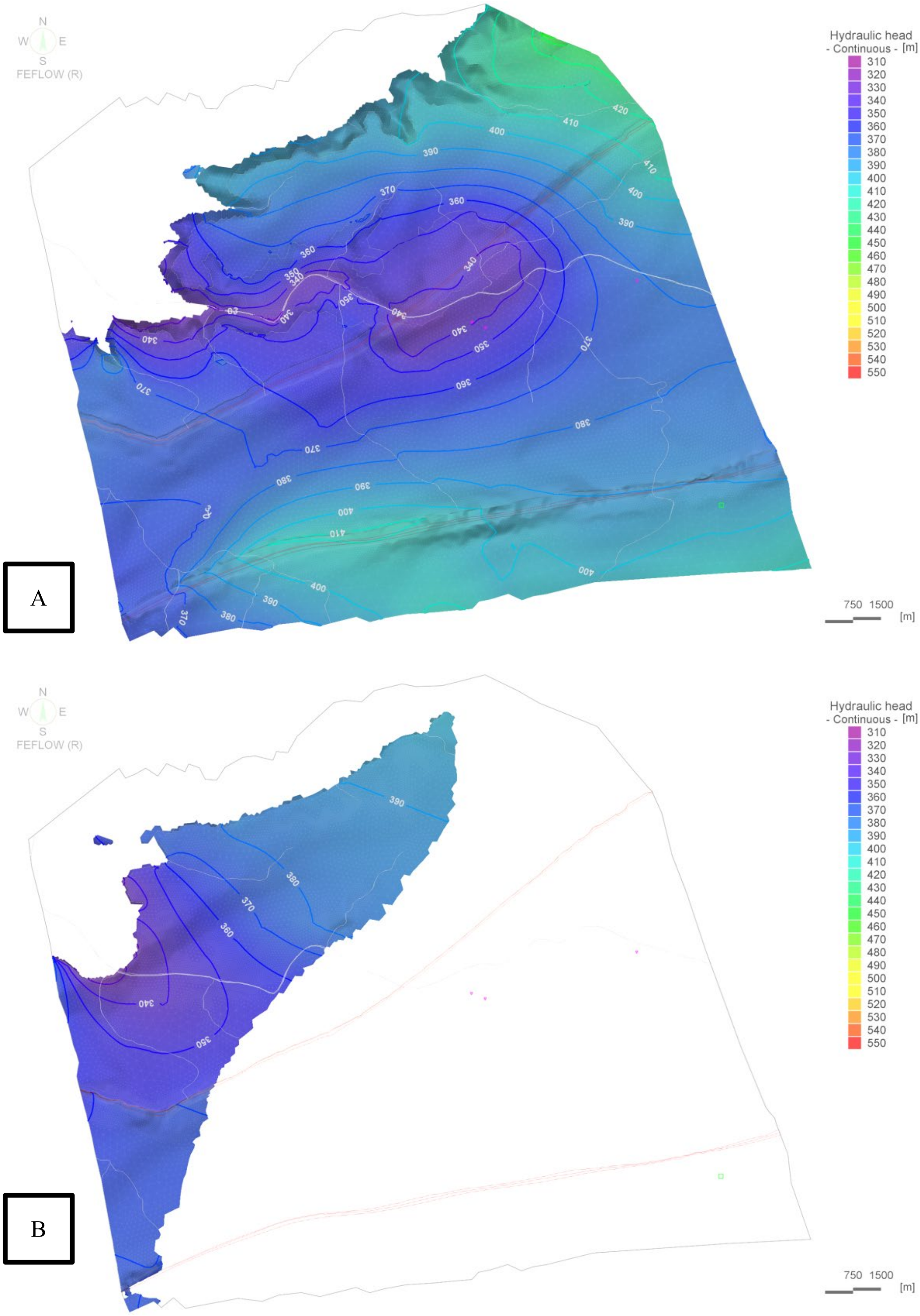


Fig. 4-36: Base Case C3a - Simulated Head Fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

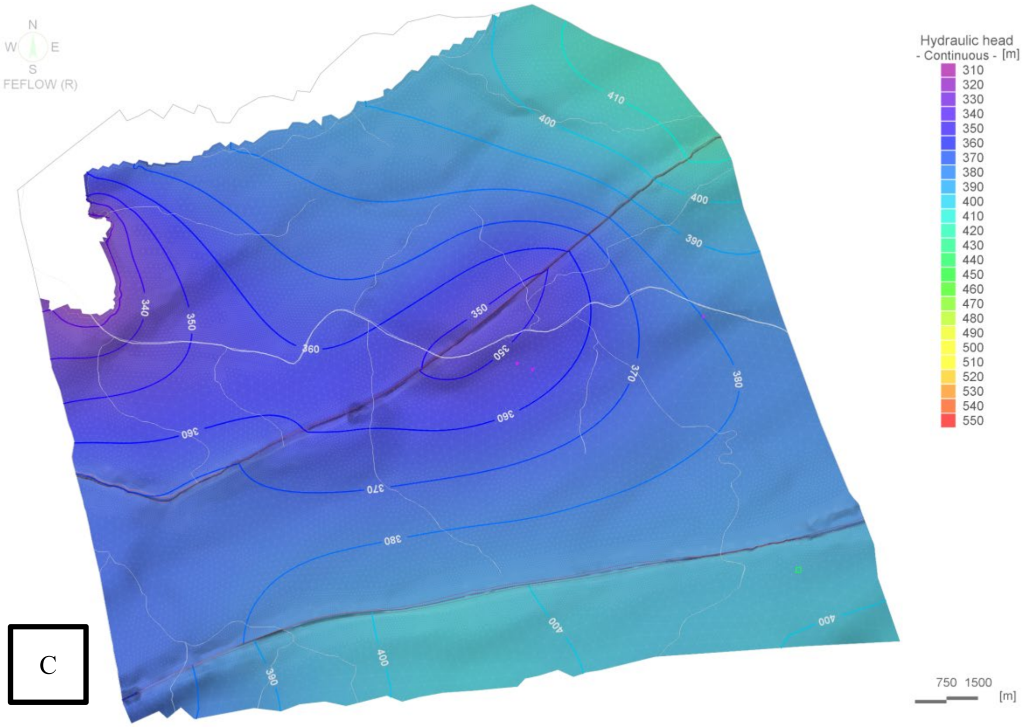


Fig. 4-36: (cont.) Base Case C3a - Simulated Head Fields along aquifers above the Opalinus Clay. A – Malm aquifer, B – Hauptrogenstein (BD2), C – Sissach Member (BD5).

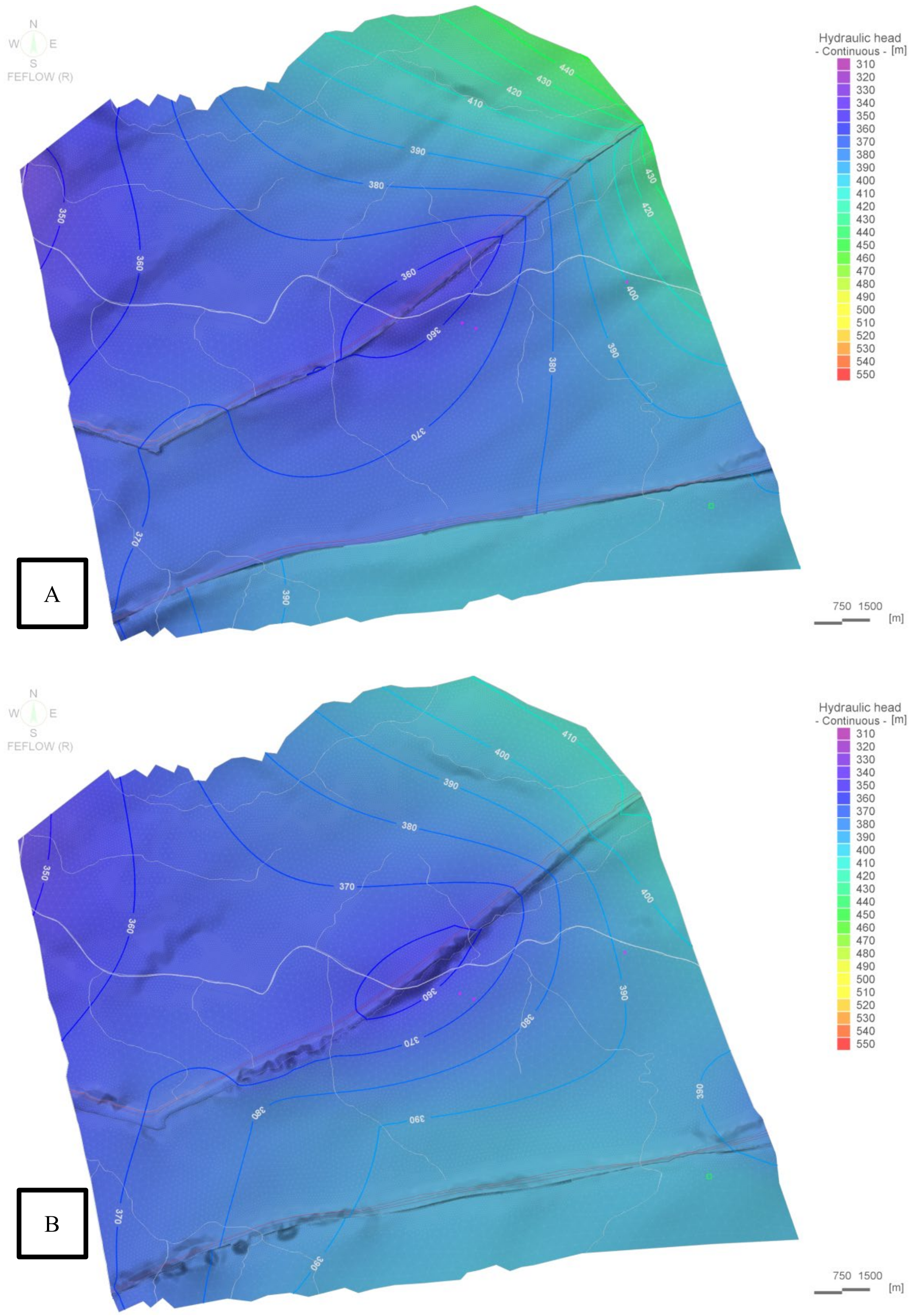
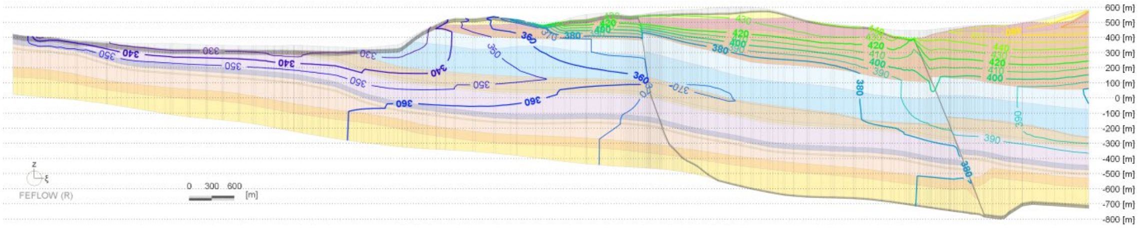
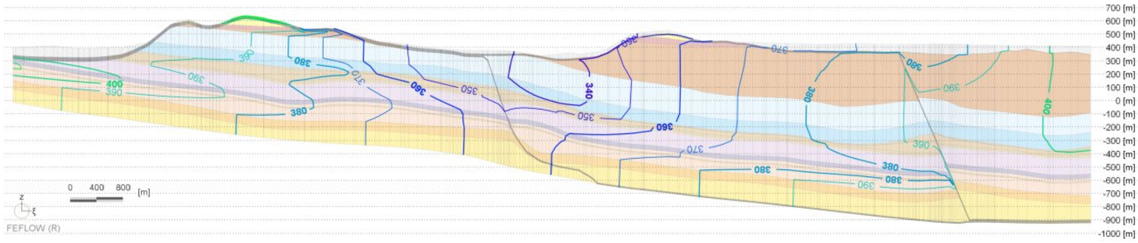


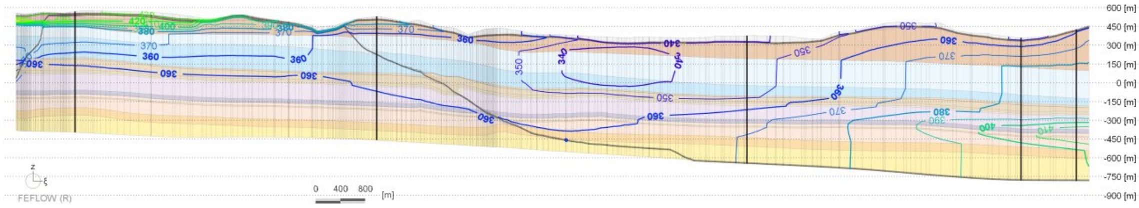
Fig. 4-37: Base Case C3a - Simulated Head Fields along aquifers below the Opalinus Clay. A – Keuper aquifer, B – Muschelkalk aquifer.



a. Section R13 (NS)



b. Section R15 (NS)



c. Section W2 (WE)

Fig. 4-38: Base Case C3a - Simulated Head Fields along Vertical Sections.
(Location see Fig. 4-3, 2x vertical exaggeration).

As mentioned earlier, no completely independent flow field above and below the low conductive Opalinus Clay develops. In order to assess vertical flow through the host rocks, head differences of the BD5 above minus the Keuper aquifer below the Opalinus Clay were evaluated as shown in Fig. 4-39.

The head difference patterns of C3a are comparable to that of C3. Due to additional cross flow through the fault plane, the patterns look more continuous and smooth in the immediate surroundings of the faults when compared to the head difference patterns of C3 (Fig. 4-39 and Fig. 4-29, respectively). The computed head distributions in BD5 and the Keuper aquifer are displayed in Fig. 4-40 and Fig. 4.-41, with comparison to the corresponding head distributions of Base Case C3.

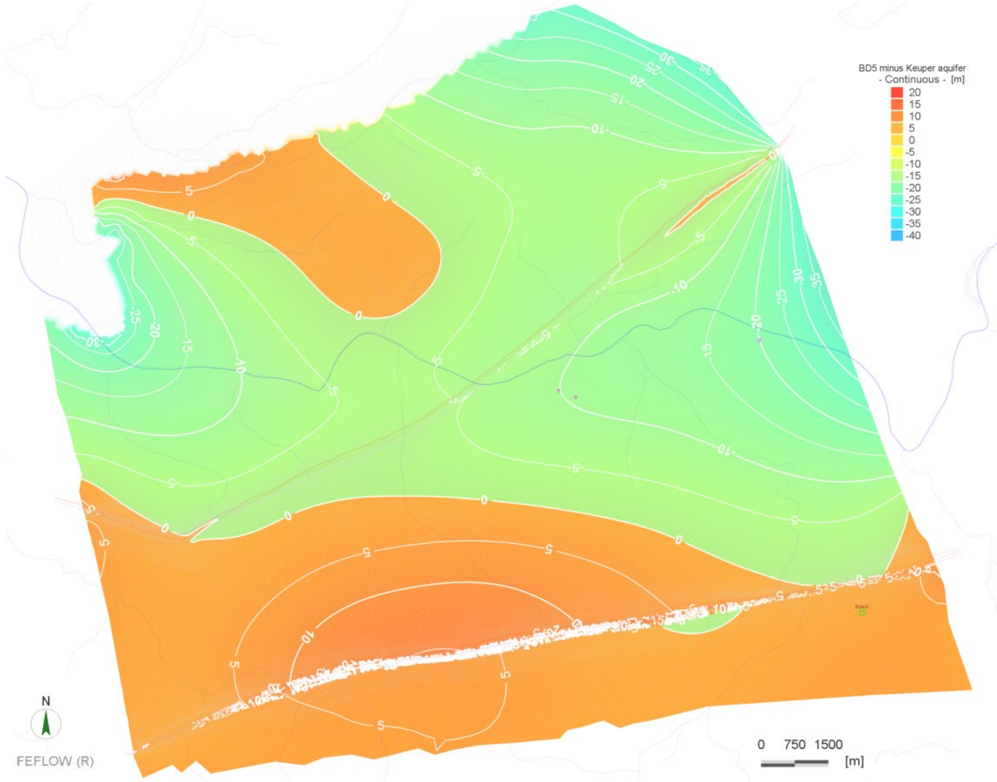


Fig. 4-39: Base Case C3a - Evaluation of Head Differences between the Sissach Member (BD5) and Keuper aquifer.

The orange coloured regions indicate a positive head difference meaning that vertical groundwater flow is directed downwards. The vertical component of groundwater flow points upwards in regions coloured light green.

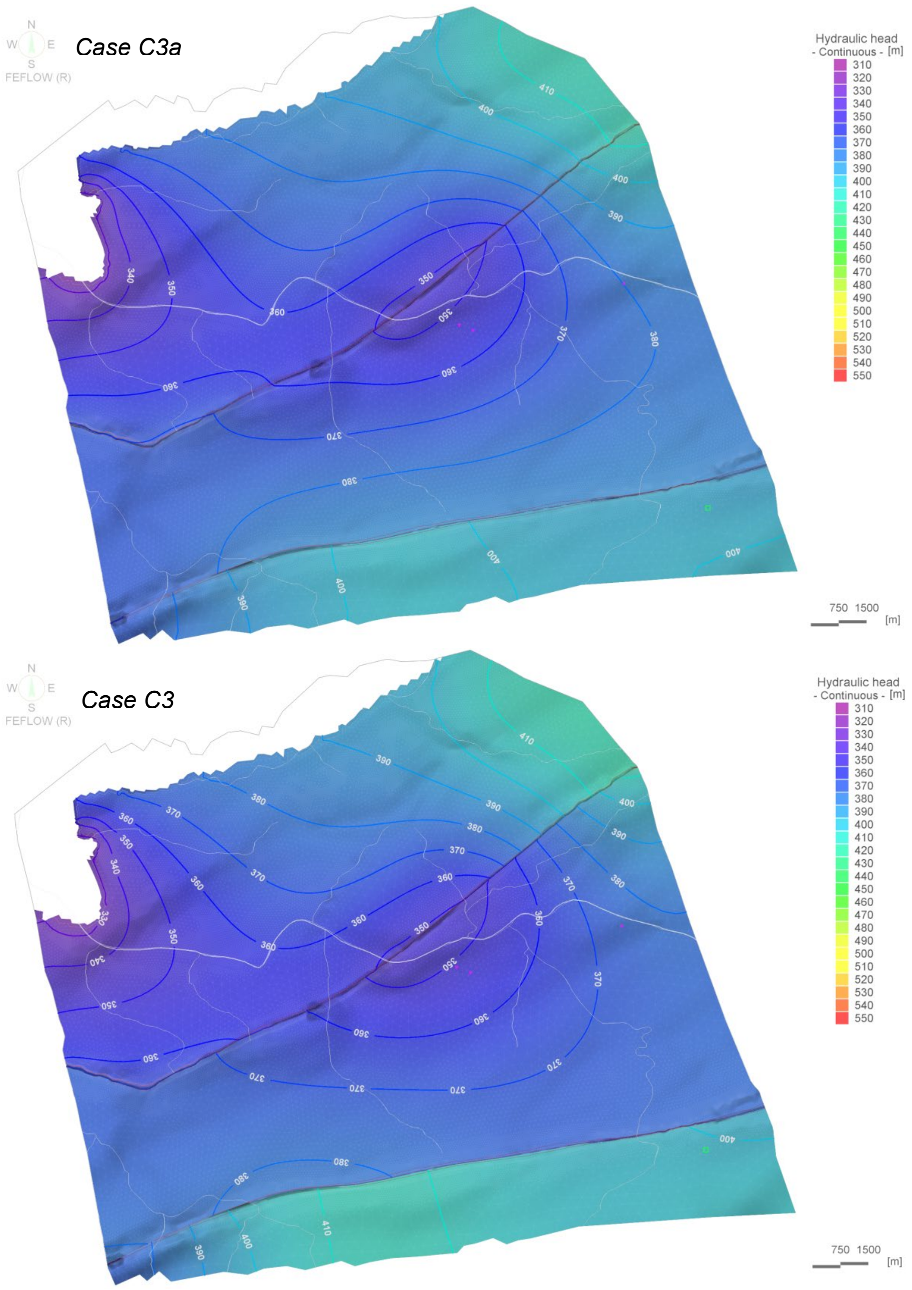


Fig. 4-40: Base Case C3a - Head in BD5 compared to Base Case C3.

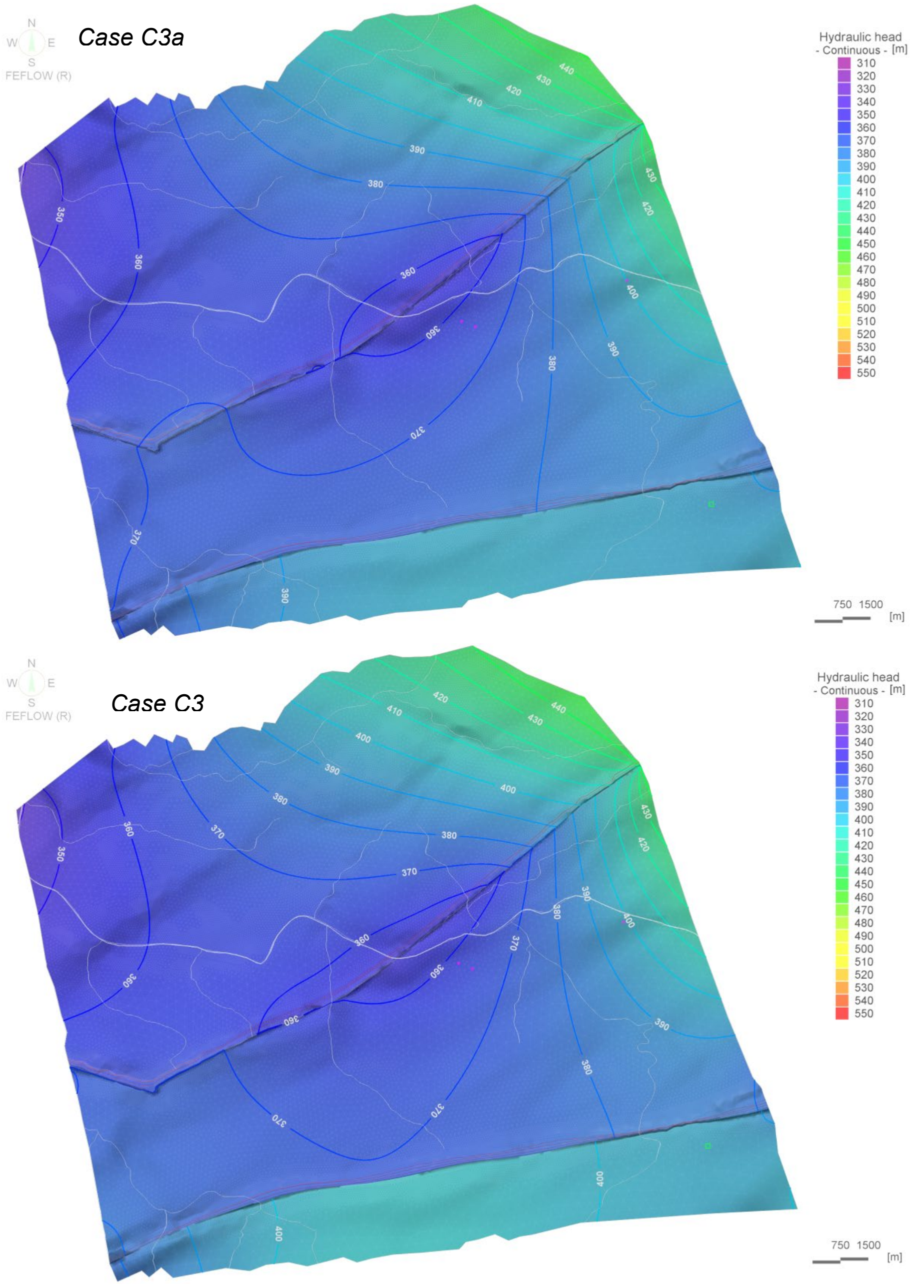


Fig. 4-41: Base Case C3a - Head in the Keuper aquifer compared to Base Case C3.

4.5.2 Recharge and Discharge Paths

In order to assess discharge paths of groundwater from the main aquifers Malm and Muschelkalk, particle tracking has been carried out. The particles were started from given points in the aquifers considered. While tracking along the direction of flow (i.e. forward tracking) the paths run to discharge points at a model boundary. Tracking in the opposite direction (i.e. backward tracking) the particles follow the recharge paths until a model boundary is reached indicating where groundwater originates from. Fig. 4-9 shows the used starting points in the area of the siting region Nördlich Lägern.

Fig. 4-42 shows calculated discharge paths (forward tracking) starting from the Malm aquifer as well as recharge paths obtained by backward tracking. The resulting path lines show that the discharge areas of the Malm aquifer are mainly located along the Rhine valley, a few path lines leave the model area at the western boundary. Recharge paths within the Malm aquifer arrive at the eastern, western and southern boundary from outside of the model domain. Recharge also occurs through the Molasse (from the south) and down the BIH into the Malm aquifer.

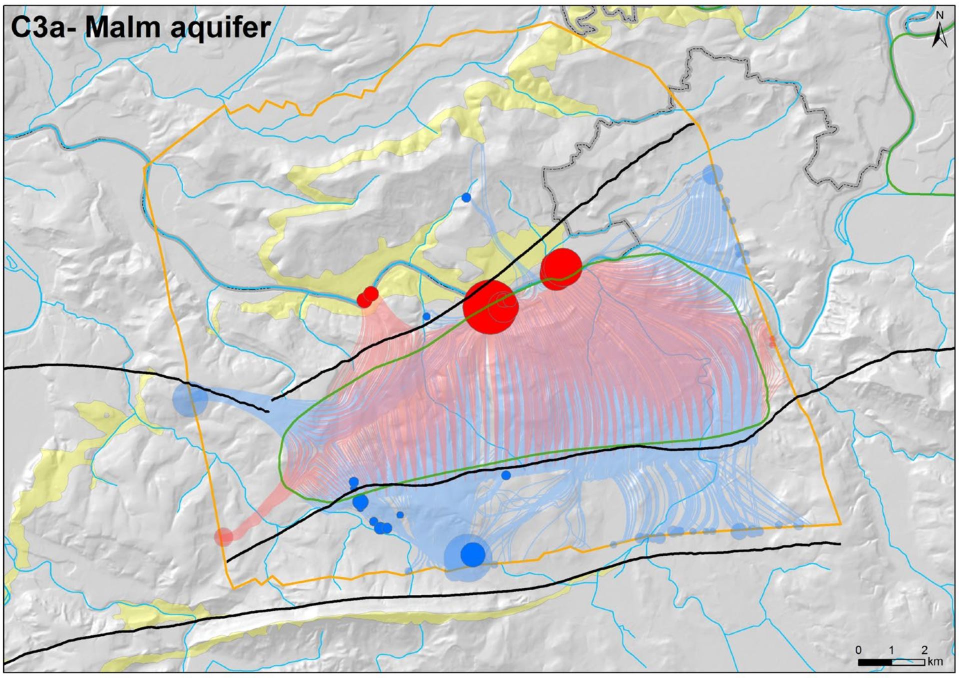


Fig. 4-42: Base Case C3a - Calculated Path Lines Starting from the Malm aquifer.

(Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

The forward path lines starting in the Muschelkalk aquifer show that a part of the path lines reach the top of the Molasse in the Rhine valley (Fig. 4-43) or leave the model area towards the west and east. Again, the influence of the different conductivity zones within the Muschelkalk aquifer are reflected by the different discharge paths (compare Fig. 3-13C). The backward tracks show recharge paths originating from the lateral boundaries (east and south) only.

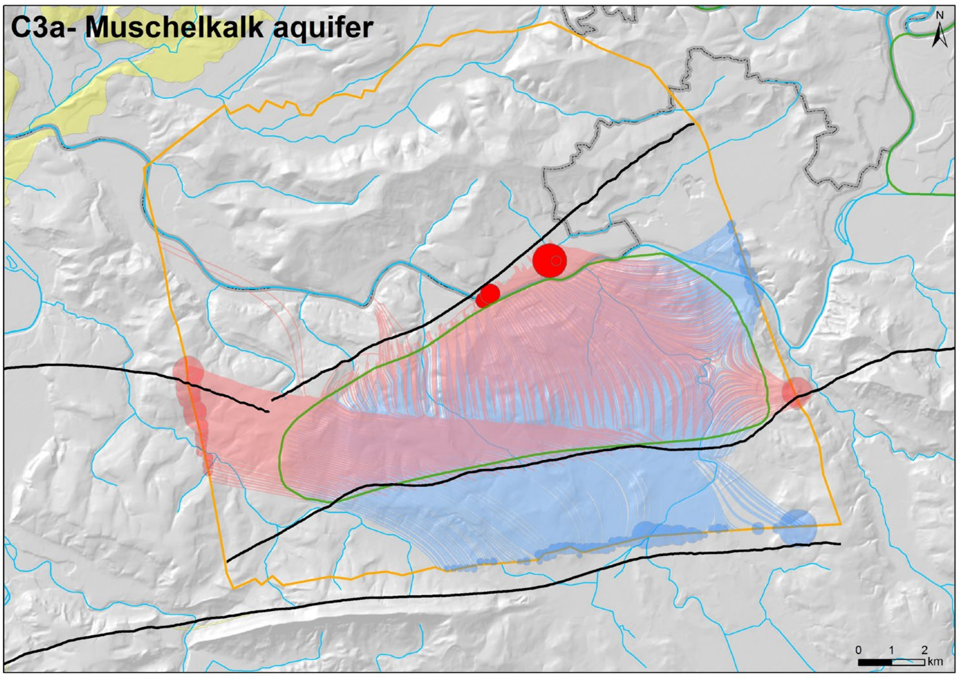


Fig. 4-43: Base Case C3a - Calculated Path lines Starting from the Muschelkalk aquifer.

(Blue: recharge path; red: discharge paths. Size of circles is a measure for the number of path lines reaching the respective point. Pale coloring indicates path lines reaching the side of the model, strong colors indicate path lines reaching the top of the model domain.)

5 Discussion of Results

Based on the implemented hydrogeological model, the corresponding hydraulic reference parameters and boundary conditions (see Chapter 3), four model hypotheses have been investigated to account for the general uncertainty related to the hydraulic behaviour of the 2 modelled faults zones, the Siglistorf Anticline and the BIH Lineament. In this context, four Base Cases have been modelled, namely:

- Base Case C1 ("throw only"): Potential groundwater flow along and across the fault is suppressed unless aquifers are (sub-/horizontally) connected, i.e. the geological offset either is to small to offset the aquifer so that it abuts against an aquitard or the offset is large enough so that two different aquifers are directly connected
- Base Case C2 ("sealing fault"): Any groundwater flow along and across the fault is suppressed
- Base Case C3 ("connecting fault"): Groundwater flow can exclusively occur in the fault plane meaning that multiple-aquifer systems are (sub-/vertically) connected but flow across (i.e. perpendicular to the fault plane) is suppressed
- Base Case C3a ("fully connecting fault"): Groundwater can flow along and across the fault

Comparison with Existing Hydraulic Data Bases

The number of head measurements in the deep aquifer systems of the siting region Nördlich Lägern is very limited. Only four head measurements could be used for comparison with the modelling results, namely measurements from the borehole Eglisau (USM), from Weiach (Malm aquifer and Muschelkalk aquifer) and from Zurzach (Muschelkalk aquifer), which is located at the boundary of the model domain (see Nusch et al. 2013). The comparison of these values with simulated values in the four Base Case simulations C1, C2, C3 and C3a is shown in Fig. 5-1.

Fig. 5-1: Comparison of Measured Head Values vs. Simulated Head Values of the Base Cases in Eglisau (USM), Weiach (Malm and Muschelkalk (abbreviated as MU)) and Zurzach (Muschelkalk, abbreviated as MU).

The measurements indicate (sub)hydrostatic to slightly artesian conditions, suggesting that groundwater flow is controlled by the local/regional discharge level of the Rhine valley. All Base Case simulations account reasonably well for this fact; a clear discrimination in model performance is not possible, even though the Case C3 ("connecting fault") may match slightly better the head measurements in the Malm aquifer and Muschelkalk aquifer of the Weiach borehole.

In summary, a clear preference for one of the Base Case models C1 - C3a cannot be made, even though special features of local groundwater flow might be better represented by one or the other model. Consequently, the full spectrum of modelling results, comprising all Base Case simulations and the corresponding sensitivity needs to be considered to define the range of expectations on ground water flow conditions in the siting region Nördlich Lägern.

Discussion

Horizontally the, on average, 110 m thick Opalinus Clay divides the sediment succession in the model domain into an upper and a lower groundwater system.

The **upper groundwater system** is mainly driven by surface water seeping through the outcrops and mountains outside of the model domain. In the south, recharge mainly originates from the northern limb of the Lägern while in the north the main recharge areas are the outcrops of the respective aquifers along the Laufenberg and Randen (SW and N of Schaffhausen, see Gmünder et al. 2013b).

The Malm aquifer, as the uppermost regional aquifer in the model, shows the strongest dependence of the head field on the local topography. The implemented regional faults are governing the general flow direction, which is in line with the boundary conditions derived from the regional hydrogeological model. Consequently, the differences in the head distribution are moderate in all Base Cases. The faults in the model have been implemented such that they do not reach the topography. Since the Malm aquifer is in direct contact with the medium permeable Molasse layers, the local recharge levels in the south of the model area near the BIH Lineament (Wehntal) may recharge the Malm aquifer by seepage through the Molasse. The main discharge areas of the Malm aquifer are located along the Rhine valley close to the Hohentengen am Hochrhein and in the Rhine valley close to Rümikon. A few forward path lines leave the model area in the vicinity of Freienwil, most likely towards the Malm outcrops west of the model area in the vicinity of the Aare and the Limmat.

The Hauptrogenstein, below the Malm aquifer, only covers a small portion of the model area. In all Base Cases, the head distribution indicates a recharge originating from the NE of the model domain, discharge is mainly directed towards the Rhine valley in the area of Bad Zurzach. The offset of the Hauptrogenstein along the Siglistorf Anticline is larger than the layer thickness so path lines cannot cross the fault. As the area south of the Siglistorf Anticline, where the Hauptrogenstein occurs, is very small, the groundwater flow direction is not well-defined but it

The deepest potentially water conducting sequence of the upper groundwater system is the BD5 (Sissach Member). As the sequences above and below have been implemented as aquitards, the Sissach Member shows the strongest influence of the implemented faults on the head distribution though the topography still plays a minor role. Recharge areas are comparable to those of the Malm aquifer (water supply from the NE and SE) and discharge is controlled by the low head levels along the Rhine valley (also in the vicinity of Hohentengen am Hochrhein). Overall, the lowest head values were simulated in the NW of the model domain close to Bad Zurzach. In case of the BD5 unit, the main discharge areas depend on the hydraulic significance of the faults. The offset of the BD5 unit along the Siglistorf Anticline is smaller than the layer thickness so groundwater can, in Cases C1 and C3a, cross the fault and discharge in the area of Bad Zurzach. In Cases C2 and C3 however, the faults are implemented as (horizontally) sealing faults so groundwater flows towards the area of Hohentengen am Hochrhein, comparable to discharge areas of the Malm aquifer. In all Base Cases, discharge towards the south is unlikely because the highest head values can be found in the south of the model domain (as this is an area of recharge) and the offset of the BD5 unit along the BIH is larger than the layer thickness so groundwater could not cross the fault. In the sensitivity cases, where a higher conductivity was assigned to the BD5, the difference of the head distribution is mostly negligible. The only notable difference occurs in the NW where higher heads were simulated. These higher heads are probably due to an increased recharge just outside of the model domain where the BD5 crops out along the Acheberg. However, it is likely that any water from this recharge area immediately discharges into the Rhine valley.

The **lower groundwater system** includes the Keuper aquifer and the Muschelkalk aquifer as well as the Arietenkalk (the latter only as a potentially local transmissive unit in the sensitivity cases). They are, to a large extent, influenced by the hydraulic properties of the faults. Generally, artesian conditions created by higher hydraulic heads imposed from the regional NE-W flow in connection with the relatively impermeable host rocks were simulated.

The Keuper aquifer is the uppermost local aquifer in the lower groundwater system. The offset of the Keuper aquifer along the Siglistorf Anticline is less than the layer thickness so groundwater could flow across the fault. At the BIH however, offset is larger than the layer thickness, so an N-S (or vice versa) flow across the fault is not permitted. In addition, the faults are oriented more or less normal to the flow field imposed by the lateral boundary conditions. Therefore, in Base Cases C1 and C2, the flow field is largely determined by the boundary conditions, showing high heads in the NE and low heads in the W and SW. No (Base Case C1) or only a small (Base Case C2) offset of heads develops along the Siglistorf Anticline while the BIH, as it effectively prohibits flow across the fault because of large vertical offsets, shows a drop of head values across the fault. As stated earlier, recharge occurs outside the model domain, and, at least for Base Cases C1 and C2, discharge within the model domain is limited to an area SE of Bad Zurzach in the Rhine valley. Although the flow field between the two Base Cases C1 and C2 are comparable, the lateral gradients differ to a large extent. This is mainly due to the imposed boundary conditions. While for Base Case C1 the largest head values are in the order of 440 - 450 m at the NW corner of the model domain, these values reach 540 - 550 m in Base Case C2. This is caused by the parameter assignment of the faults in a regional context. To calculate the necessary boundary conditions for the local model, faults in the regional model have also been assigned with very low permeabilities. The Randen Fault, situated to the W of the local model, and the BIH completely block any lateral connection across these faults. Therefore, the high heads indirectly reflect the elevation of the outcrops of the Keuper aquifer SW of the Wutach valley (see Gmünder et al. (2013b) for more information). In Cases C3 and C3a, the artesian conditions in the Keuper aquifer are relieved through the permeable faults. Simulated heads in the area above the repository site indicate a possible discharge into the Rhine valley (close to Hohentengen am Hochrhein/Kaiserstuhl) along the Siglistorf Anticline.

The head distribution north of the Siglistorf Anticline also indicates a flow along the fault plane in the direction of Bad Zurzach, most likely towards discharge areas in outcrops along the Rhine valley (Aareberg, Laubberg and/or the Bürgerwald S of Tiengen) just outside the model domain.

The Muschelkalk aquifer, as the lowest regional aquifer in the model domain, shows a comparable head distribution as the Keuper aquifer. However, since the offset along both, the Siglistorf Anticline and the BIH, is smaller than the layer thickness, path lines may cross the faults in Base Cases C1 and C3a. In all 4 Base Cases, recharge of the Muschelkalk aquifer occurs outside the model domain (towards the NE), leading to high head values along the NE boundary of the model domain. In the south, recharge also occurs from outside the model domain (Wehntal) or from the area south of the BIH (but within the model domain) which also acts as a seepage zone in Base Cases C2, C3 and C3a. This leads to a sharp bend of the head isolines between the two faults in Base Case C3a (where flow across the fault is also allowed) and C2 (sealing fault) and to only very low lateral gradients in Base Case C3. In Base Case C1, recharge of the Muschelkalk aquifer occurs outside the model domain (to the S) leading to higher head values along the S boundary of the model domain. Due to the interacting recharge areas, path lines originating from below the siting region mainly leave the model domain on its western lateral boundary. In Base Case C3a, the faults also deflect some path lines towards the eastern boundary of the model domain. In addition, the artesian conditions in Base Cases C3 and C3a are relieved along the Siglistorf Anticline, leading to possible discharge into the higher aquifers or even to the surface in the area of Hohentengen am Hochrhein.

While the Base Cases described above refer to structural uncertainties regarding the role and significance of the faults zones, additional sensitivity cases have been investigated to account for parameter uncertainties related to the conductivity of potential aquifers above and below the host rocks. In this context, the conductivity of the BD5 (Sissach Member, factor 2) and/or the Arietenkalk (4 orders of magnitude) was increased for Base Cases C1, C2 and C3 and the resulting head differences were analysed compared to the Base Cases. In all cases, the effect of a more conductive BD5 (Sissach Member) is of minor importance and only small changes of the lateral flow field (mainly the gradients but not the general directions) arise. Increasing the conductivity of the Arietenkalk also has only very small effects on the lateral gradient compared to the less conductive Base Cases. An increased conductivity in the Arietenkalk results in higher heads directly below the siting region and therefore in a slight increase of the vertical gradient through the Opalinus Clay in the siting region. With respect to vertical head gradients, the "sealing" hypothesis (Base Case C2), where faults prevent any cross-flow through the zones, computes the maximum value caused by corresponding regional (boundary) conditions. In contrast, the "connecting" hypotheses (Base Case C3 and C3a) largely break up the vertical separation of the flow system by relieving the artesian conditions through the (vertical) conductive fault zones. As a result, the head gradients through the host rocks largely disappear. Maximum and minimum vertical gradients for the different Base Cases in the area of the siting region have been calculated using the head distribution on the top Keuper aquifer and the top Opalinus Clay (equals bottom BD5) using an average distance between these two layers of 160 m. The maximum gradient that was calculated was 0.6 (directed upward) for Base Case C2 while for some Base Cases an insignificant vertical gradient (gradient of approx. 0) was calculated. However, the high gradient (upward) coincides with the worst fit between measured and simulated values (see above) so it is likely that this value really represents an unlikely case and that usually gradients are lower (the second highest, upward directed gradient has been calculated to 0.25 for Base Case C1). Some downward directed gradients have also been calculated for Base Cases C1, C3 and C3a. These usually only occur in the western part of the siting region and range between 0 (Base Case C1) to 0.03 (Base Case C3).

The results of the various simulations shortly summarized above show that the hydrological conditions in the upper groundwater system are mainly influenced by the topography and also by the hydrology of the regional faults. The lower groundwater system is largely controlled by the hydrology of the faults; this not only includes the offset of the head field but also the general flow field hinted at by the head distributions. The hydrological conditions of the local, potentially transmissive units (e.g. Arietenkalk) only play a minor role for the lateral flow field. However, higher conductivities in units directly above and below the Opalinus Clay (BD5 and Arietenkalk) increase the head difference across the Opalinus Clay and therefore increase the vertical flux through it.

6 Conclusions

A hydrogeological model of the siting region Nördlich Lägern was elaborated, aimed at evaluating the local groundwater flow conditions for a variety of hypothesis regarding the hydraulic behaviour of faults and the role of local aquifers and potentially transmissive units. In the present study, the time of validity of the hydrogeological modelling results is inherently associated with the assumption that the regional topography remains largely unchanged, implying that the local recharge and discharge conditions are subjected to moderate changes only.

The model analyses are elaborating on the hydraulic state conditions in the proposed host rocks and the aquifer systems of the siting region, particularly including:

- The assessment of the Opalinus Clay and the 'Brown Dogger' as flow barriers, separating the groundwater flow systems of the deep regional aquifers Malm aquifer and Muschelkalk aquifer. Emphasis of the investigations has been on the direction (up/downward) and magnitude of hydraulic gradient in the two proposed host rocks. The impact of the two regional fault systems has been analysed by parametric studies.
- The detailed evaluation of groundwater flow in the aquifer systems/transmissive units above and below the Opalinus Clay formation. The hydraulic significance of the Sissach Member, the Arietenkalk and the Keuper aquifer is adressed with particular focus on their potential role as locally important aquifers/transmissive units. The impact of the Siglistorf Anticline and the BIH Lineament on groundwater flow in the regional Malm aquifer and Muschelkalk aquifer is analysed in terms of prevailing flow direction and representative ranges of hydraulic gradients. Finally, the closest discharge areas are inferred.

The host rock formations Opalinus Clay and 'Brown Dogger'

The Opalinus Clay formation in the siting region is characterized by a typical thickness of 100 - 110 m, a high clay content and a uniform lithology, giving rise to an effective separation of the regional groundwater flow systems of the Malm aquifer and Muschelkalk aquifer. The simulated vertical hydraulic gradient in the Opalinus Clay is controlled by the hydraulic heads in the local/regional aquifer systems above and below. The following conclusions can be drawn:

- The local and regional aquifers in the siting region are partitioned by the regional fault systems (Siglistorf Anticline and BIH Lineament), resulting in lateral fragmentation of the groundwater flow systems. Consequently, the head differences between the regional aquifer systems are bracketed by the local/regional recharge and discharge levels rather than by far-off recharge and discharge areas (e.g. Alpine region).
- In the western part of the siting region, a downward directed hydraulic gradient is expected due to local recharge from the Wehntal to the North of the Lägern, giving rise to elevated heads in the Malm aquifer, whereas the Muschelkalk aquifer is characterised by hydrostatic conditions. The corresponding vertical hydraulic gradient in the Opalinus Clay ranges between .1 and 1, depending on the assumed model scenario. Table 6-1 displays the spectrum of expectations on vertical hydraulic gradients in the Opalinus Clay of the western part of the siting region.

- In the eastern part of the siting region, upward directed gradients are expected in the Opalinus Clay. The Muschelkalk aquifer is supplied mainly by recharge areas in the southern Black Forest (upper Wutach valley) and exhibits more or less hydrostatic heads. The heads in the Malm aquifer are controlled by the discharge levels in the Rhine valley (near Hohentengen), resulting in subhydrostatic conditions. The corresponding vertical gradients in the Opalinus Clay range between .1 and 1, depending on the flow scenario (see also Table 6-1).

The 'Brown Dogger' in the siting region Nördlich Lägern is composed of clay-rich and some calcareous sequences, revealing an average thickness of 70 - 80 m and variable clay content. Vertical flow through the 'Brown Dogger' is controlled by the low hydraulic conductivity of the clay-rich sequences, which are comparable with the Opalinus Clay. The calcareous layers may exhibit higher conductivities, depending on the lithological variability of the sedimentary structures, respectively on the intensity of tectonic overprint. In this context, the Sissach Member (called BD5 in the hydrogeological model Nördlich Lägern) is of particular relevance because it is located above the Opalinus Clay and has been identified as a potentially transmissive unit. The hydraulic gradient in the 'Brown Dogger' of Nördlich Lägern exhibits similar general features as in the Opalinus Clay, such as downwards directed flow in the western part and upflow in the eastern part of the siting region. The magnitudes of the gradients are generally lower due to the lower burial depth. Table 6-1 summarises the spectrum of expectations on vertical hydraulic gradient in the 'Brown Dogger' of the siting region Nördlich Lägern.

Tab. 6-1: Hydrogeological Characteristics of the Opalinus Clay and the 'Brown Dogger' in the Siting Region Nördlich Lägern.

RV: Reference value (best guess, defendable value).

AV: Alternative value (pessimistic value; complementary model assumption).

Host rock	Parameter	RV	AV	Remarks
Opalinus Clay	Hydraulic head/mid of the formation [m]	*	-	RV: * Hydrostatic conditions, defined by the ground level at the location of interest
	Vertical gradient in the host rock [m/m] - western part of the siting region	0.1	0.5	RV: Downflow derived from pressure difference between Sissach Member and Keuper aquifer AV1: Downflow derived from pressure difference between Sissach Member and Arietenkalk (pessimistic assumptions)
			0.1	AV2: Up- or downflow possible; pressure difference between Malm and Muschelkalk aquifer
	Vertical gradient in the host rock [m/m] - eastern part of the siting region	0.1	1	RV: Upflow derived from pressure difference between Sissach Member and Keuper aquifer AV1: Upflow derived from pressure difference between Sissach Member and Arietenkalk
			0.1	AV2: Upflow derived from pressure difference between Malm and Muschelkalk aquifer
'Brown Dogger'	Hydraulic head/mid of the formation [m]	*	-	RV: * Hydrostatic conditions,, defined by the ground level at the location of interest
	Vertical gradient in the host rock [m/m] - eastern part of the siting region	0.1	0.1	RV: Upflow derived from pressure difference between Sissach Member and Malm aquifer AV1: Downflow derived from pressure difference between Sissach Member and the Malm aquifer
	Vertical gradient in the host rock [m/m] - western part of the siting region	0.1	0.1	RV: Downflow derived from pressure difference between Sissach Member and Malm aquifer AV1: Upflow derived from pressure difference between Sissach Member and Malm quifer

Groundwater Flow in the Local and Regional aquifer Systems

The evaluation of groundwater flow in the aquifer systems above and below the host rock formations is motivated by the safety assessment, which requires a complete description of the composite radionuclide release path from the disposal system through the host rock and the aquifer systems, finally discharging into the biosphere. Since the present model was used to simulate the local scale hydrogeological system, some of the recharge and discharge areas mentioned below are outside of the model domain of the local scale model. In that case, the respective information was taken from the hydrogeological regional model which is explained in detail in Gmünder et al. (2013).

The following conclusions can be drawn with respect to the local and regional aquifer systems:

- The lateral continuity of the regional aquifers Muschelkalk aquifer and Malm aquifer is broken by the regional fault systems Siglistorf Anticline and BIH, forming the legs of a funnel like zone which opens towards NE. The resulting fragmentation governs the local and regional groundwater flow systems in the siting region, shielding largely the aquifers from recharge areas in the South (Swiss Alps) and in the North, respectively. The regional faults may show a simple offset disrupting the continuity of the hydrogeological units (Case C1; see Chapter 4). Otherwise they could act as sealing faults (Case C2) or leaky faults (Cases C3 and C3a). In all cases, the hydraulic heads in the regional aquifer systems are defined by the local/regional recharge and discharge levels, giving rise to more or less hydrostratic conditions and low hydraulic gradients in the central part of the siting region.
- Depending on the assumed hydraulic characteristics of the faults, the main discharge areas of the Muschelkalk aquifer and Malm aquifer appear along the Rhine valley and the lower Aare valley (Muschelkalk: Koblenz, Hohentengen am Hochrhein, Kaisten and lower Aare valley; Malm: Hohentengen am Hochrhein and the Limmat valley close to Wettingen). The expected discharge areas, together with the expected ranges of the horizontal hydraulic gradient in the Muschelkalk aquifer and Malm aquifer are given in Table 6-2.
- The hydraulic significance of the Sissach Member, the Arietenkalk and the Keuper aquifer as potential local groundwater flow systems has been subjected to data interpretations (packer tests in Weiach) and model analyses. Recalling the packer test results in the Weiach borehole with artesian heads and an interval conductivity of 9E-11 m/s it seems plausible to treat parts of the Keuper as a local aquifer system. This is in line with experience from the borehole Benken, were parts of the Keuper were clearly identified as a local aquifer. Reference values and alternative values for the hydraulic gradient in the Keuper aquifer are given in Table 6-2 together with the expected discharge areas.
- The Arietenkalk is represented as sequence of 3 m thickness in the hydrogeological model Nördlich Lägern, located around 20 m above the Keuper aquifer. Model analyses exhibit a similar head distribution as in the Keuper aquifer and consequently, similar discharge areas.
- The Sissach Member is represented as sequence of 10 m thickness in the hydrogeological model Nördlich Lägern, located directly above the Opalinus Clay. Model analyses exhibit a similar head distribution as in the Malm aquifer and, consequently, similar discharge areas.

Tab. 6-2: Hydrogeological Characteristics of the Regional and Local aquifer Systems/ Potentially Transmissive Units in the Siting Region Nördlich Lägern.

Note that only the most prominent discharge areas are given in the table.

RV: Reference value (best guess, defendable value).

AV: Alternative value (pessimistic value; complementary model assumption).

Hydrogeological unit	Parameter	RV	AV	Remarks
Muschelkalk aquifer (Regional aquifer)	Hydraulic head/mid of the formation [m]	*	-	RV: * Hydrostatic conditions
	Horizontal component of hydraulic gradient [m/m]	.001	.01	RV: Value deduced from Case 1-3 AV: pessimistic scenario
	Discharge area	-	-	AV1: Hohentengen am Hochrhein AV2: Area between Laufenburg and Sisseln AV3: Aare valley (close to Koblenz/Döttingen)
Keuper aquifer (Local aquifer)	Hydraulic head/mid of the formation [m]	*	+50 m	RV: * Hydrostatic conditions AV: * Artesian conditions (taken from base Case C2)
	Horizontal component of hydraulic gradient [m/m]	0.01	0.1	RV: Value deduced from Cases 1-3a AV: Pessimistic value
	Discharge area	-	-	AV1: Hohentengen am Hochrhein /Bad Zurzach AV2: Aareberg/Laubberg AV3: Frick
Malm aquifer (Regional aquifer)	Hydraulic head/mid of the formation [m]	*	-	RV: * Hydrostatic conditions
	Horizontal component of hydraulic gradient [m/m]	0.01	0.1	RV: Value deduced from Cases 1,2 AV: Value deduced from Case 3, 3a (pessimistic scenario)
	Discharge area	-	-	AV1: Hohentengen am Hochrhein/Rümikon AV2: Limmat valley (Wettingen)

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Appendix 1: Gradients

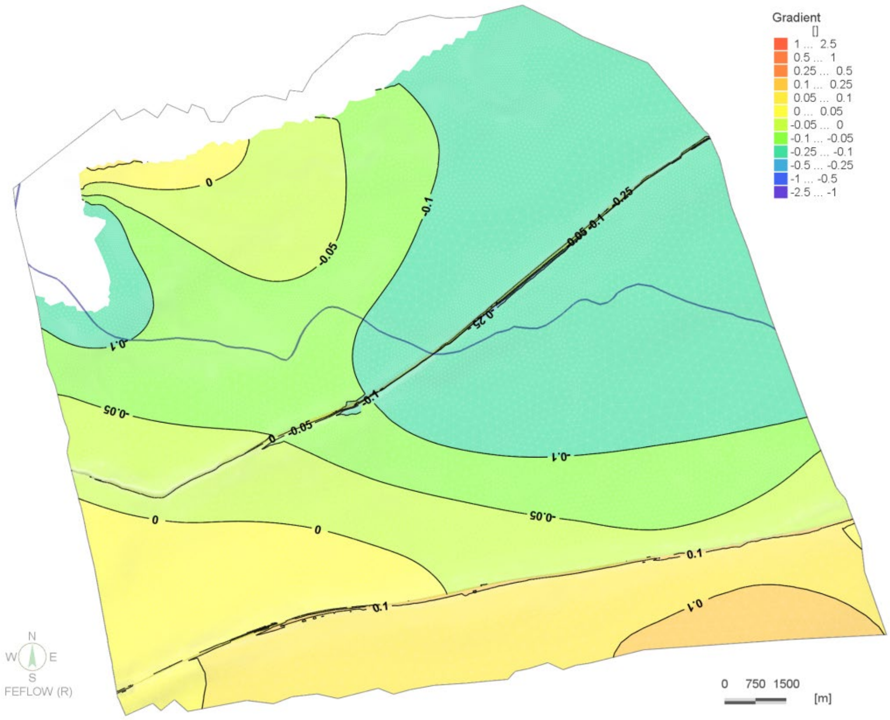

Fig. A1: Gradient for Base Case C1 between the BD5 (Sissach Member) and the Keuper aquifer.

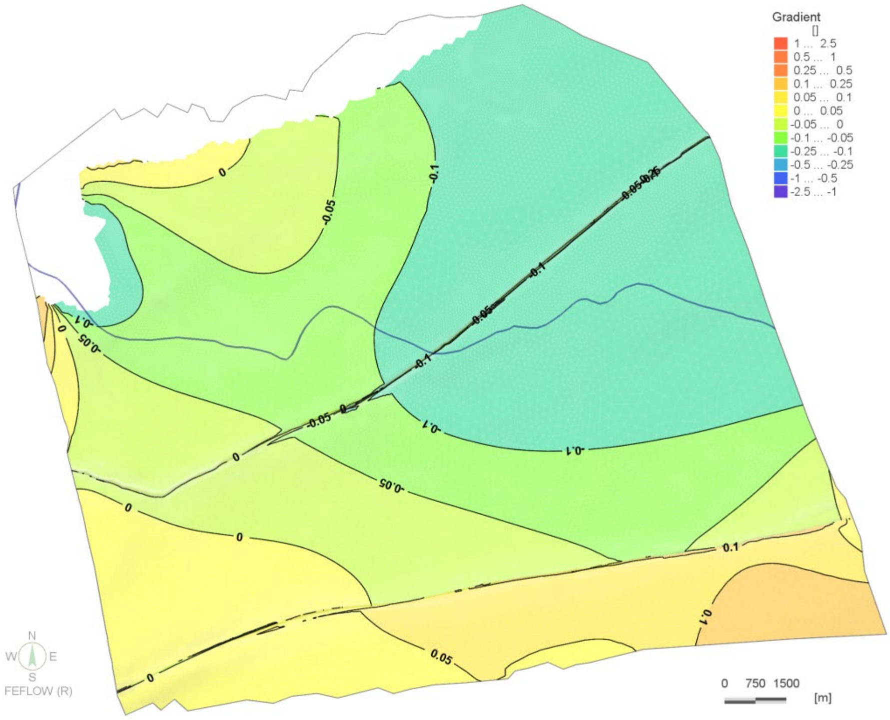

Fig. A2: Gradient for Sensitivity Case C1-BD5 between the BD5 (Sissach Member) and Keuper aquifer.

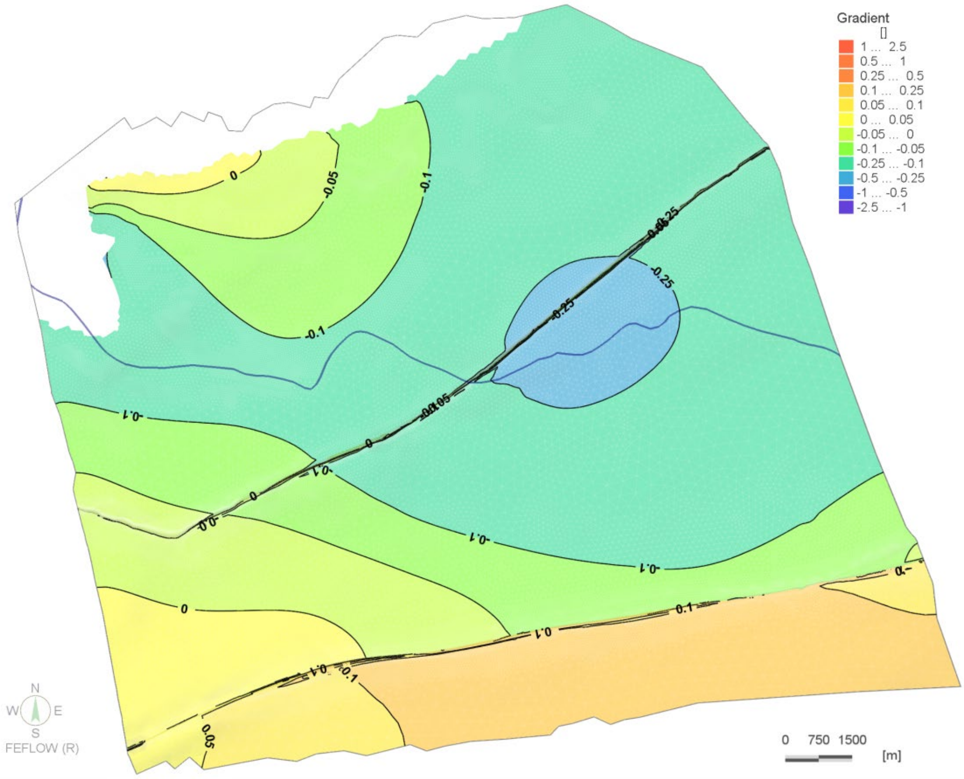

Fig. A3: Gradient for Sensitivity Case C1-AKA between the BD5 (Sissach Member) and the Arietenkalk.

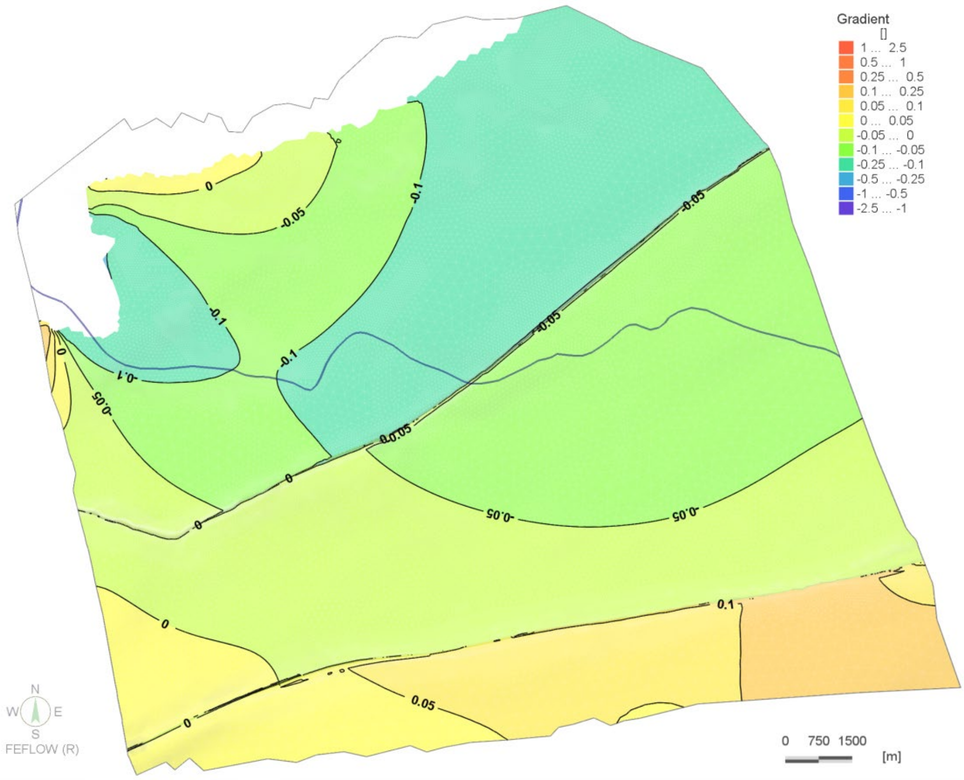

Fig. A4: Gradient for Sensitivity Case C1-BD5-AKA between the BD5 (Sissach Member) and the Arietenkalk.

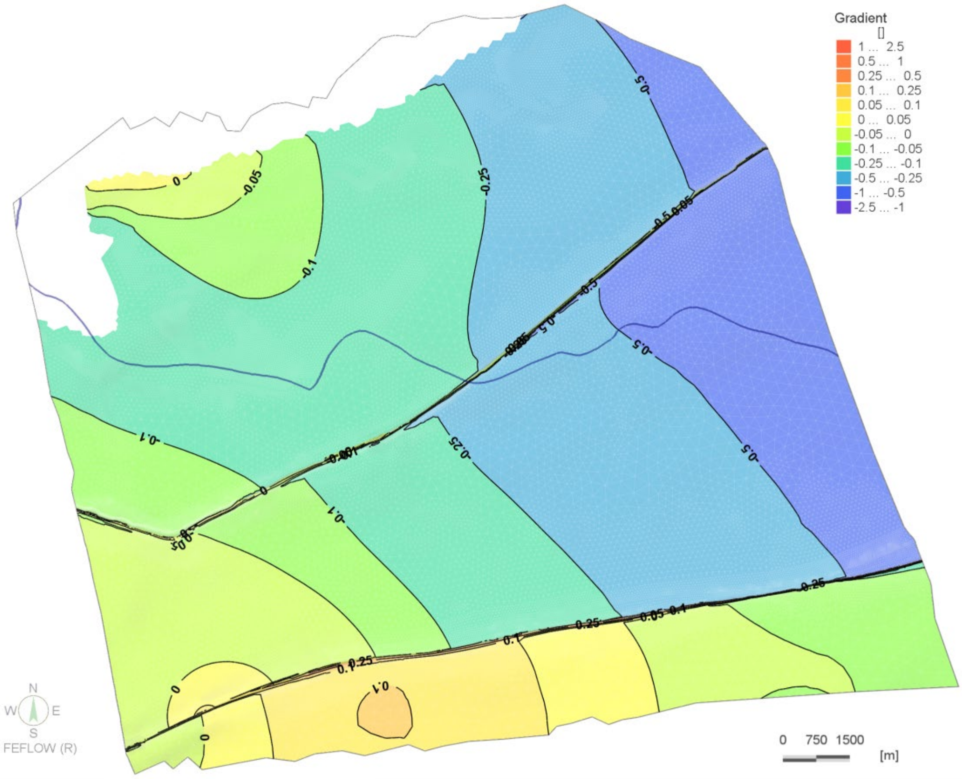

Fig. A5: Gradient for Base Case C2 between the BD5 (Sissach Member) and the Keuper aquifer.

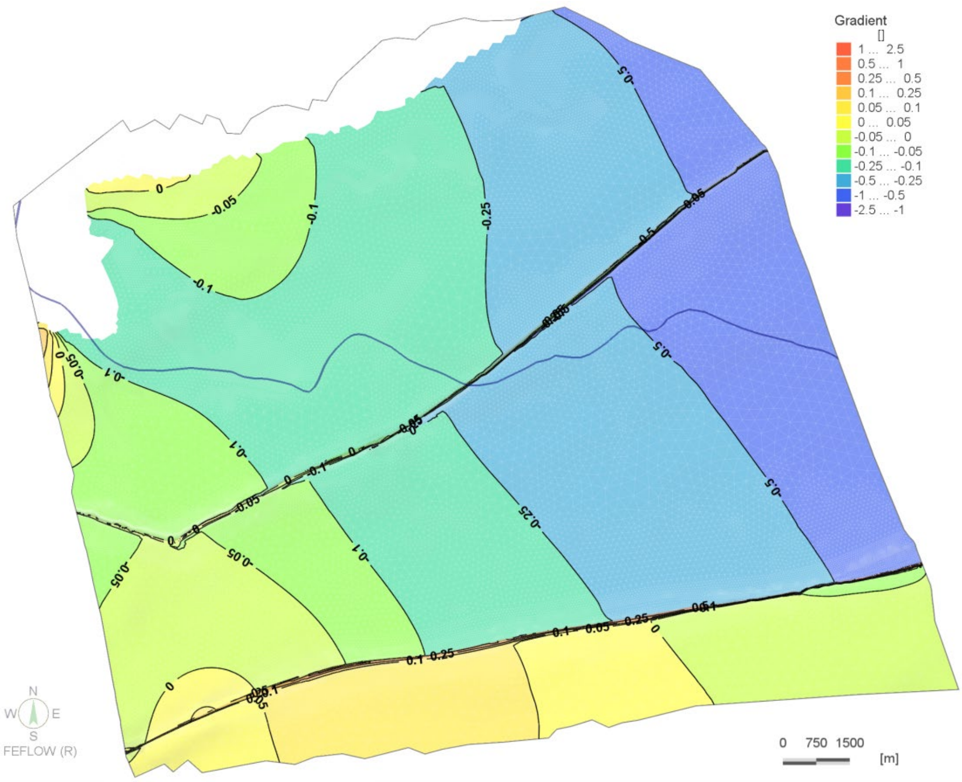

Fig. A6: Gradient for Sensitivity Case C2-BD5 between the BD5 (Sissach Member) and the Keuper aquifer.

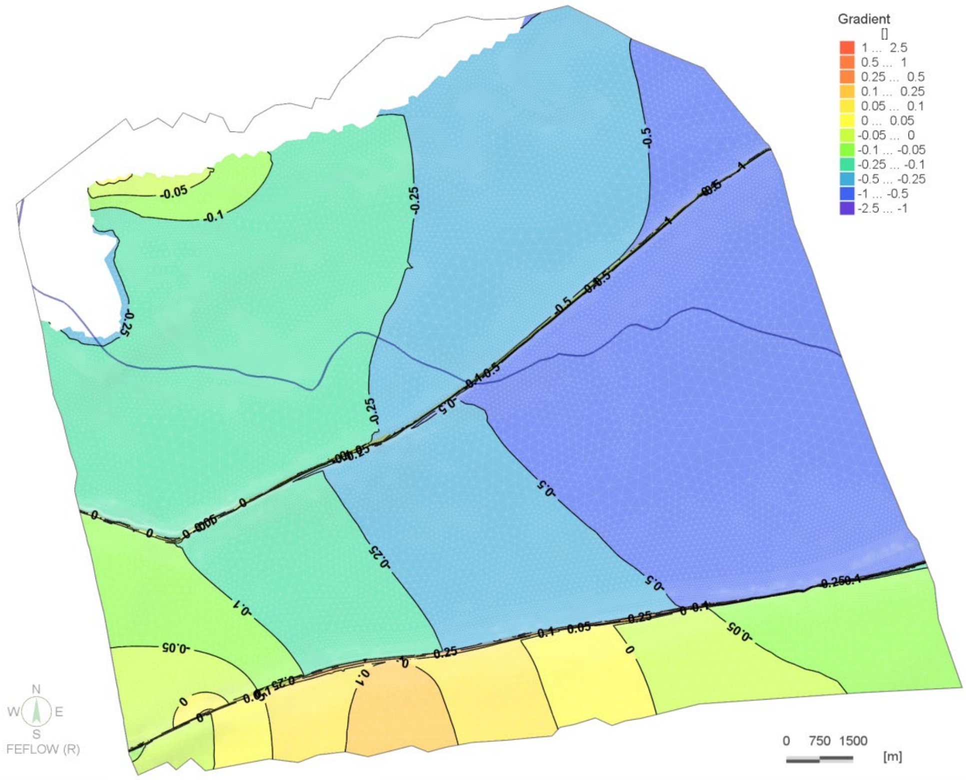

Fig. A7: Gradient for Sensitivity Case C2-AKA between the BD5 (Sissach Member) and the Arietenkalk.

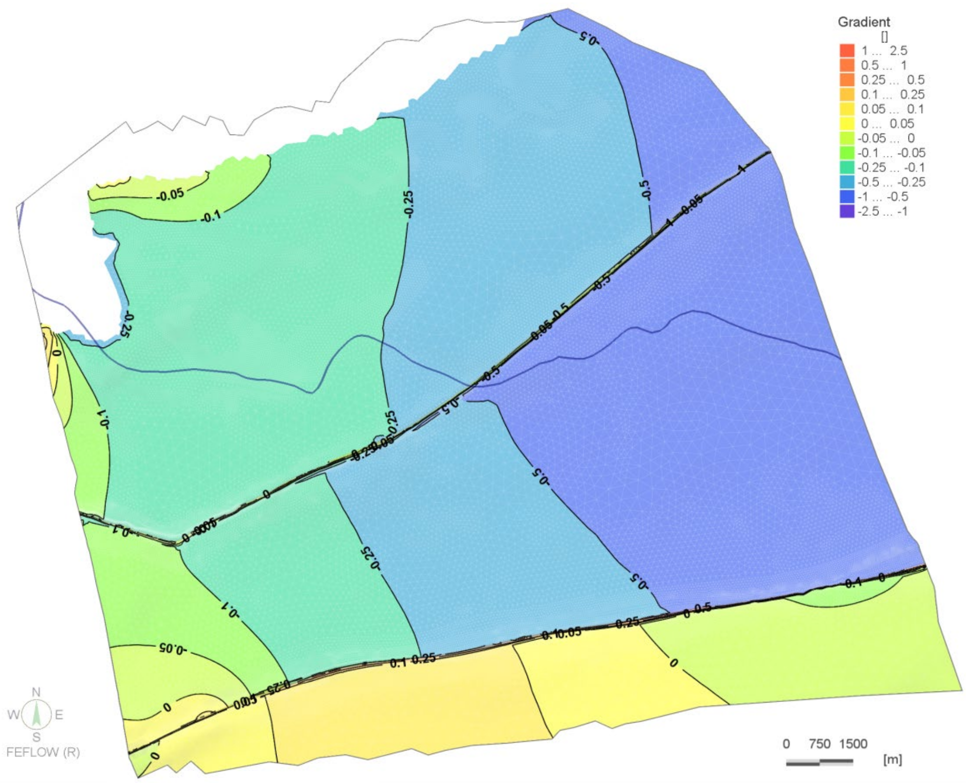

Fig. A8: Gradient for Sensitivity Case C2-BD5-AKA between the BD5 (Sissach Member) and the Arietenkalk.

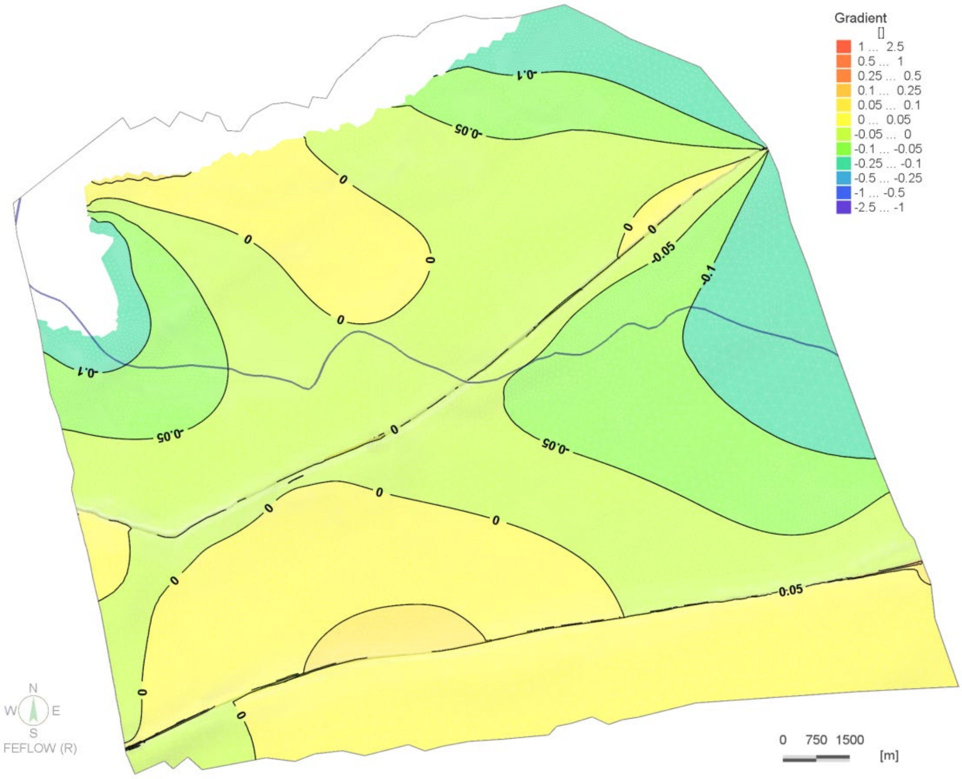

Fig. A9: Gradient for Base Case C3 between the BD5 (Sissach Member) and the Keuper aquifer.

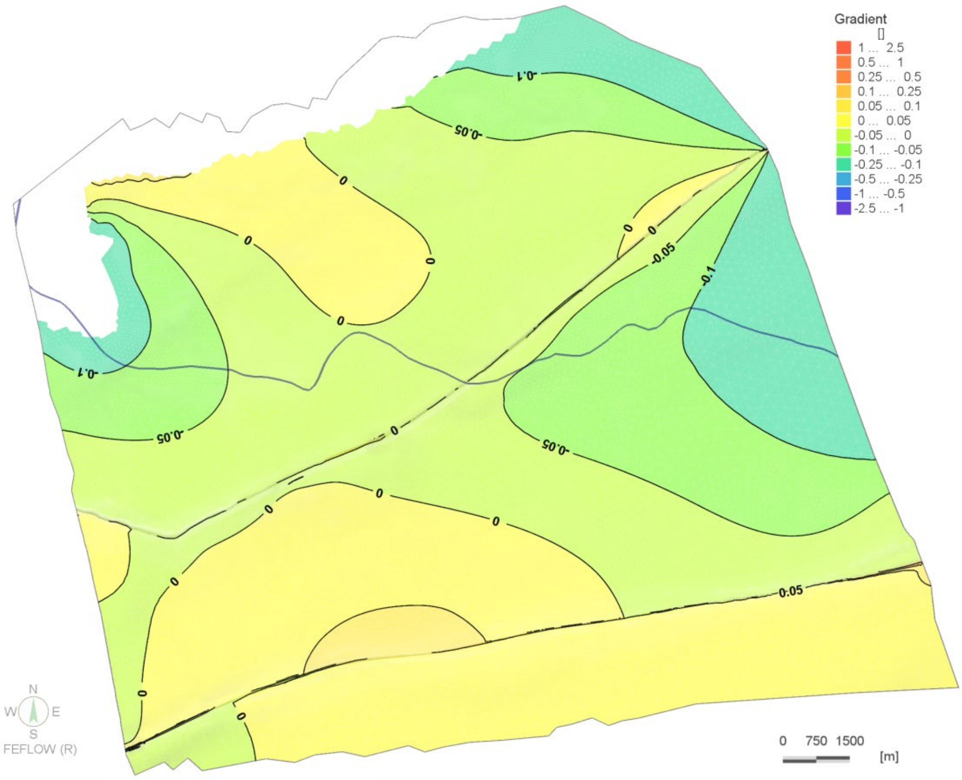

Fig. A10: Gradient for Sensitivity Case C3-BD5 between the BD5 (Sissach Member) and the Keuper aquifer.

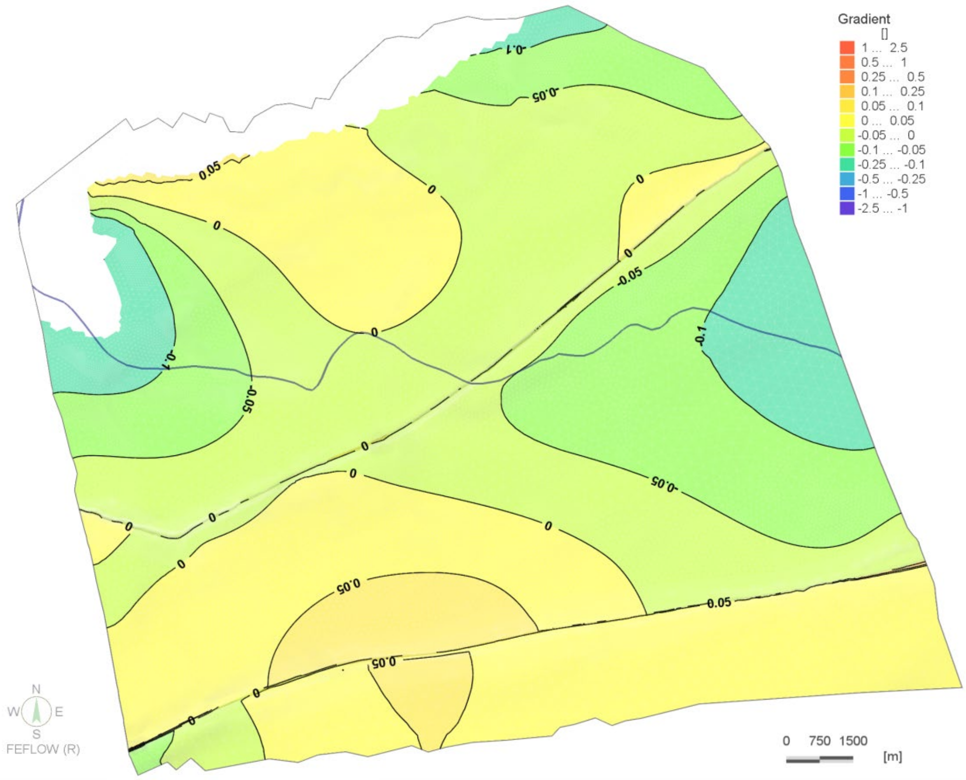

Fig. A11: Gradient for Sensitivity Case C3-AKA between the BD5 (Sissach Member) and the Arietenkalk.

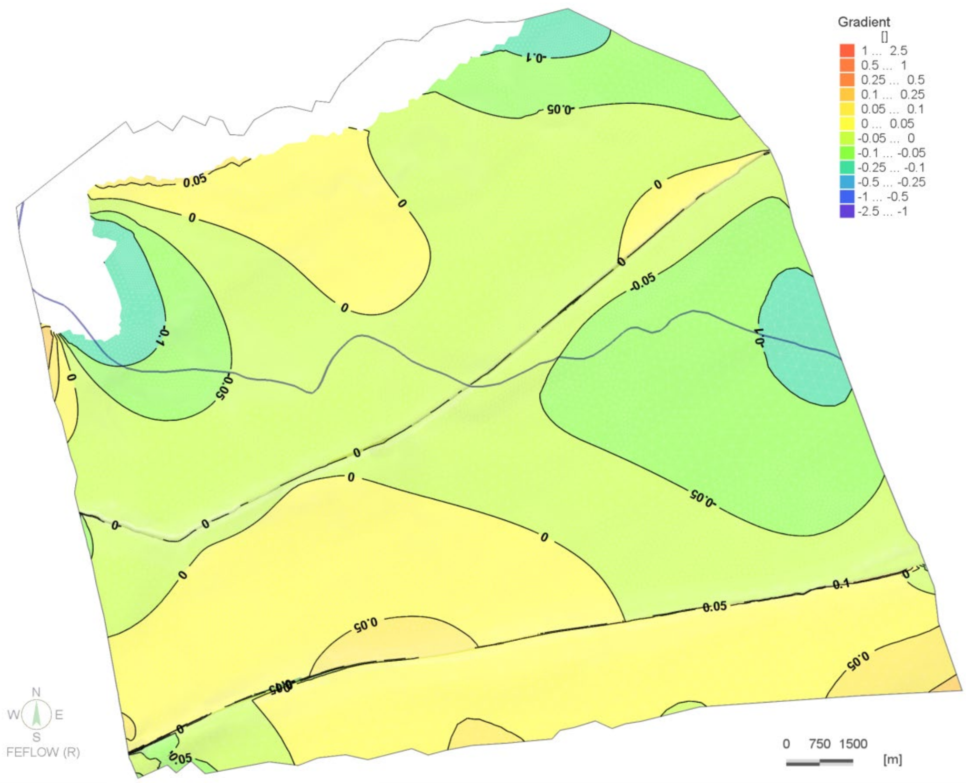

Fig. A12: Gradient for Sensitivity Case C3-BD5-AKA between the BD5 (Sissach Member) and the Arietenkalk.

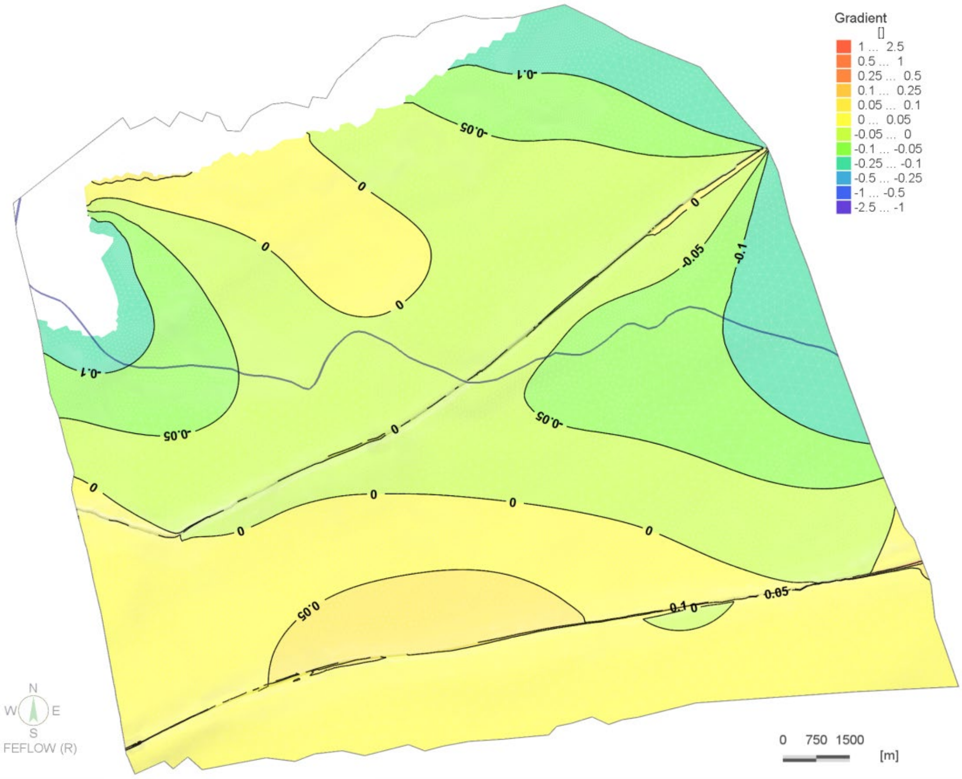

Fig. A13: Gradient for Base Case C3a between the BD5 (Sissach Member) and the Keuper aquifer.