



ARBEITSBERICHT NAB 24-16

Hydrogeological Model of
Northern Switzerland

November 2024

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
+41 56 437 11 11 | info@nagra.ch | nagra.ch



ARBEITSBERICHT NAB 24-16

Hydrogeological Model of
Northern Switzerland

November 2024

KEYWORDS

Hydrogeology, groundwater head, flow path, gradient, discharge,
recharge, numerical model

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
+41 56 437 11 11 | info@nagra.ch | nagra.ch

Nagra Arbeitsberichte ("Working Reports") present the results of work in progress that have not necessarily been subject to a comprehensive review. They are intended to provide rapid dissemination of current information.

Abstract

A regional steady-state hydrodynamic model was developed to examine the groundwater flow system in Northern Switzerland, focusing on aquifers above and below the Opalinus Clay and the influence of regional-scale faults on groundwater flow. The model geometry was based on existing geological models and extended with hydrogeologically significant layers. Except for the Jura Main Thrust, which was modelled in more detail, faults have been implemented as vertical zones with a constant width of 150 m. Model boundaries were determined using hydraulic data and conceptual considerations and a sensitivity study was performed to test various boundary conditions to determine the best-fit model. The best-fit model was selected based on performance metrics such as mean absolute error and correlation coefficients between modelled and observed head values. Using the best-fit model as the base, a careful calibration of the model parameters was performed using the PEST algorithm. This calibrated model is the base case. The sensitivity of the model was also explored with additional cases.

The base case is marked by a piezometric depression located in the area of the lower Aare Valley and Hochrhein Valley in the region of Kaiserstuhl – Hohentengen (close to the Nördlich Lägern siting region, NL), separating the hydraulic flow system in the northern part of the model domain into an eastern (including the Zürich Nordost siting region, ZNO) and western part (including the Jura Ost siting region, JO). This depression can be observed in all aquifers and is the result of the topography, the surface waters and the location of outcrops. Generally, flow occurs from topographically higher outcrops in the west or northeast towards the piezometric depression.

For the Malm aquifer in the eastern part (ZNO), recharge areas are mainly located along the topographically higher outcrops in the north, discharging into the Rhine Valley. In the western part of the model, flow is directed towards the Aare Valley and other, smaller river valleys. The area between these two (including the NL siting region) is characterised by low hydraulic heads where recharge of the Malm mainly occurs through the thick Molasse units along the northern part of the Lägern Anticline and discharge along the Rhine River in the area of Kaiserstuhl – Hohentengen.

The Hauptrogenstein aquifer, only present in the western part of the model, shows recharge areas in the topographical elevation zones (areas of Frickberg and Internal Jura (Folded Jura) to the south of JO) and discharges into the river valleys (lower Aare Valley and Sissle Valley).

The local Keuper aquifer was implemented in the model with different zonations of the hydraulic properties (based on geological and hydrogeological observations). For the NL siting region, the calibration results suggest lower hydraulic conductivities than in ZNO and JO. Recharge areas for the Keuper aquifer are located between the Wutach and the Klettgau Valleys north of the NL and ZNO siting regions, and locally in outcrops north of the JO siting region. Comparable to the Muschelkalk aquifer below the Keuper aquifer, discharge areas for the Keuper aquifer in JO are mainly located in the lower Aare Valley and the Sissle Valley. From the NL and ZNO siting regions, flow is directed southwards. In NL, flow velocities are particularly low, reflecting the low hydraulic conductivities and gradients.

Finally, the Muschelkalk aquifer represents the lowest aquifer implemented in the model. In the western part, recharge is mainly located in topographically higher outcrops to the north and to the south of JO, while flow is directed towards the Aare and Sissle Valleys. In the eastern part, a large-scale flow system occurs extending from the recharge area along the Wutach Valley, across the ZNO and NL siting regions towards the regional discharge area located at the confluence of the Aare and Rhine Rivers.

A set of additional cases addressed the local Keuper aquifer. Lithological and hydrogeological data show that the nature of this aquifer varies between the siting regions with marked variations in hydraulic conductivity. These differences and the related uncertainties were accounted for by different parametrisations: isotropic and variants of anisotropic K_{xx}/K_{yy} . The anisotropic cases are based on the observation that in parts of the Keuper aquifer, sand-rich channels seem to be mainly responsible for groundwater flow. To account for the resulting flow direction depending on the orientation of the channels (which are not known), two additional cases, with preferred E-W- or N-S-directed flow, have been simulated. These additional cases show that the details of flow direction and gradients locally change depending on the parametrisation, but the flow field remains stable with respect to the recharge and discharge areas. Generally, the fit of these additional cases to observations is not as good as in the base case.

In the base case, the Malm aquifer consists of the «Felsenkalke» and «Massenkalk», the Schwarzbach Formation and the Villigen Formation. As an additional case, only the «Felsenkalke» and «Massenkalk» were assigned with a higher transmissivity, however, this has little to no effect on the regional recharge/discharge areas compared to the base case.

The effects of regional-scale faults on the flow system were assessed performing sensitivity analyses. Using various permeability scenarios, conceptually accounting for the orientation of the faults with respect to the current stress field, show that the Baden – Irchel – Herdern Lineament and the Jura Main Thrust (roughly E-W-trending faults) effectively separate the model into a southern and northern hydrogeological system. Roughly N-S-trending faults (especially the Randen Fault) may locally channel flow from the recharge areas in the northern part of the model to the southeast. However, the resulting simulated head distributions of the sensitivity analyses show that faults appear to have only minor and local effects on the regional flow patterns.

Overall, the hydraulic situation in the model area is very robust, changes of parametrisation show only localised impacts. The comparison of simulation results with observation data supports the accuracy of the hydraulic simulations and shows that the model boundaries do not impede the reliability of the model.

Table of Contents

Abstract	I
Table of Contents	III
List of Tables.....	V
List of Figures	V
List of Enclosures.....	VIII
List of Acronyms.....	IX
1 Introduction	1
2 General hydrogeology	3
3 Model building/construction	7
3.1 Definition of model limits	7
3.1.1 Upper and lower model boundary	9
3.1.2 Southern model limit	9
3.1.3 Eastern model limit.....	12
3.1.4 North-eastern model limit.....	13
3.1.5 North-western model limit.....	15
3.1.6 Western model limit	16
3.2 Regional faults.....	17
3.3 3D geological model.....	19
3.4 Finite element mesh construction	20
4 Preliminary sensitivity analyses for selection of base case.....	23
4.1 Surface recharge spreading layer.....	23
4.1.1 Surface flow boundary estimation	24
4.1.2 Estimation of surface parameters.....	25
4.2 Preliminary parametrisation of units.....	28
4.3 Lateral flow boundary conditions.....	32
4.4 Main results of the boundary condition sensitivity analysis (preliminary sensitivity analysis).....	35
4.5 Selected model.....	36
5 Fault sensitivity analyses	39
5.1 Regional faults in the model area	40
5.2 Fault parametrisation	40
5.2.1 Hydromechanical arguments	40
5.2.2 Fault / rock parameter relationships.....	41
5.3 Definition of scenarios for fault sensitivity analysis	42

5.4	Simulation results	43
5.4.1	Main results	43
5.4.2	Analysis of specific scenario: IT100_C (14)	45
5.4.3	General observations from fault hydraulics.....	49
6	Model calibration.....	51
7	Base case	55
7.1	Muschelkalk aquifer	55
7.2	Keuper aquifer	60
7.3	Hauptrogenstein aquifer.....	67
7.4	Malm aquifer	72
7.5	Hydraulic gradients in the Opalinus Clay.....	77
7.6	Discharge/Recharge from particle tracking	81
7.6.1	Muschelkalk aquifer	81
7.6.2	Keuper aquifer	83
7.6.3	Hauptrogenstein aquifer.....	85
7.6.4	Malm aquifer	87
8	Additional cases	91
8.1	Introduction	91
8.2	Case homogeneous and isotropic Keuper aquifer.....	92
8.2.1	Case rational	92
8.2.2	Definition of model.....	92
8.2.3	Simulation results	93
8.2.4	Summary.....	98
8.3	Case anisotropic Keuper aquifer.....	99
8.3.1	Case rational	99
8.3.2	Definition of model.....	99
8.3.3	Simulation results	100
8.3.4	Summary.....	103
8.4	Case Malm.....	103
8.4.1	Case rational	103
8.4.2	Definition of model.....	104
8.4.3	Simulation results	104
8.4.4	Summary.....	106
9	Summary and conclusions	107
10	References.....	111

List of Tables

Tab. 4-1:	Initial horizontal and vertical K values of the modelled layers	29
Tab. 4-2:	Multipliers used to increase contrasts between some aquifers/aquitards.....	30
Tab. 4-3:	Definition of lateral flow boundary conditions for model limits.....	33
Tab. 4-4:	Definition of model variants based on lateral flow boundary conditions.....	34
Tab. 4-5:	Lateral flow boundary conditions' (Fbcs) definitions for model 53/54	36
Tab. 5-1:	Scenario definitions for the fault sensitivity analysis using the base case.....	43
Tab. 5-2:	Difference between mean absolute error [m] of the model 53/54 (ID 0) and all tested scenarios (ID 1 – 19) calculated for each aquifer separately.....	44
Tab. 7-1:	Hydraulic conductivities and horizontal anisotropy ratio in the Muschelkalk aquifer.....	55
Tab. 7-2:	Hydraulic conductivities and horizontal anisotropy ratio in the Keuper aquifer.....	61
Tab. 7-3:	Hydraulic conductivities and horizontal anisotropy ratio in the Hauptrogenstein aquifer.....	67
Tab. 7-4:	Hydraulic conductivities and horizontal anisotropy ratio in the Malm aquifer	72

List of Figures

Fig. 2-1:	Schematic hydrogeological profile of Northern Switzerland (Nagra 2024f).....	4
Fig. 2-2:	Geological map of Northern Switzerland with the siting regions and major faults (from Nagra 2024f).....	5
Fig. 3-1:	Shaded digital elevation model of Northern Switzerland overlain by a schematic map of groundwater domains with the extension of the regional model (stippled black line)	8
Fig. 3-2:	Cross-section through the western model area indicating the geology of the Jura Main Thrust with the outcrops of the evaporitic Muschelkalk (from Nagra 2024f).....	9
Fig. 3-3:	Simplified tectono-geological map with the southern model limits following the frontal thrust of the Subalpine Molasse	10
Fig. 3-4:	Aerial view of the eastern part of the southern model limit with Subalpine Molasse units drawn to the SE of the frontal thrust.....	12
Fig. 3-5:	Digital elevation model of the Bodensee area	13
Fig. 3-6:	Geological Map of southern Germany and Northern Switzerland (position shown in close-up bottom-right) overlain by a digital elevation model with northeastern model limits	14
Fig. 3-7:	Close up of the north-western model limit portion.....	15

Fig. 3-8:	Western model limit along the Säcking Fault and the Aare, Langete and Emme Rivers	16
Fig. 3-9:	Geological map including the regional-scale faults implemented in the hydrogeological model in a simplified way (modified from Nagra 2024f).....	18
Fig. 3-10:	View of the 2D mesh of the hydrogeological model	20
Fig. 3-11:	The area of the Jura Main Thrust has been modelled in detail (orange polygon, also see inset of the specifically modelled part) since it includes outcrops of important regional aquifers and aquitards	21
Fig. 3-12:	Semi-transparent 3D view of the hydrogeological model, together with cross-sections, of the northeastern part of the hydrogeological model	22
Fig. 4-1:	Basic principle of a catchment water balance, assuming identical hydrological and hydrogeological catchments extends, with the discharge rate Q reflecting the effective precipitation, i.e. $P - ET$	24
Fig. 4-2:	Map of the spatial variability of the groundwater recharge [m/s] implemented in the model	25
Fig. 4-3:	Initial model – calibrated hydraulic conductivities in the spreading layer on the model surface ($\log_{10}(K \text{ [m/s]})$).....	26
Fig. 4-4:	Comparison between simulated and measured near-surface hydraulic heads	27
Fig. 4-5:	Simulated near-surface hydraulic head distribution	28
Fig. 4-6:	Depth dependency of K values observed in the Malm and Muschelkalk aquifers	31
Fig. 4-7:	Calculated correlation coefficients $R [-]$, mean absolute errors $MAE [m]$ and sum of squared errors $[m^2]$ for all tested scenarios.....	35
Fig. 4-8:	Mean absolute error for the different aquifers (compared to observations) after the sensitivity analyses (but before calibration)	37
Fig. 5-1:	Conceptual fault architecture (centre), 2D representation of the fault zone with the evolution of fracture density (dF) and hydraulic conductivity (KF) with respect to the fault axis (left), anisotropy of fault parameters (modified after Bense et al. 2013) (right).....	39
Fig. 5-2:	Vertical variability of the hydraulic properties of the regional faults in model scenario 14.....	41
Fig. 5-3:	Scenario 14 – Comparison between simulated and measured hydraulic heads.....	45
Fig. 5-4:	Model results for the Muschelkalk aquifer in Scenario 14 – Top: Simulated hydraulic heads in the Muschelkalk aquifer. Bottom: Differences with model 53/54	46
Fig. 5-5:	Model results for the Malm aquifer in Scenario 14 – Top: Simulated hydraulic heads in the Muschelkalk aquifer	47
Fig. 5-6:	3D view of the hydraulic perturbation in the Malm and Muschelkalk aquifers compared to model 53/54 (only where difference is $< -10 \text{ m}$ or $> 10 \text{ m}$).....	48
Fig. 6-1:	Conceptual zones in the Malm, Keuper and Muschelkalk aquifers.....	51
Fig. 6-2:	Comparison between simulated and measured hydraulic heads with uncertainty intervals.....	53

Fig. 6-3:	Groundwater flow budgets (Log10 Inflows and Outflows [m ³ /yr]) at different model boundaries.....	54
Fig. 7-1:	Calibrated hydraulic conductivities in the Muschelkalk aquifer horizon	56
Fig. 7-2:	Observed versus simulated hydraulic heads in the Muschelkalk aquifer	57
Fig. 7-3:	Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Muschelkalk aquifer	59
Fig. 7-4:	Boxplot of the Darcy fluxes calculated by the model in the Muschelkalk aquifer horizon of the siting regions.....	60
Fig. 7-5:	Calibrated hydraulic conductivities in the Keuper aquifer horizon	62
Fig. 7-6:	Observed versus simulated hydraulic heads in the Keuper aquifer	63
Fig. 7-7:	Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Keuper aquifer	65
Fig. 7-8:	Boxplot of the Darcy fluxes calculated by the model in the Keuper aquifer horizon of the siting regions	66
Fig. 7-9:	Calibrated hydraulic conductivities in the Hauptrogenstein aquifer horizon	68
Fig. 7-10:	Observed versus simulated hydraulic heads in the Hauptrogenstein aquifer	69
Fig. 7-11:	Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Hauptrogenstein aquifer.....	71
Fig. 7-12:	Calibrated hydraulic conductivities in the Malm aquifer horizon	73
Fig. 7-13:	Observed versus simulated hydraulic heads in the Malm aquifer	74
Fig. 7-14:	Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Malm aquifer.....	76
Fig. 7-15:	Boxplot of the Darcy fluxes calculated by the model in the Malm aquifer horizon of the siting regions	77
Fig. 7-16:	Vertical hydraulic gradient across the Opalinus Clay	78
Fig. 7-17:	Difference in hydraulic heads between aquifers above and below the Opalinus Clay	80
Fig. 7-18:	Simulated hydraulic heads and particle tracking identifying recharge and discharge areas in the Muschelkalk aquifer.....	82
Fig. 7-19:	Simulated hydraulic heads and particle tracking identifying recharge and discharge areas in the Keuper aquifer.....	84
Fig. 7-20:	Stacked histogram of the total distance travelled by the backward (left figure) and forward (right figure) particles released in the Keuper aquifer of the JO, NL and ZNO siting regions	85
Fig. 7-21:	Simulated hydraulic heads and particle paths identifying recharge and discharge areas in the Hauptrogenstein aquifer	86
Fig. 7-22:	Simulated hydraulic heads and the particle paths identifying recharge and discharge areas of the Malm aquifer.....	88
Fig. 7-23:	Hydraulic head differences between the Malm aquifer and the Lower Freshwater Molasse (USM).....	89

Fig. 8-1:	Cross plot of the simulated and observed hydraulic heads for the case of a homogeneous isotropic Keuper aquifer	93
Fig. 8-2:	Hydraulic head difference between the homogeneous isotropic case and the base case	95
Fig. 8-3:	Simulated hydraulic heads and backward particle tracking identifying recharge areas in the Keuper aquifer for the base case (upper figure) and the homogeneous isotropic case (lower figure).....	96
Fig. 8-4:	Simulated hydraulic heads and forward particle tracking identifying discharge areas in the Keuper aquifer for the base case (upper figure) and the homogeneous isotropic case (lower figure).....	97
Fig. 8-5:	Stacked histogram of the total distance travelled by the backward (left figure) and forward (right figure) particles released in the Keuper aquifer of the JO, NL and ZNO siting regions	98
Fig. 8-6:	Simulated hydraulic heads and backward particle tracking identifying recharge areas in the Keuper aquifer for the base case (figure a), the anisotropic K W-E case (figure b), and the anisotropic K N-S case (figure c).....	101
Fig. 8-7:	Simulated hydraulic heads and forward particle tracking identifying recharge areas in the Keuper aquifer for the base case (fig. a), the anisotropic K W-E case (fig. b), and the anisotropic K N-S case (fig. c).....	102
Fig. 8-8:	Simulated hydraulic heads and the particle paths identifying recharge and discharge areas of the Malm aquifer.....	105

List of Enclosures

Encl. A Compilation of hydraulic heads in the Mesozoic aquifers and Molasse units

Note: The enclosures are only included in the digital version of this report and can be found under the paper clip symbol.

List of Acronyms

a.s.l.	Above sea level
BAC1	Bachs-1-1 borehole
BOZ1	Bözberg-1-1 borehole
BOZ2	Bözberg-2-1 borehole
BUL1	Bülach-1-1 borehole
b.g.l.	Below ground level
Fbcs	Flow boundary conditions
JO	Jura Ost siting region
K	Hydraulic conductivity [m/s]
MAE	Mean absolute error
MAR1	Marthalen-1-1 borehole
NAB	Nagra Work Report ('Nagra Arbeitsbericht')
NL	Nördlich Lägern siting region
NTB	Nagra Technical Report ('Nagra Technischer Bericht')
OMM	Upper Freshwater Molasse Group
OSM	Upper Marine Molasse Group
PEST	Parameter estimation and uncertainty analysis
R	Correlation coefficient
RSL	Surface recharge spreading layer
SGT	Sectoral Plan for Deep Geological Repositories
SSE	Sum of squared errors
STA2	Stadel-2-1 borehole
STA3	Stadel-3-1 borehole
T	Transmissivity [m^2/s]
TRU1	Trüllikon-1-1 borehole
UMM	Lower Marine Molasse Group
USM	Lower Freshwater Molasse Group
ZNO	Zürich Nordost siting region

1 Introduction

This report details the modelling effort to characterise the hydrogeological situation in north-eastern Switzerland, covering the Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO) siting regions. The general objectives of the hydrogeological model are aimed at characterising the regional groundwater flow conditions which also are used to determine more local-scale hydraulic states in the different siting regions. The steady-state hydrogeological model also is a useful tool to test the consistency of the available hydrogeological dataset and to investigate the impact of different conceptual models in cases where the available hydrogeological data is too limited to develop a precise conceptual understanding.

Results of the steady-state hydrodynamical modelling are used to determine the regional flow field and locate recharge and discharge areas as well as fluxes in the modelled hydrogeological units. The results support the hydrogeological chapters of the Geosynthesis (Nagra 2024f), which integrates the results from the hydraulic modelling with results from lithological, structural, geological and hydrogeochemical analyses and interpretations.

It is important to note that the hydrogeological model presented here has been tailored to the specific purposes shortly detailed above. To minimise the intrinsic model uncertainty, boundary conditions have been carefully evaluated and model parameters have been chosen with the above-mentioned general objectives in mind. This regional-scale model is hence fit for the purpose of evaluating the regional flow system and analysing the impact of different conceptual models on the flow field, thereby increasing the general hydrogeological understanding of the modelled area. On this scale, the groundwater velocity field is mainly influenced by the upscaled hydrogeological properties of the included geological layers, outcrops or intersections of layers with rivers. On a smaller scale, local flow patterns are more influenced by small-scale hydrogeological features such as structural or lithological heterogeneities resulting in a spatially heterogeneous distribution of hydraulic conductivities. To analyse these small-scale flow patterns, the regional hydrogeological model is not detailed enough.

This report first summarises the general hydrogeological situation and the hydrogeological stratigraphy of the model area (Chapter 2). Chapter 3 details the reasoning for setting the lateral and vertical boundaries of the model and the general model setup. Since there is a number of uncertainties with respect to the different boundary conditions and parameters, a preliminary sensitivity analysis has been performed to determine the best fitting combination of boundary conditions. This is described in more detail in Chapter 4. The preliminary sensitivity analyses lead to an initial model choice which was used to test the impact of different parametrisations of the implemented regional faults, for which no observations were available, on groundwater flow (Chapter 5). The resulting best-fit model was further calibrated to observations (Chapter 6) and is described in Chapter 7 (the base case). Additional cases testing different conceptual models and parametrisations compared to the base case have been performed and are detailed in Chapter 8. Finally, a summary and conclusions of the modelling effort are given in Chapter 9.

2 General hydrogeology

The hydrogeological system modelled here is defined by the topographic situation, the river network, the sedimentary sequence with its respective hydrogeological properties and the (regional) fault system and associated hydrogeological properties of the faults.

Fig. 2-1 shows the general hydrogeological profile of Northern Switzerland. The Mesozoic sedimentary sequence from the Buntsandstein to the Malm displays a wide variety of vertically and, in some cases also horizontally, different lithological units resulting in important variations of hydraulic conductivities. The main aquifers included in the hydrogeological model in the Mesozoic sedimentary sequence are, from bottom to top, the Muschelkalk and the Keuper aquifers and the Hauptrogenstein and Malm aquifers. The sedimentary concepts and hydrogeological properties used in the hydrogeological model are described in detail in Nagra (2024f, Section 4.5) and Nagra (2024e). The most striking feature of the model domain arguably is that the upper and lower regional aquifers, the Malm/Hauptrogenstein and Keuper/Muschelkalk aquifers, are separated by the thick, low-permeable Opalinus Clay and the adjacent low-permeable units, which effectively lead to the occurrence of an upper and lower hydrogeological system. From a conceptual point of view, due to the clay-rich and hence low-permeable Opalinus Clay in between the major aquifers, faults do not provide relevant vertical shortcuts but are expected to be characterised by low vertical hydraulic conductivities within the Opalinus Clay (Nagra 2024f, 2024h).

The Mesozoic sediments are covered by the Molasse. The Molasse is separated into the Plateau Molasse within the model domain and the Subalpine Molasse south of the model domain. For simplicity, mentioning of Molasse in this report always refers to the Plateau Molasse and the three Molasse main units occurring in the study area (from bottom to top), the Lower Freshwater Molasse Group (Untere Süsswassermolasse, USM), the Upper Marine Molasse Group (Obere Meeresmolasse, OMM) and the Upper Freshwater Molasse Group (Obere Süsswassermolasse, OSM). The OMM is more homogeneous and permeable than the USM and OSM and is also considered as a regional aquifer (Nusch et al. 2013). The thickness of the (Plateau) Molasse increases towards the Alps to more than 4 km. Along the Alps, the Plateau Molasse is truncated by the Subalpine Molasse (see Nagra 2008 or Nagra 2024f for a more detailed description). A hydrogeological description and available hydrogeological data for the Molasse is described in detail in Nusch et al. (2013) and Nagra (2024e).

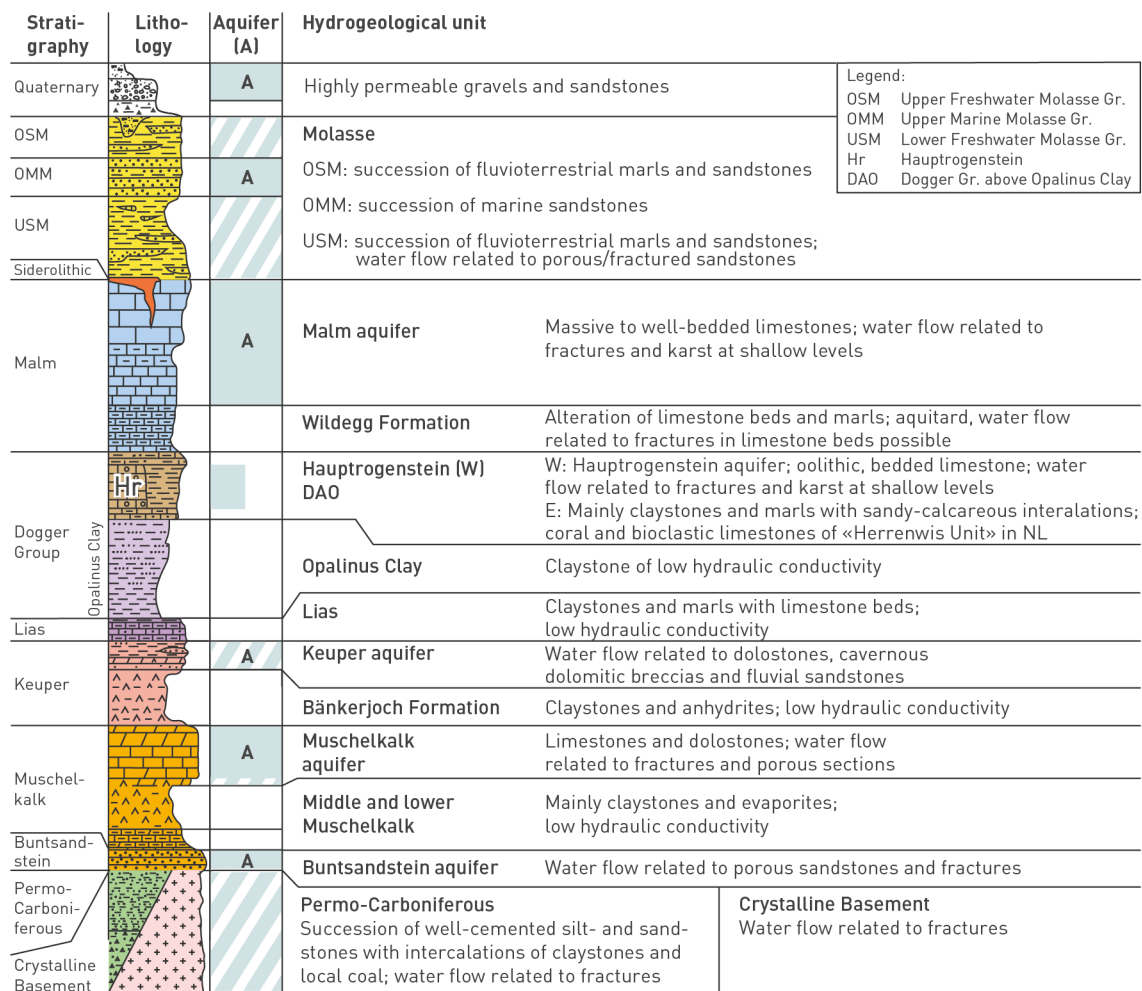


Fig. 2-1: Schematic hydrogeological profile of Northern Switzerland (Nagra 2024f)

The figure focuses on the situation relevant to the siting regions. Hatched areas indicate local aquifers or units in which the water flow is linked to a specific lithology (e.g. sandstones in the USM). Gr.: Group.

The uppermost Moraine and alluvial deposits of the Quaternary also comprise very variable lithologies, hence the hydraulic properties vary significantly. Most of the river valleys in Northern Switzerland are characterised by a several decametres thick infill of unconsolidated Quaternary sediments, including highly permeable gravels, which represent important shallow aquifers. Some of the valleys are glacially overdeepened; the infill of these overdeepenings is complex and often heterogeneous and can reach depths of more than 200 m below the actual terrain (Nagra 2024d).

Fig. 2-2 gives an overview of the main regional-scale faults in Northern Switzerland. Most of the faults are steeply inclined, with the exception of the Jura Main Thrust, and mainly affect the outcrop situation and the continuity of the implemented units. Within the Jura Main Thrust, outcrops down to the Anhydrite group of the Muschelkalk can be observed. A summary of the tectonic evolution, leading to the various regional, large-scale faults included in the model, and, more importantly, their orientation, is given in Nagra (2024f). In general, the hydrogeological model includes all relevant regional-scale faults (see Section 3.2 and Fig. 3-9), including, but not limited to, the Jura Main Thrust and Baden – Irchel – Herdern Lineament (as roughly E-W-trending faults) and the Randen and Neuhausen Faults (as roughly N-S-trending faults).

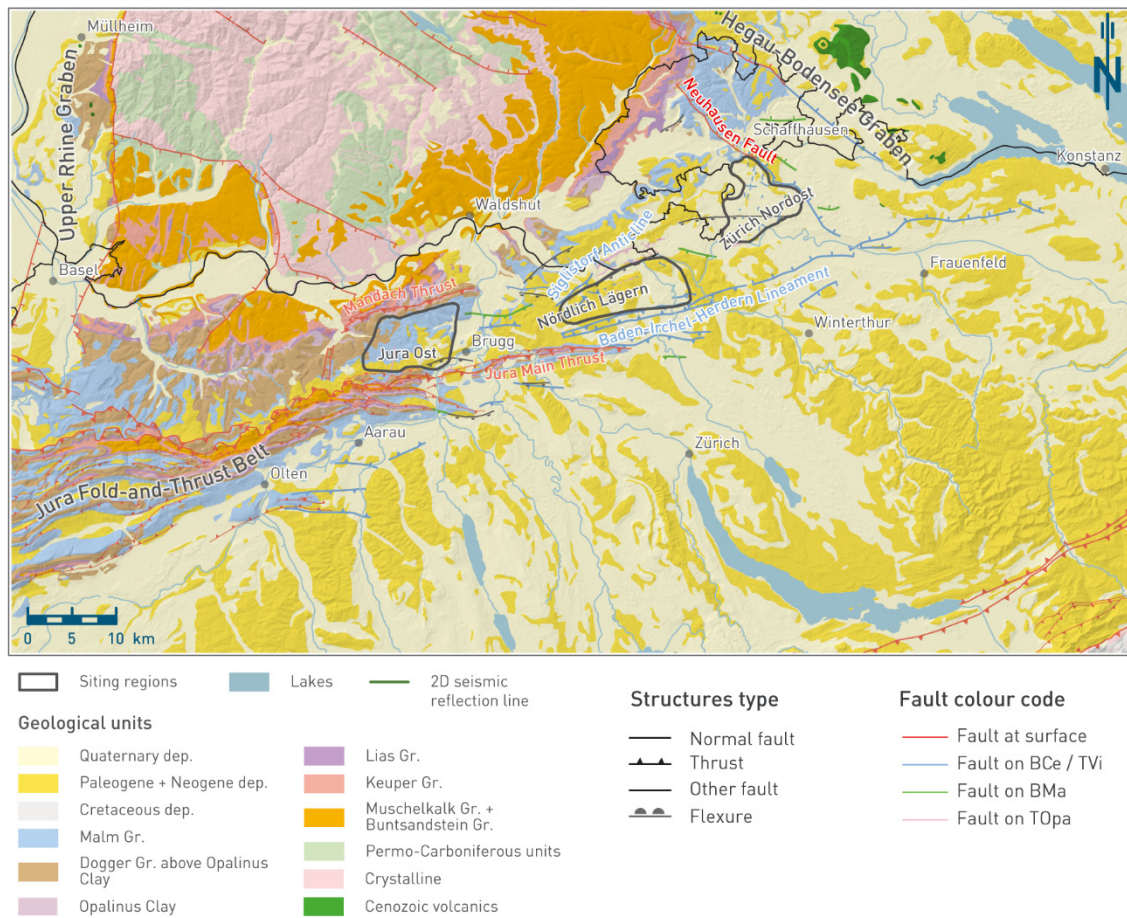


Fig. 2-2: Geological map of Northern Switzerland with the siting regions and major faults (from Nagra 2024f)

Geological units from 1:500'000 geological map with the addition of Opalinus Clay outcrops in Northern Switzerland (©swisstopo). Fault traces at the surface based on Nagra (2014). Fault traces at the base Cenozoic are derived from an integration of 2D seismic reflection lines and current 3D seismic reflection interpretation (Nagra 2014, 2024a, 2024b, 2024c). Gr.: Group.

3 Model building/construction

3.1 Definition of model limits

A crucial aspect in any modelling approach is the definition of the model extent, since it is along the model boundaries that all interactions with areas outside the model have to be managed through boundary conditions. Seeking hydrogeologically 'natural' limits is therefore of particular importance, as it allows to test different physically reasonable hypotheses with respect to the hydrogeological situation to decrease the inherent model uncertainty.

With the main objective of the hydrogeological model being the general understanding of the regional hydrogeological situation (see Fig. 3-1) and, more particular, the assessment of the regional flow fields around the potential repository sites, both the lateral and vertical model extensions are of prime importance. The lateral limits should be chosen sufficiently far away from the area of interest to allow groundwater flow fields to develop 'naturally' (uninfluenced by the boundary conditions) in the simulated environment. Vertically, the model delimitation should include all project-relevant units, in this case from the top surface down to, and including, the Muschelkalk aquifer as the next regional aquifer below the Opalinus Clay.

Model delimitation, both lateral and vertical, comprises a balancing act between uncertainty related to boundary conditions' definition and parametrisation of the units as well as computing time. The smaller the model size, the higher the uncertainty related to boundary conditions but the smaller the uncertainty related to the geological setting and the parametrisation of all relevant units will be, and vice versa.

To estimate the actual boundary conditions for each of the boundaries described here, and hence to decrease the inherent uncertainty of said boundary, a preliminary sensitivity analysis concerning the parametrisation of the boundaries has been performed (see Chapter 4).

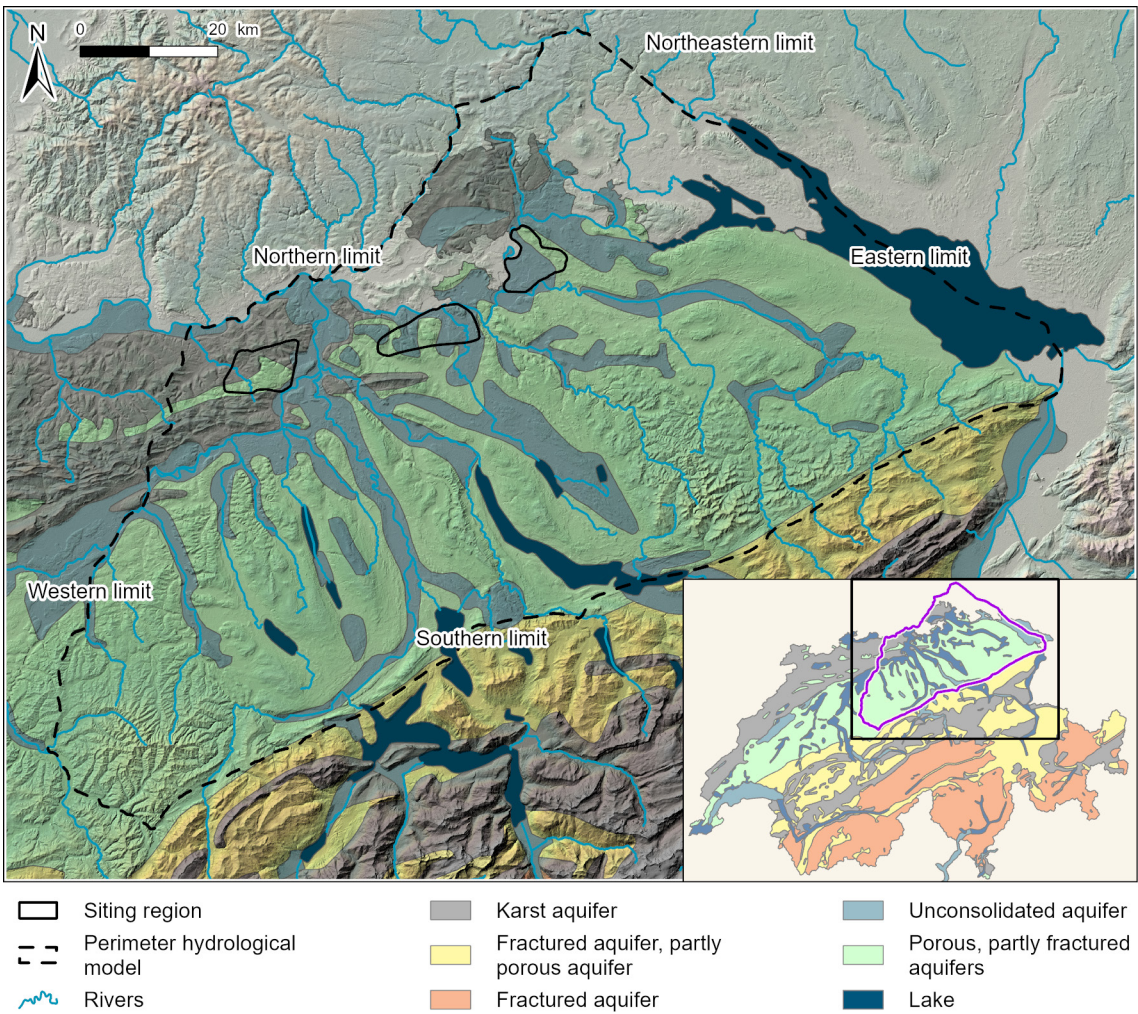


Fig. 3-1: Shaded digital elevation model of Northern Switzerland overlain by a schematic map of groundwater domains with the extension of the regional model (stippled black line)

Extract of the hydrogeological map of Switzerland (©swisstopo). See inset on bottom right for a larger overview of Switzerland. Black polygons outline the siting regions.

3.1.1 Upper and lower model boundary

The upper limit of the model is defined by the topography which allows the introduction of surface boundary conditions to simulate interaction with surface water bodies as well as spatially distributed diffuse groundwater recharge. The model uses the concept of a surface recharge spreading layer, a thin layer on top of the model which distributes recharge by precipitation to the deeper aquifers or as runoff into the included rivers and lakes (see Section 4.1 for more detail).

The lower limit was selected based on the aim of the model and taking into account technical feasibility and hydrogeological considerations. The Muschelkalk aquifer is the next large, regional aquifer below the Opalinus Clay and just above a thick, impermeable, evaporitic and clay-mineral-rich unit. The base of the model has therefore been defined at the base of the Muschelkalk aquifer (with a no-flow boundary condition). This is in agreement with the hydrogeochemical dataset indicating a dominating aquifer specific evolution of the Muschelkalk groundwater (Nagra 2024f). The selection of the basal limit defines the northern lateral boundary along the Rhine and the Wutach Rivers which have incised the Mesozoic units down to the Middle and Lower Muschelkalk. The base of the evaporitic unit of the Muschelkalk will also be included in the hydrogeological model within the Jura Fold-and-Thrust Belt along the Jura Main Thrust, where it crops out (Fig. 3-2). A possible influence of inflow from the units below the model via the regional faults is tested during the preliminary sensitivity analyses (see Chapter 4).

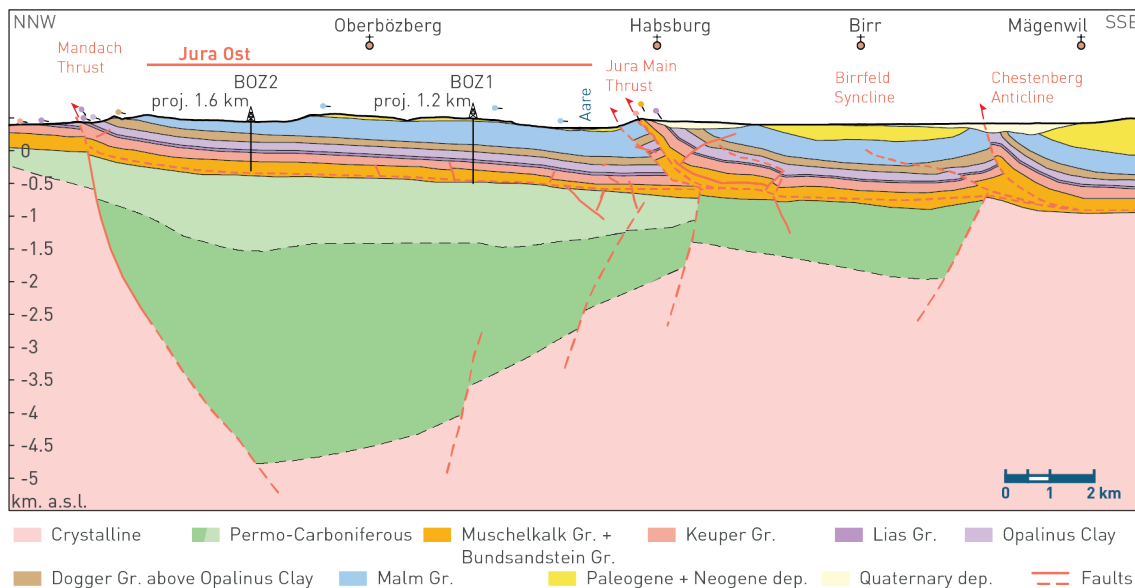


Fig. 3-2: Cross-section through the western model area indicating the geology of the Jura Main Thrust with the outcrops of the evaporitic Muschelkalk (from Nagra 2024f)

3.1.2 Southern model limit

The frontal thrust of the Subalpine Molasse forms a distinctive limit between the Alpine hydrogeological domain, within which groundwater flow is dominated by tectonic features, and the Molasse Basin, dominated by combined interstitial-fractured groundwater flow within a mostly undeformed sedimentary stack. Hence, the southern limit of the model has been defined roughly along the frontal thrust of the Subalpine Molasse (see Fig. 3-3) reaching from the Bodensee in the east all the way to the Emmental, close to Lake Thun, in the west.

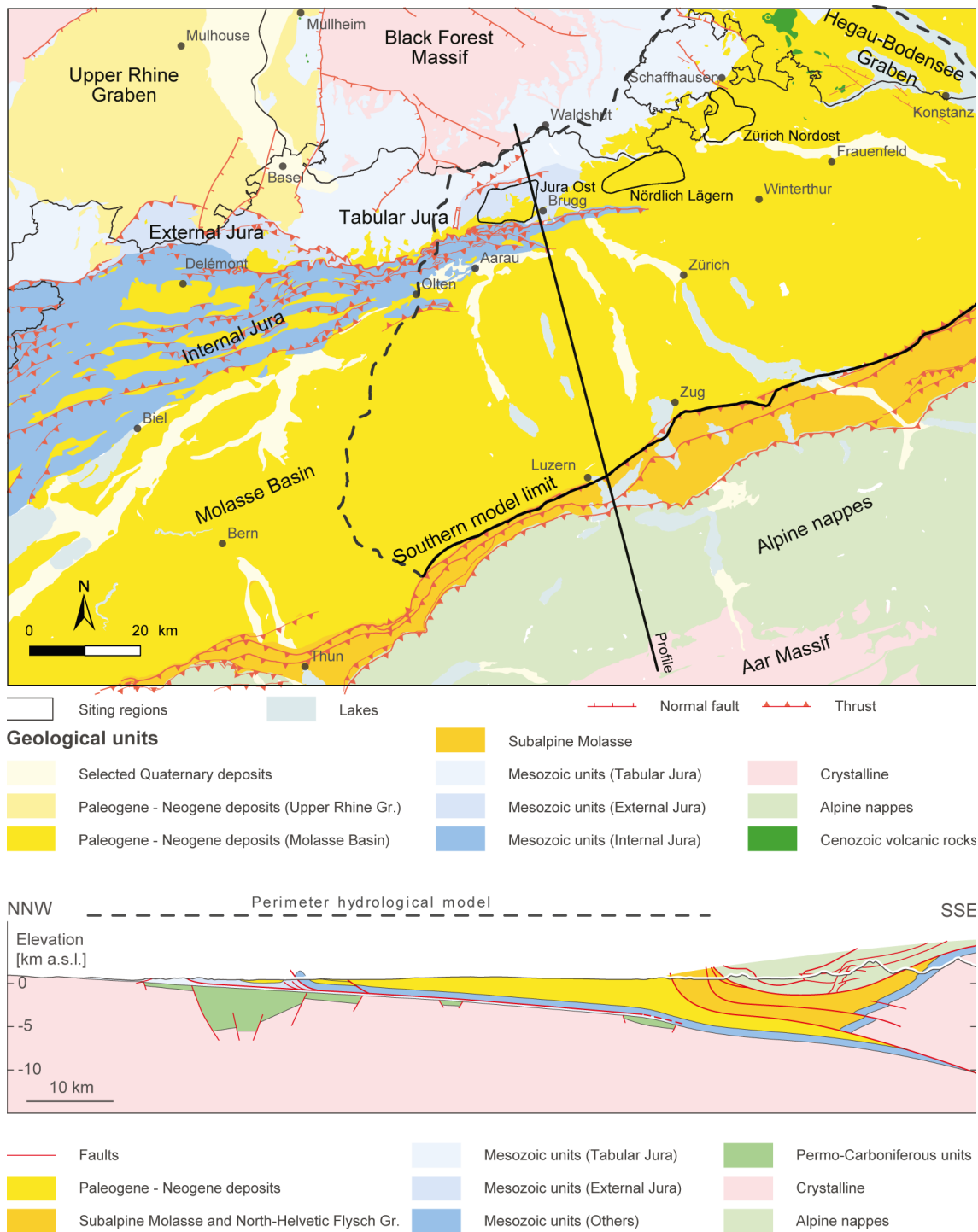


Fig. 3-3: Simplified tectono-geological map with the southern model limits following the frontal thrust of the Subalpine Molasse
Modified from Nagra (2014). Gr.: Graben (map above) or Group (cross-section below).

Qualitative observations support the hypothesis of lateral SW-NE-trending groundwater flow within the tilted Subalpine Molasse, rather than northward-directed flow towards the model, as shown in Fig. 3-4 (blue arrow), where recharge area features are laterally aligned with discharge area features. The black dots in Fig. 3-4 indicate areas within the exposed USM Group where karstic dolines, i.e. recharge area features, are aligned parallel to the frontal thrust (Flehtner & Scholz 2012, Pochon & Zwahlen 2003), suggesting that the UMM Group acts as hydraulic barrier leading to lateral groundwater flow. Possible associated discharge area features suggesting the same spatial trend are shown as white dots in Fig. 3-4, highlighting localities with names which include 'Bad' or 'Brunn'. Although these highly qualitative observations do not exclude the possibility of groundwater interaction between the southern hydrogeological domain at the foot of the Alps with the Molasse Basin, they support the assumption that the chosen southern limit is hydrogeologically meaningful. To decrease uncertainty due to the two possible settings concerning the southern boundary (no NS-directed flow possible, or possible NS-directed recharge in the Malm and Muschelkalk aquifers), both scenarios have been tested in the preliminary sensitivity analyses (see Section 4.3).

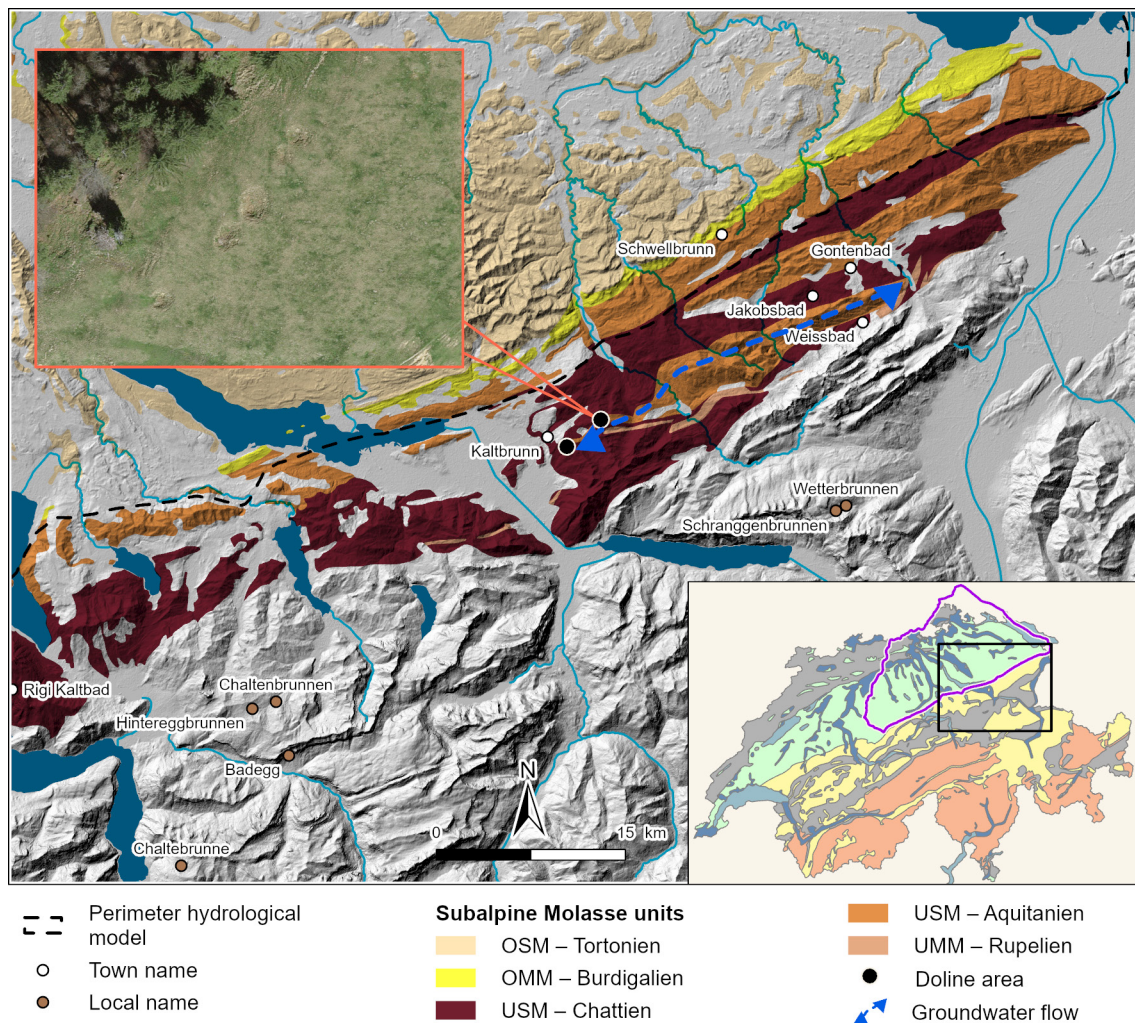


Fig. 3-4: Aerial view of the eastern part of the southern model limit with Subalpine Molasse units drawn to the SE of the frontal thrust

Black dots: areas where dolines and small karstic systems have developed (indicative for recharge) within the tilted upper member of the USM Group (Aquitanien), surrounded by the low-permeable lower member of the USM (Chattien), probably forcing groundwater flow along SW-NE direction (indicated as blue stippled arrow). White dots: Place names which include '...bad', '...brunnen' or '...brunn' in their names (*well* or *bath* in English), indicative for discharge, with a relatively high density within the Subalpine Molasse wedges.

3.1.3 Eastern model limit

The eastern model limit joins the southern model limit where the frontal thrust of the Subalpine Molasse coincides with the southern end of the Bodensee. Wessels et al. (2015) describe large and irregular depressions with sharp upslope edges and smoother lake-ward boundaries (see inset in Fig. 3-5) in deeper waters of the upper lake ('Überlinger See', in about 80 to 100 m depth), the north-western arm of the main basin of the Bodensee. These depressions lack any characteristic indications for mass movements and are interpreted by Wessels et al. (2015) to be caused by groundwater discharge into the lake. To account for such groundwater discharge into the lake, the model limit follows the bathymetric axis of the lake floor, as shown in Fig. 3-5. This allows the definition of constant head boundary conditions along the lake floor and will thereby allow for possible interactions with the intersecting units.

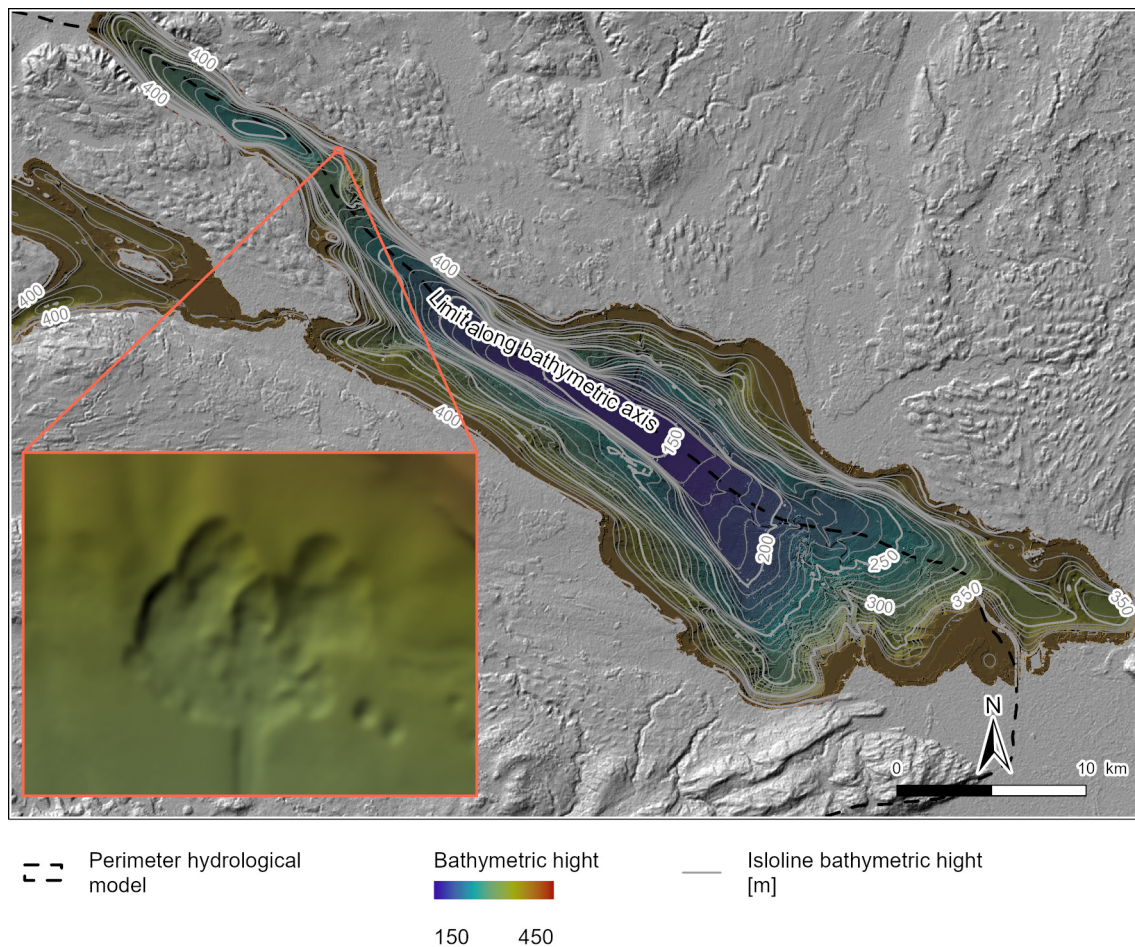


Fig. 3-5: Digital elevation model of the Bodensee area

The indicated eastern model boundary follows the bathymetric axis of the lake floor (shown with grey contour lines), with its lowest parts at altitudes of 180 m a.s.l. The close-up (lower left) is taken from Wessels et al. (2015) showing an irregular depression at depths of 80 – 100 m, interpreted as groundwater discharge areas into the upper lake ('Überlinger See').

3.1.4 North-eastern model limit

The northeastern model limit shown in Fig. 3-6 starts in the southeast at the Bodensee from where it runs along NW-SE-striking fault systems related to the Hegau – Bodensee – Graben all the way to the main Danube sinkhole in Immendingen. This boundary coincides with a hydraulic boundary in the Malm aquifer indicated by the infiltration of the Danube into the karstic Malm aquifer in the sinkhole in Immendingen.

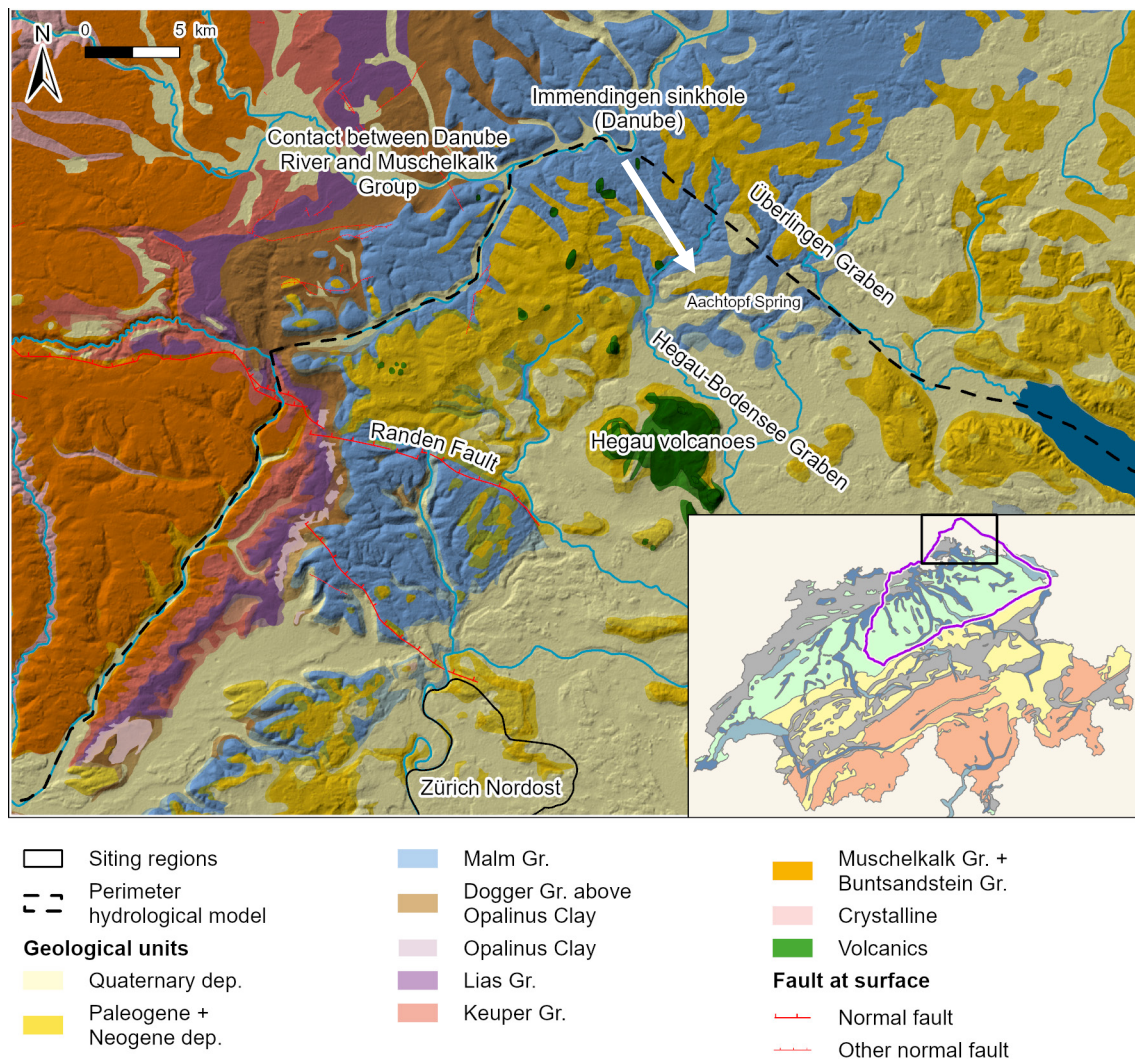


Fig. 3-6: Geological Map of southern Germany and Northern Switzerland (position shown in close-up bottom-right) overlain by a digital elevation model with northeastern model limits

Gr.: Group.

The hydraulic connection (shown as a white arrow in Fig. 3-6) between the Danube sinkhole and the Aachtopf spring (one of the most prominent karst springs in Germany) suggests that the Hegau – Bodensee Graben acts as a drain. The Danube sinkhole right on the model boundary allows for a natural definition of the recharge hydraulic boundary condition for the Malm aquifer. Outcrops for the Muschelkalk in that area are further to the north. Extending the model to these outcrops would have considerably increased the model uncertainty because of the complex geological situation.

3.1.5 North-western model limit

The northwestern model limit runs south from the village of Blumberg (Fig. 3-7) crossing a small portion of the Triassic Muschelkalk to join the Wutach Valley where the valley forms a sharp bend towards the southwest. Along the Wutach Valley, the upper Muschelkalk has been eroded down by the Wutach River into the low-permeable Anhydrite group of the Muschelkalk, which forms the base of the regional hydrogeological model. The model limit within the Wutach Valley therefore follows the top Anhydrite group wherever it crops out, or the Wutach River otherwise. The Wutach River becomes either a no-flow boundary (where cut into the Anhydrite group), or it is a natural head boundary along the portions where it is connected to the upper Muschelkalk.

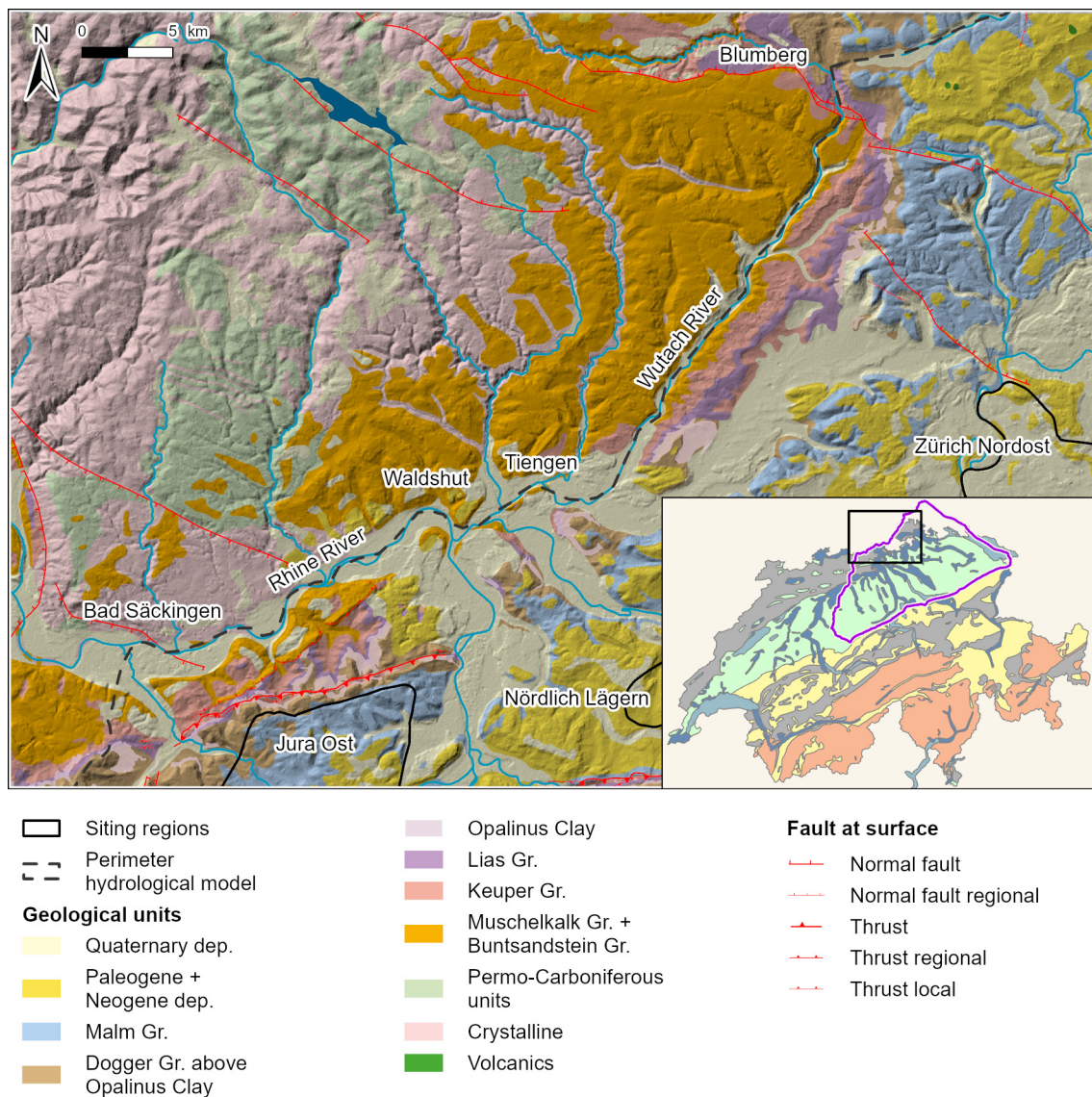


Fig. 3-7: Close up of the north-western model limit portion

Along the Wutach Valley, the model limit follows the surface intersection between the base of the Muschelkalk aquifer whenever above the river. Westwards from the junction between the Wutach and Rhine Rivers, the limit follows the Rhine River down to Bad Säckingen. Gr.: Group.

From the junction with the Rhine River in Waldshut, the model limit follows westwards along the Rhine River to Bad Säckingen. Between Waldshut and Laufenburg, the Rhine River partially has a hydraulic connection with the Muschelkalk aquifer. At Bad Säckingen, the model boundary turns south and runs parallel to N-S-trending fault systems.

3.1.6 Western model limit

The northernmost point of the western model limit is located slightly east of Bad Säckingen, where the EW-trending Eggberg basement fault intersects the Rhine River (Fig. 3-8). From there, the western model boundary roughly runs parallel to the NNE-SSW-oriented faults that become more and more dominant towards the west (Upper Rhine Graben). Further to the south, the model limit follows the Aare, Langete and Emme Rivers, thereby connecting via a surface-defined hydrogeological feature (rivers) to the tectonically defined southern model limit.

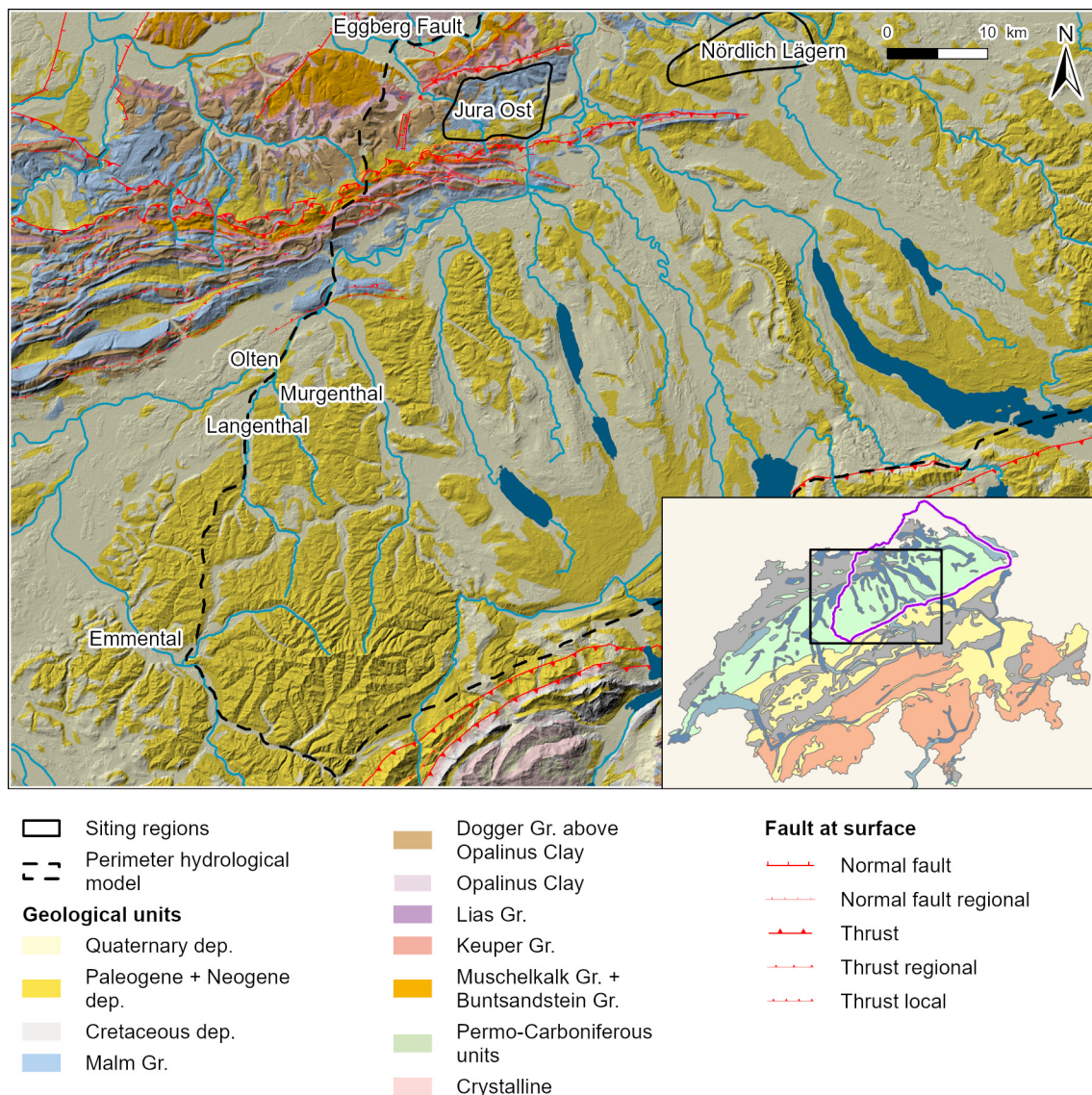


Fig. 3-8: Western model limit along the Säckingen Fault and the Aare, Langete and Emme Rivers

3.2 Regional faults

Faults can be important hydrogeological elements, either because they may have an increased/reduced hydraulic conductivity compared to the surrounding rocks or, because of the offset of aquifers and aquitards along the fault, they may change the continuity of such hydrogeologically important layers. While the strike and dip of faults and possible offsets along faults can be determined using e.g. seismic images or outcrops, the hydraulic properties of a fault can only be measured very locally, e.g. by placing a packer test in a borehole. In the area of the hydrogeological model discussed here, no datasets exist that would allow the derivation of representative transmissivities on a scale of hundreds of metres or larger, i.e. hydraulic properties that would be indicative for the whole fault. This lack of direct measurements can be addressed by using conceptual approaches and sensitivity analyses. In the hydrogeological model, different fault concepts were considered in addition to the effect of changes in the flow cross-section of the faults in the sense that the faults have homogeneous high or low permeabilities. These cases cannot usually be further justified solely by comparing them to measured hydraulic heads, and at many locations, they are primarily influenced by nearby infiltration and exfiltration zones.

In the model, only regional-scale faults have been implemented (see Fig. 3-9). These large-scale faults may have an impact on the regional flow system as they may prohibit flow across fault planes or act as water conducting pathways, depending on parametrisation, and hence their role needs to be analysed and accounted for. A sensitivity analysis concerning the parametrisation of faults depending on their orientation with respect to the dominant regional stress field was performed and is described in more detail in Chapter 5.

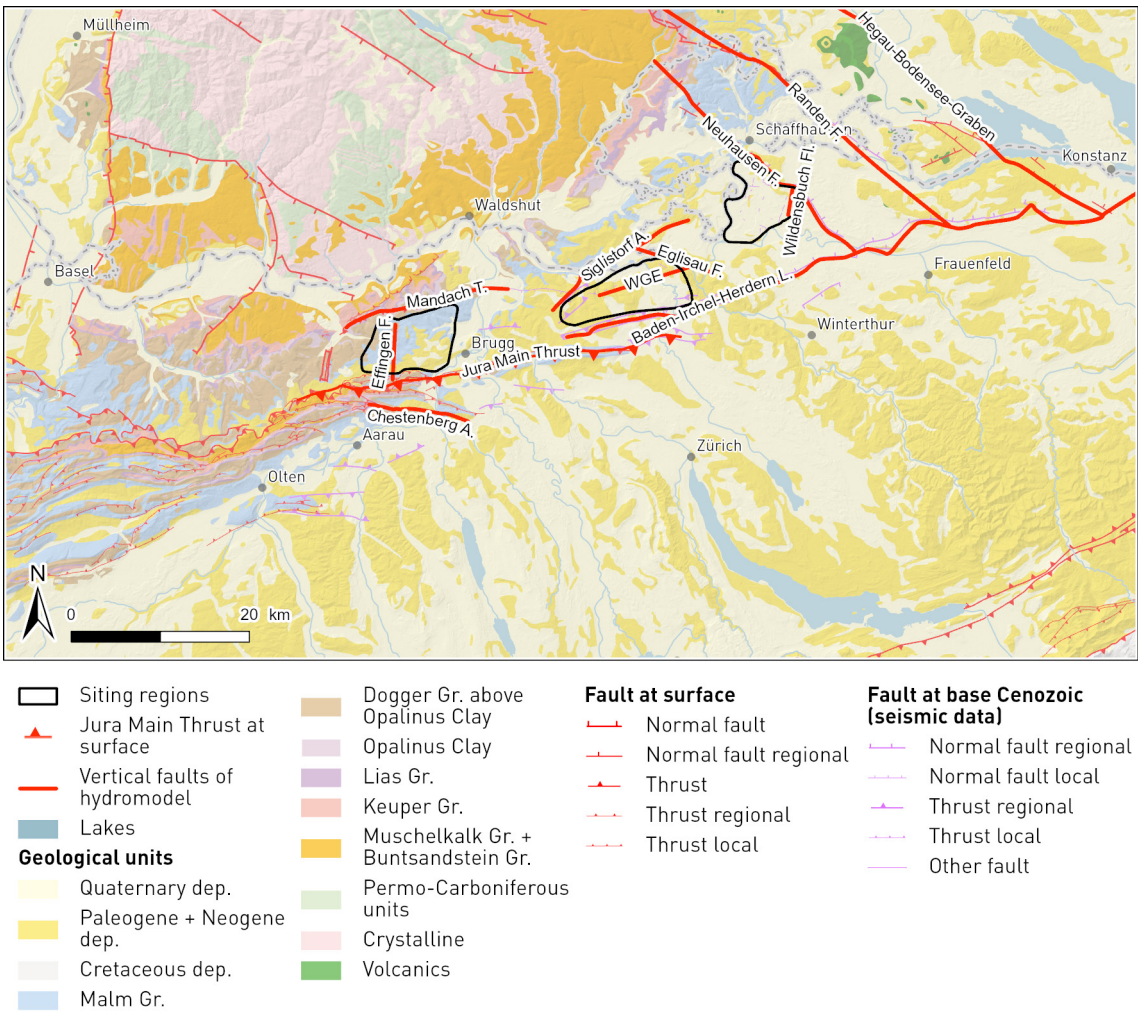


Fig. 3-9: Geological map including the regional-scale faults implemented in the hydrogeological model in a simplified way (modified from Nagra 2024f)

WGE: Weiach – Glattfelden – Eglisau Lineament, A: Anticline, F: Fault, Fl: Flexure, T: Thrust

3.3 3D geological model

The geological models used as a starting point to build the hydrogeological model and implement the abstracted hydrostratigraphy summarised in Chapter 2 were a regional-scale geological model detailed in Gmünder et al. (2013) (termed Nagra model below) and the geological model GeoMol detailed in Allenbach et al. (2017). These models include, next to a digital elevation model (DEM) the following main surfaces:

- Top Upper Freshwater Molasse Group (OSM, from GeoMol)
- Top Upper Marine Molasse Group (OMM, from GeoMol)
- Top Lower Freshwater Molasse Group (USM, from GeoMol)
- Top Lower Marine Molasse Group (UMM, from GeoMol)
- Base Cenozoic (from GeoMol)
- Top Malm Group (from Nagra model)
- Top Effingen Member (from Nagra model)
- Top Dogger Group (from Nagra model)
- Top Opalinus Clay (from Nagra model)
- Top Lias Group (from Nagra model)
- Top Keuper Group (from Nagra model)
- Top Muschelkalk Group (from Nagra model)
- Base Mesozoic (from Nagra model)
- Regional-scale faults (from Nagra model)

However, both the Nagra model as well as the GeoMol predate an extensive borehole campaign from 2020 – 2022 where 9 new boreholes have been drilled and analysed. The models also predate a 3D seismic campaign from 2016 – 2017. The hydrogeological model includes the newly acquired information from these two field campaigns. A seismic quick look interpretation of the three siting regions was introduced into the hydrogeological model. The geological surfaces mentioned above were integrated from the seismic quick-look interpretations into the existing geological surfaces by replacing the respective areas in the old geological surfaces with the new interpretation. A buffer zone of 1 km around the surfaces was used to adjust for any depth mismatch between the new and old surfaces.

According to the hydrostratigraphic abstraction, several intermediate units, in addition to the surfaces detailed above, were included in the hydrogeological model. These additional units include, where applicable:

- Upper Muschelkalk
- Passwang Formation
- Klingnau Formation
- Hauptrogenstein Formation
- Upper Dogger

These units were implemented based on (relative) thickness models determined from borehole thicknesses and conceptual considerations.

3.4 Finite element mesh construction

The 3D mesh construction is based on the implementation of a so-called super-mesh. This super-mesh integrates all constraints related to relevant geometrical and structural features of the hydrogeological model, geological interfaces and important topographical features. These data of different types, i.e. polygons, lines, points, were first prepared in a geographic information system (GIS), and included rivers, faults traces, contours of geological outcrops, contours of areas of interest, locations of observation boreholes, etc. Having defined the super-mesh, a 2D mesh was then created (see Fig. 3-10). The latter was progressively refined in the vicinity of the rivers and faults and, in particular, around the target areas.

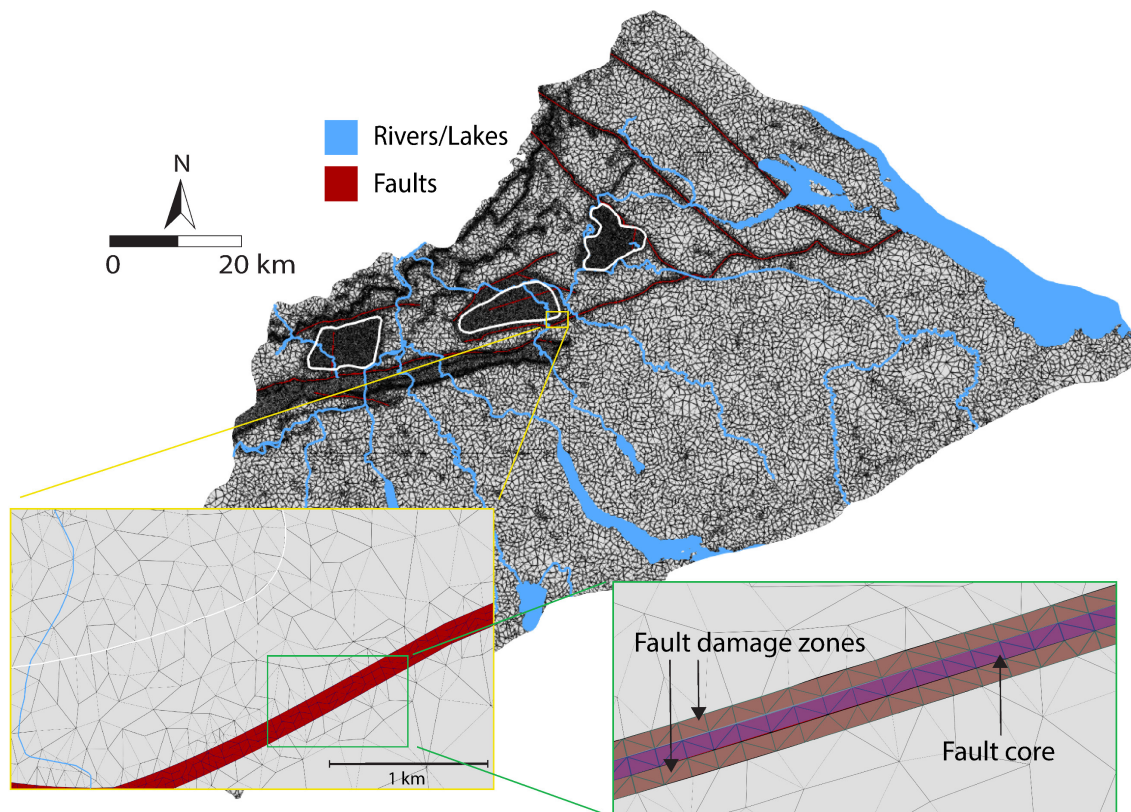


Fig. 3-10: View of the 2D mesh of the hydrogeological model

Insets show the higher resolution in the area of the siting region (example of an area close to NL) and the 3-layer setting along vertical faults. Siting regions are shown as white polygons.

The 2D mesh was then extended to 3D using geological interfaces and adjusting the depth-values of each point as necessary. In total, 22 geological layers, from the lower middle Muschelkalk to the top Quaternary, were discretised into a 3D finite element mesh. Regional faults have been implemented as three rows of vertical elements of 50 m thickness each: a fault-core layer surrounded by two damage-zone layers (see inset in Fig. 3-10). This setting allows to assign and test different fault parametrisations, for example fully transmissive, impervious or combined transmissive-impervious faults. The exception here is the area of the Jura Main Thrust. The Jura Main Thrust is inclined and includes a number of important outcrops of the local and regional aquifers (see Fig. 3-2). Hence, this fault zone was modelled separately keeping the inclined faults (see Fig. 3-11).

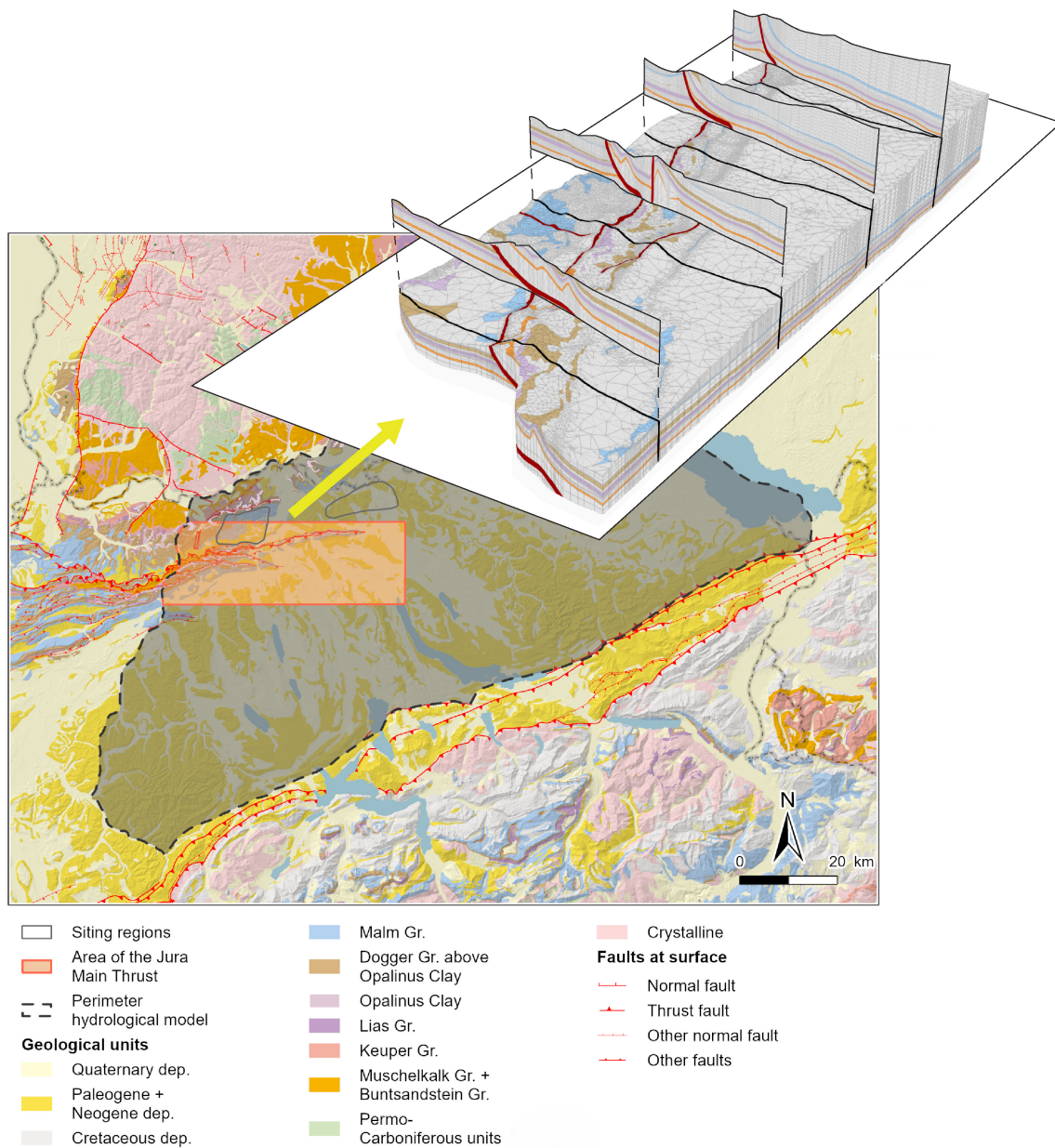


Fig. 3-11: The area of the Jura Main Thrust has been modelled in detail (orange polygon, also see inset of the specifically modelled part) since it includes outcrops of important regional aquifers and aquitards

2× vertical exaggeration of the inset.

The final step in the 3D FE mesh construction was to refine the resulting layers representing geological formations or members. Some of the layers have a (very large) thickness (e.g. USM Group) and need to be numerically subdivided to better reproduce e.g. vertical hydraulic gradients. Some units include distinct geological layers that may have to be parametrised separately (e.g. in the Lias and Dogger Groups). Of note here is the «Herrenwis Unit» which was implemented within the Dogger Group above Opalinus Clay.

The final hydrogeological model hence represents 22 geological units using 41 numerical layers (see Fig. 3-12 for the main aquifer units). The total number of 3D elements in the mesh is almost 4.5 million which, in terms of computation time, is manageable.

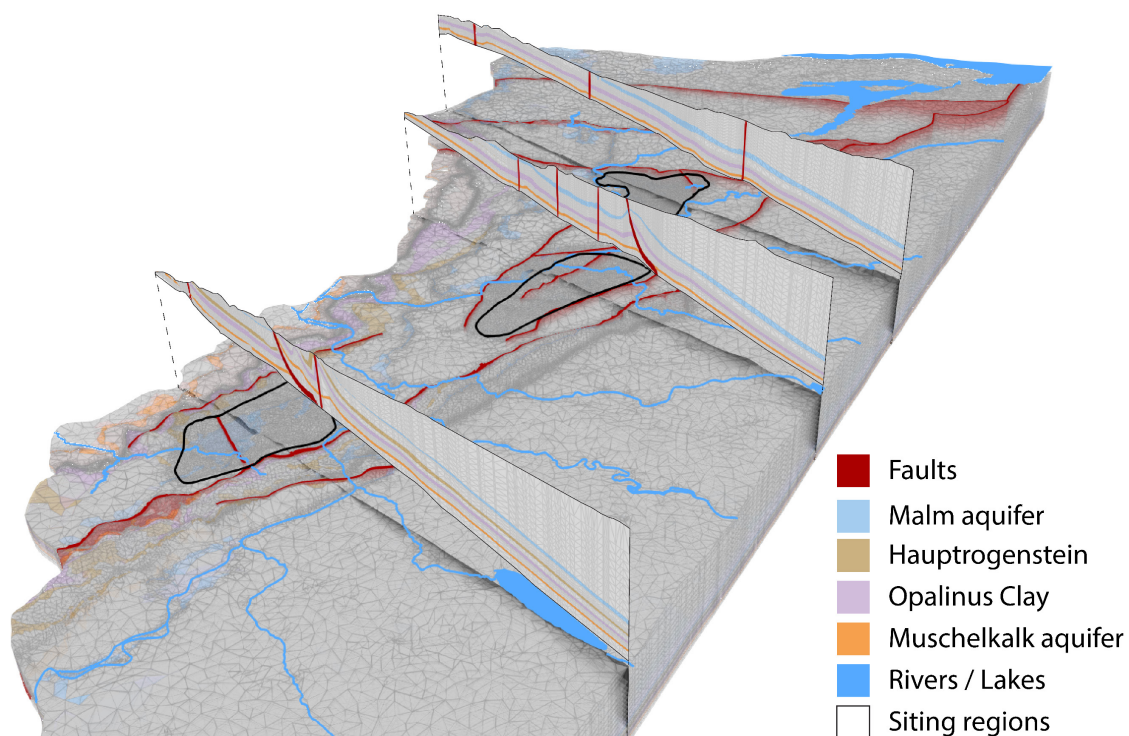


Fig. 3-12: Semi-transparent 3D view of the hydrogeological model, together with cross-sections, of the northeastern part of the hydrogeological model

Shown are the main regional Malm, Hauptrogenstein and Muschelkalk aquifers together with the Opalinus Clay aquitard. Siting regions are shown with black polygons. The volumetric model is 2× vertical exaggerated, the cross-sections are exaggerated 3×.

4 Preliminary sensitivity analyses for selection of base case

The main objective of the preliminary sensitivity analysis is to define robust outer flow boundary conditions that are consistent with both, the conceptual understanding of the hydrogeological system and the available data. The preliminary sensitivity analysis is based on an iterative process including the adjustment of the flow boundary conditions and the adjustment of the hydraulic conductivities. A total of 72 steady-state flow simulations, each with a different set of outer boundary conditions and model parametrisations, were performed. The simulated hydraulic heads were then compared with a set of 77 observed hydraulic heads in the Mesozoic aquifers of the Muschelkalk, Keuper, Hauptrogenstein and Malm, as well as in the Molasse units (Appendix 1). The dataset consists of a selection of robust hydraulic heads that were selected based on the criteria described in Nusch et al. (2013). For the comparison between the model results and the observations, various calibration criteria were calculated to compare, sort and classify the simulation results. These criteria are the correlation coefficient R , the mean absolute error (MAE), the sum of squared errors (SSE), and the mean squared error (MSE). Groundwater flow budgets were also calculated in selected nodes/limits of the model. Based on these metrics, the simulation that best fits the available observation data was chosen as a base case and used for a more detailed parameter calibration using the well-known PEST-algorithms (Doherty 2004).

In the following, the different outer boundary conditions and initial model parameters are described, with special attention to the surface boundary conditions.

4.1 Surface recharge spreading layer

The model employs a surface recharge spreading layer (RSL) which is considered to be the topmost groundwater flow system occurring at very shallow depths (Fig. 4-1). The thickness E of the RSL is poorly known (it can vary between 10 m to several hundreds of metres). However, what matters most is that its transmissivity ($T \text{ [m}^2\text{/s]} = K \text{ [m/s]} \times E \text{ [m]}$) is far higher than those of the deeper aquifers since it is exposed to weathering and surface erosion processes. The hydrogeology in the RSL is topography-driven and connected to the topographical drainage system. The RSL ensures that groundwater recharge can either percolate to deeper aquifers or flow to rivers and lakes depending on the hydraulic characteristics of the local geology and topography.

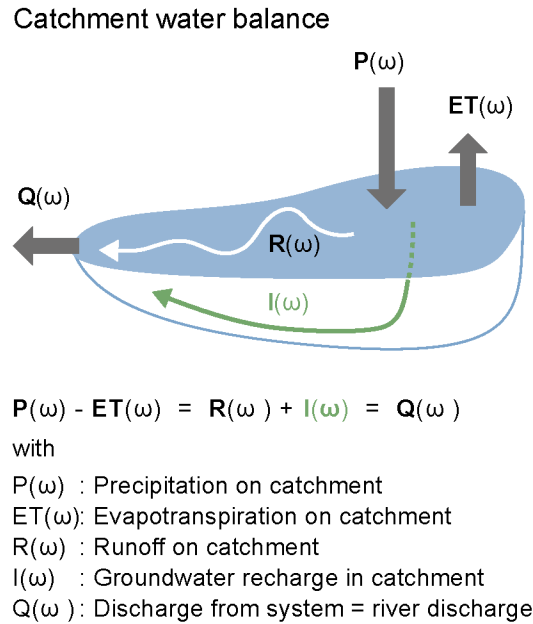


Fig. 4-1: Basic principle of a catchment water balance, assuming identical hydrological and hydrogeological catchments extends, with the discharge rate Q reflecting the effective precipitation, i.e. $P - ET$

4.1.1 Surface flow boundary estimation

The diffuse groundwater recharge to be applied to the RSL was estimated based on water balance calculations in which each component of the water balance, i.e. precipitation, evapotranspiration and runoff, was spatially mapped. The spatial distribution of rainfall comes from CHIRPS (Climate Hazards group InfraRed Precipitation with Station data; Funk et al. 2015). The runoff component was assessed by soil types and combined with analysis of the digital elevation model to obtain the runoff coefficients (see Bussard et al. 2004 for details). The evapotranspiration, however, which is the most uncertain component, was estimated using Modis satellite imagery from Nasa (Modis is a Moderate-resolution Imaging Spectroradiometer capable of measuring, amongst other things, the total precipitable water and the vegetation and land-surface cover). These satellite images allow the estimation of evapotranspiration using calibration and validation with ground data from reference catchments for which water balances are established by hydrograph separation in order to obtain the correction factor which is then applied to the entire satellite image.

These data were used to calculate spatially distributed water balances. The mean annual diffuse groundwater recharge has been calculated to 337 mm/yr, representing 28% of the average annual precipitation. The estimated diffuse and spatially distributed groundwater recharge was applied to the RSL as a Neumann boundary condition. Fig. 4-2 shows the spatial variability of the groundwater recharge as implemented in the model as the surface boundary condition. The highest values are encountered along the southern boundary where rainfall intensities are well above the average, resulting in higher groundwater recharge. Using the surface recharge estimated from satellite data, hydraulic heads equal to the topographic elevations of the surface water bodies (for rivers and lakes) were assigned as a Dirichlet boundary condition. This modelling approach is equivalent to coupling surface waters to groundwater flow, but with a much lesser degree of numerical complexity. In the regional model, this has led to a total of 5'511 Dirichlet boundary nodes and 70'453 Neumann boundary nodes on the surface.

A second surface boundary condition was also constructed for the sensitivity analyses where the estimated mean annual value of 337 mm/yr was applied uniformly over the whole model domain.

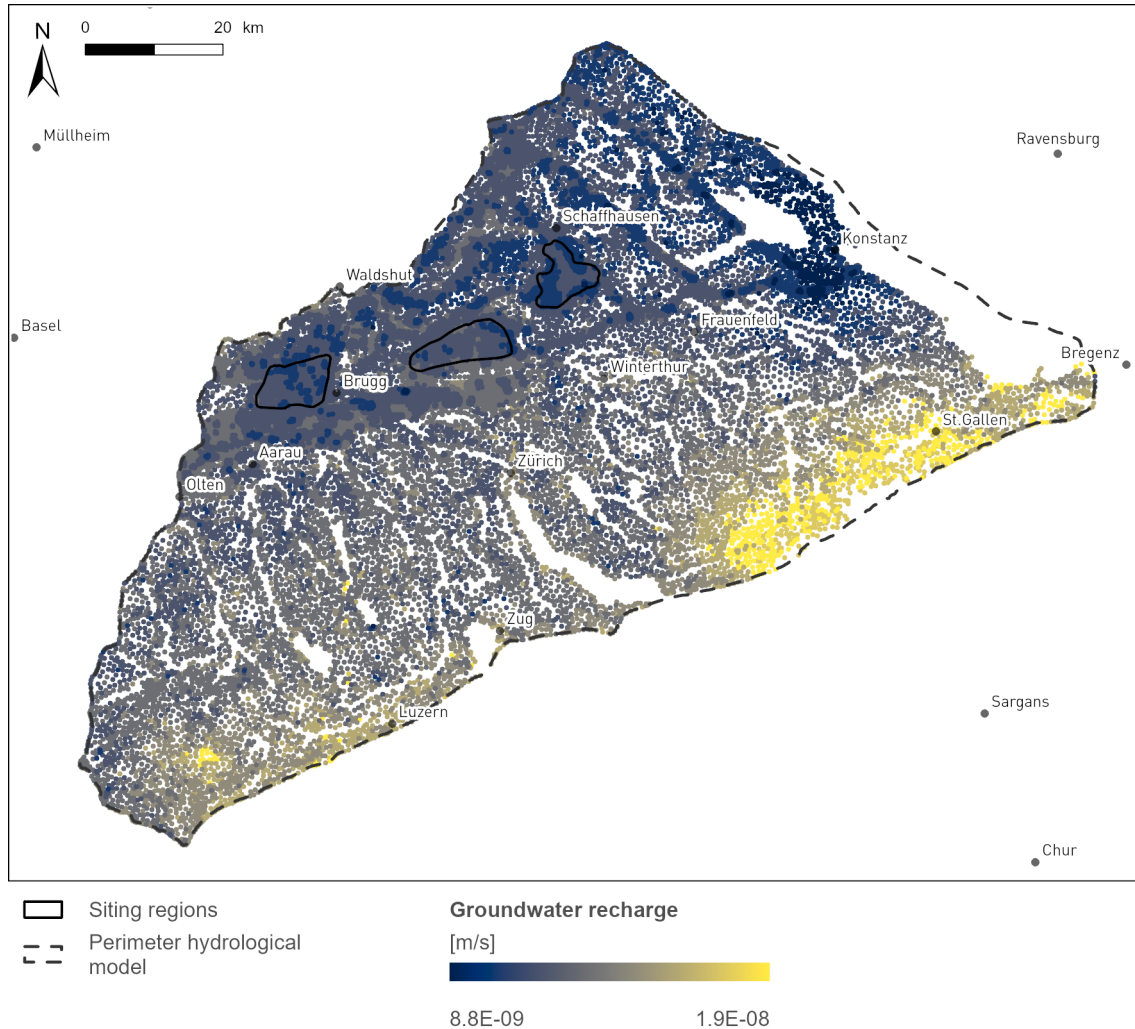


Fig. 4-2: Map of the spatial variability of the groundwater recharge [m/s] implemented in the model

Areas with no visible points relate to rivers and lakes where fixed heads were assigned as Dirichlet boundary conditions.

4.1.2 Estimation of surface parameters

The estimation of surface parameters is essential for the construction of the regional hydrogeological model, ensuring that the surface flow boundary conditions as well as the transmissivities of the recharge spreading layer are consistent with the outcropping geological units and the regional water balance. In other words, the observed surface hydraulic heads must be reproduced with reasonable residual errors. The parametrisation of the surface layer is an integral part of the setup of the initial/starting model in order to avoid any parametric bias and hence must be carried out before the definition of lateral flow boundary conditions, followed by the calibration of aquifers.

After assigning the surface flow boundary conditions and attributing the initial parameters to the modelled layers (see Section 4.2), the calibration of the hydraulic conductivities of the recharge spreading layer was carried out by means of inverse modelling using the PEST algorithm (Doherty 2004). 23 calibration zones were defined, corresponding to the geological outcrops of the modelled layers (see Fig. 4-3). The lithology of each outcrop was used to determine the range of plausible solutions of the hydraulic conductivity. More than 3500 hydraulic head data, mainly provided by the cantons Aargau and Zürich from their cantonal databases, were used to constrain the inverse modelling algorithm PEST (see Fig. 4-3). Observation points representing springs were given a lower weight during the calibration because of the uncertainty of their influence on the source layer in the calculation of the total error. Upon convergence of the algorithm, the total error was considerably reduced compared to the initial value.

Fig. 4-3 presents the calibrated hydraulic conductivities for the spreading layer of uniform unit thickness (i.e. 23 zones corresponding to the outcropping geological units), ranging between 10^{-4} m/s and 10^{-2} m/s, reflecting a reasonable contrast of two orders of magnitude between permeable and less-permeable units.

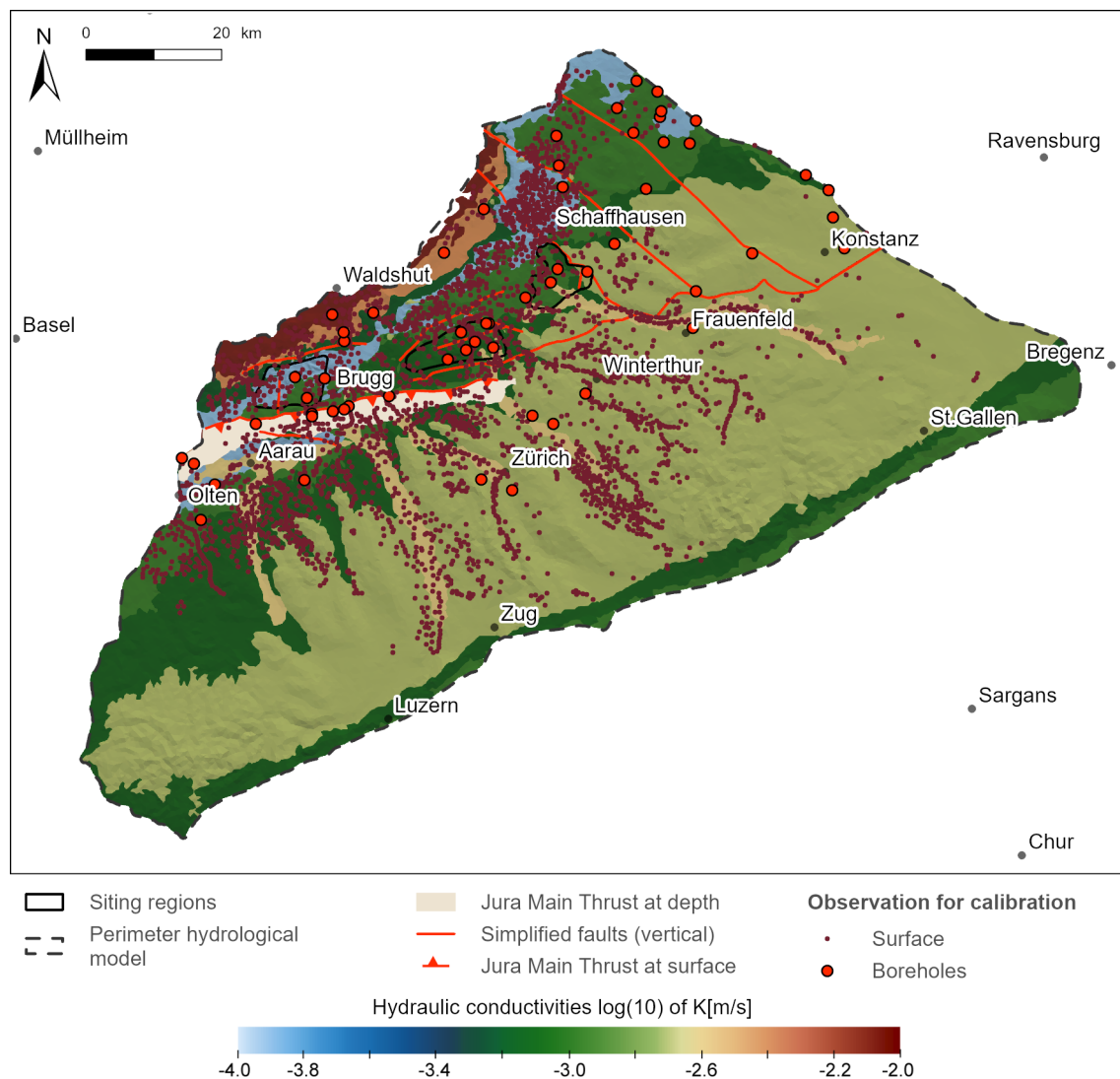


Fig. 4-3: Initial model – calibrated hydraulic conductivities in the spreading layer on the model surface ($\log_{10}(K)$ [m/s])

Fig. 4-4 shows a comparison between simulated and measured hydraulic heads after calibration of the surface parameters. It reveals a good agreement between surface hydraulic head data and simulated values. The majority of the 3'500 near-surface observation points are reproduced with calibration residuals of less than 20 m.

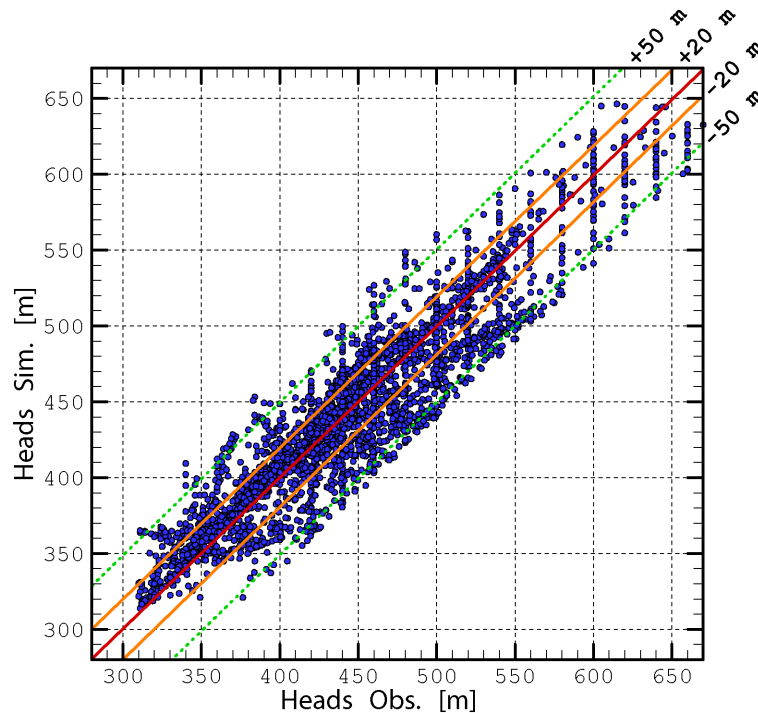


Fig. 4-4: Comparison between simulated and measured near-surface hydraulic heads

Sim.: simulated, Obs.: observed/measured.

Fig. 4-5 shows the simulated near surface piezometric map of the initial model. As expected, the flow in shallow aquifers is largely controlled by topography and the hydrologic network. High groundwater levels in alpine (e.g. St Gallen and Emmental areas) and jurassian (e.g. Wutach River) elevated topography represent recharge areas from which surface flow into rivers and lakes follows topography. The confluences between the Aare and Limmat Rivers, and between the Aare and Rhine Rivers, are most probably the major discharge areas of the regional groundwater flow system. The Bodensee also represents a discharge area of the modelled multi-layer system.

The water budget resulting from this preliminary model is, due to the modelling approach, in agreement with initial water balance estimations. The inflow from surface infiltration is equal to $2.40 \times 10^9 \text{ m}^3/\text{yr}$ ($\sim 0.30 \text{ m}/\text{yr}$ integrated over the model area.), and the inflow from Dirichlet boundary conditions is $2.85 \times 10^9 \text{ m}^3/\text{yr}$, while discharge (outflow) is $5.25 \times 10^9 \text{ m}^3/\text{yr}$. The difference between estimated diffuse recharge and simulated surface influxes is due to Dirichlet boundary nodes reducing the effective surface available for infiltration. With the cumulated in- and outflows being balanced, the net groundwater discharge to rivers is $1.36 \times 10^9 \text{ m}^3/\text{yr}$ and $5.96 \times 10^8 \text{ m}^3/\text{yr}$ to lakes. The total surface water discharge is $1.95 \times 10^9 \text{ m}^3/\text{yr}$, corresponding to 83% of the total surface infiltration. This means that 17% of the total groundwater recharge on the model area is transformed into deep percolation.

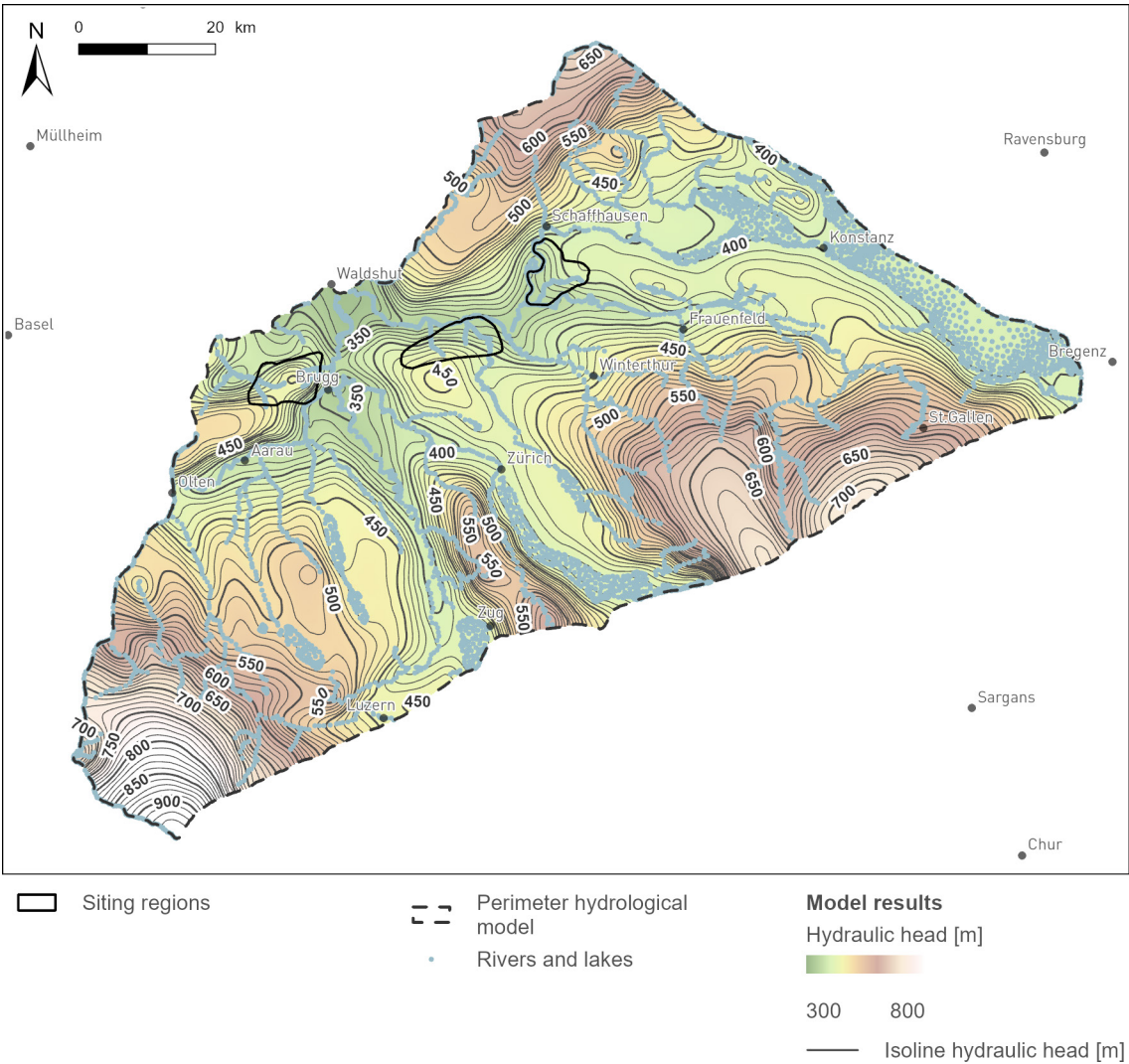


Fig. 4-5: Simulated near-surface hydraulic head distribution
Siting regions are shown as black polygons and surface water bodies by light blue points.

4.2 Preliminary parametrisation of units

For the preliminary sensitivity analyses, the available dataset consisting of hydraulic conductivity data, further referred to as K values, determined from borehole investigations, i.e. hydrotests compiled by Nusch et al. (2013) as well as new data from Nagra's recent drilling campaign (Nagra 2024f, 2024e) was used. Tab. 4-1 shows the initial horizontal and vertical hydraulic conductivities assigned to the model layers for the sensitivity analysis.

To avoid a bias during the initial sensitivity analyses stemming from the precise, but homogeneous K values reported in Tab. 4-1, another initial set of parameters was defined, based on an initial preliminary calibration, where conductivities for some hydrogeological units were either increased or decreased using a multiplier (see Tab. 4-2), leading to two sets for initial parametrisations, ID_S1 and ID_S2.

Tab. 4-1: Initial horizontal and vertical K values of the modelled layers

The K values for the main regional aquifers are further adjusted based on conceptual models (see text for further details).

Model layer	K_h [m/s]	K_v [m/s]
Anhydrite group	1×10^{-13}	1×10^{-13}
Muschelkalk aquifer	3×10^{-7}	3×10^{-7}
Gipskeuper	1×10^{-13}	1×10^{-13}
Keuper aquifer	2×10^{-9}	2×10^{-9}
Lower confining units (consists of several model units)	3×10^{-13}	3×10^{-14}
	3×10^{-13}	3×10^{-14}
	3×10^{-13}	3×10^{-14}
	3×10^{-13}	3×10^{-14}
Opalinus Clay	5×10^{-14}	1×10^{-14}
Upper confining units (consists of several model units)	3×10^{-13}	3×10^{-14}
	3×10^{-13}	3×10^{-14}
	3×10^{-13}	3×10^{-14}
Hauptrogenstein aquifer	2×10^{-8}	2×10^{-8}
Upper confining units	3×10^{-13}	3×10^{-14}
Effingen Member	1×10^{-11}	1×10^{-12}
Malm aquifer (consists of several model units)	1×10^{-7}	1×10^{-7}
	1×10^{-7}	1×10^{-7}
	1×10^{-7}	1×10^{-7}
USM	2×10^{-8}	2×10^{-11}
OMM	5×10^{-7}	1×10^{-9}
OSM	2×10^{-8}	2×10^{-11}
Quaternary	1×10^{-4}	1×10^{-5}
Jura Main Thrust	1×10^{-10}	1×10^{-10}

Tab. 4-2: Multipliers used to increase contrasts between some aquifers/aquitards
All other model layers have a multiplier of 1 even in ID_S2.

Model layer	ID_S1	ID_S2
Muschelkalk aquifer	1	10
Keuper aquifer	1	10
Malm aquifer (consists of several model units)	1	10
USM	1	2.8
OMM	1	0.1
OSM	1	0.6

These initial model parameters, or their multipliers, have been further adjusted based on conceptual considerations detailed in the following. The first consideration assumes a depth dependency of K values. Fig. 4-6 shows examples of the relationships between hydraulic conductivities and depth for the Malm and Muschelkalk aquifers.

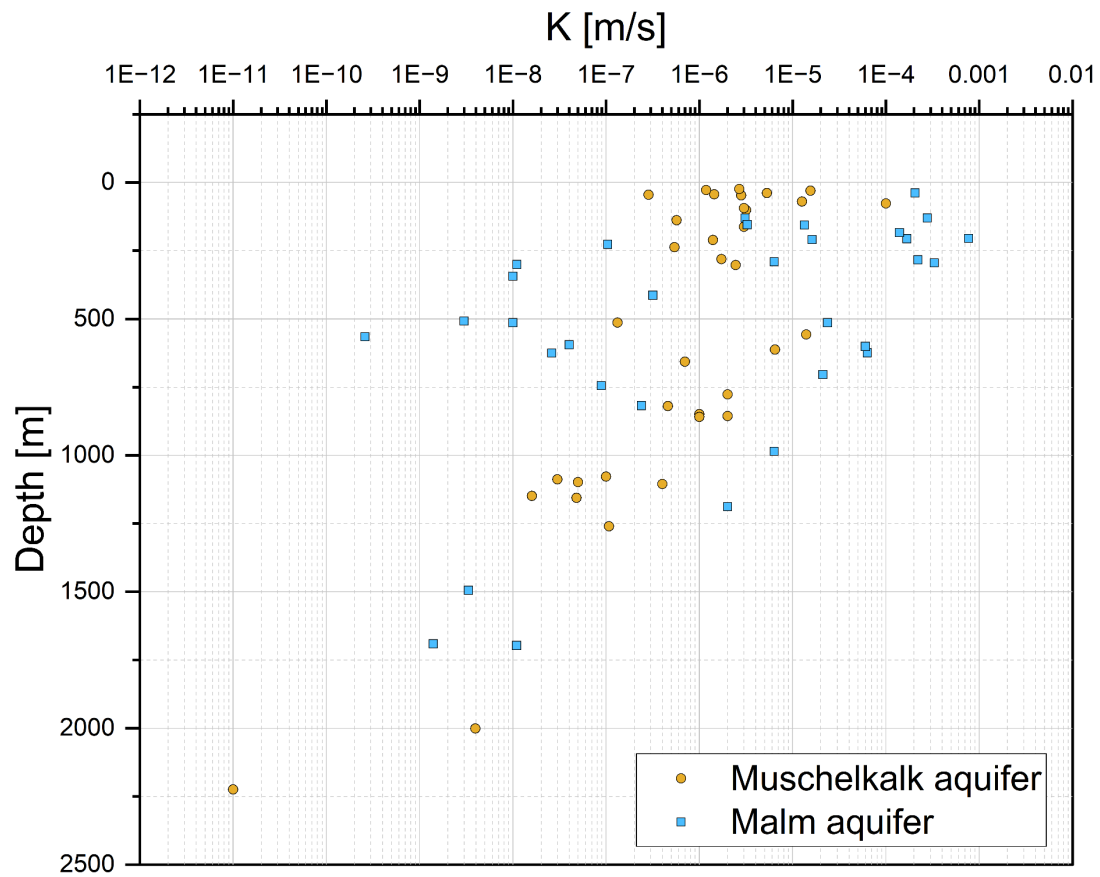


Fig. 4-6: Depth dependency of K values observed in the Malm and Muschelkalk aquifers

The dataset is presented for the well-characterised Malm and Muschelkalk aquifers. Note that a depth dependency was also implemented in the model for the Hauptrogenstein aquifer. A different approach was considered for the Keuper aquifer (see Chapter 8 and Section 7.2).

For the Muschelkalk aquifer, the depth dependency is clearly visible (see Fig. 4-6). K values range between 10^{-5} to 10^{-6} m/s near the surface to 10^{-8} m/s at depth, with one observation reaching 10^{-11} m/s. For the Malm aquifer, the depth dependency is somewhat shadowed by the large variability of K values in the model area at the near surface and the lack of data from areas where the Malm is at greater depths. However, a number of K values are available for an area outside the model area in Southern Germany. Here, the depth trend is clearly visible but in general K values are much higher than in the model area (ranging between 1×10^{-3} to 1×10^{-7} m/s). This points to regional differences in the depth of karst development and maybe also in the lithofacies (Nagra 2024f).

In general, the depth dependencies of K values are explained by fracture density and porosity (e.g. Gmünder et al. 2014). Fracture density presumably is higher, with higher hydraulic conductivities, at the surface than at depth. Hence, fracture density and porosity decrease with depth due to the increasing overburden leading to lower K values. As a guideline, surface fracture density was used which is biased because it disregards faults at depth. However, this fracture density aids in the determination of hydraulic properties of the deeper hydrogeological units. This fracture density guided approach led to values of up to one order of magnitude higher for the regions with maximum fracture densities, while retaining minimum K values for the non-fractured areas, but still consistent with the K value depth-dependency.

Similar K/depth trends can be observed in other regional aquifers in the model area; however, the number of observations is (much) smaller for these aquifers compared to the Malm and Muschelkalk aquifers.

4.3 Lateral flow boundary conditions

The calibration of the steady-state flow model, representing the final aim of this preliminary sensitivity analysis, is based on an iterative process including the adjustment of the hydraulic conductivities and the adjustment of the flow boundary conditions (Fbcs). Faults were initially considered as transparent (i.e. they have the same hydraulic conductivities as the adjacent hydrogeological unit).

To determine lateral boundary conditions, piezometric maps for the OMM, Malm and Muschelkalk aquifers have been prepared based on observed hydraulic heads. To acknowledge all available information and also the conceptual models based on the direct or indirect observations along the boundary locations (see Section 3.1 for details), two sets of lateral boundary conditions were implemented according to Tab. 4-3.

Tab. 4-3: Definition of lateral flow boundary conditions for model limits

Note that the Malm crops out in the northwestern part of the model and thus has no direct connection with the NW model limit. Similarly, the OMM has no direct connection with the northern boundaries of the model.

Boundary	BDCode	1	2
Muschelkalk S limit	MuS	H = 500 m	No flow
Muschelkalk E limit	MuE	300 m < H < 500 m	300 m < H < 375 m
Muschelkalk NE limit	MuNE	H=350 m	no flow
Muschelkalk NW limit	MuNW	no flow	Wutach River head
Muschelkalk W limit	MuW	H = 500 m	H = 600 m
Muschelkalk surface-water-outcrop intersection	MuO	fixed heads from topography	no flow
Malm S limit	MaS	H = 500 m	No flow
Malm W limit	MaE	H = 475 m	no flow
Malm NE limit	MaN	no flow	no flow
Malm W limit	MaW	no flow	H = 475 m
Malm surface-water-outcrop intersection	MaO	fixed heads from topography	no flow
OMM S limit	OMMS	no flow	no flow
OMM W limit	OMMW	no flow	no flow
OMM E limit	OMME	H = 450 m	425 m < H < 450 m
OMM surface-water-outcrop intersection	OMMO	fixed heads from topography	H on undeformed layers
Diffuse groundwater recharge	DGR	Spatially distributed recharge	homogeneous recharge
Faults	F	impervious	transmissive
Basement	B	no flow	H along fault intersections

Combining these two sets of different lateral boundary conditions with the two sets of parameters for the different hydrogeological units resulted in a total of 72 steady-state flow simulations (see Tab. 4-4).

Tab. 4-4: Definition of model variants based on lateral flow boundary conditions

Abbreviations from Tab. 4-3. Numbers 1 and 2 in the table refer to boundary conditions defined in Tab. 4-3, ID_S1 and ID_S2 refer to the two sets of multipliers shown in Tab. 4-2. For example, while e.g. model variants 1 and 37 share the exact same boundary conditions, variant 1 was calculated using ID_S1 for layer parametrisation while variant 37 was calculated using ID_S2 for the layer parameters.

ID_S1	MuS	MuE	MuNE	MuNW	MuW	MuO	MaS	MaE	MaN	MaW	MaO	OMMS	OMME	OMMW	DGR	F	B	ID_S2
1	1	2	1	2	2	1	1	1	1	2	1	1	1	1	1	1	1	37
2	1	2	1	2	2	1	1	1	1	2	1	1	1	1	1	1	2	38
3	1	2	1	2	2	1	1	1	1	2	1	1	1	1	1	2	1	39
4	1	2	1	2	2	1	1	1	1	2	1	1	1	1	1	2	2	40
5	1	2	1	2	2	1	1	1	1	2	1	1	1	1	2	1	1	41
6	1	2	1	2	2	1	1	1	1	2	1	1	1	1	2	1	2	42
7	1	2	1	2	2	1	1	1	1	2	1	1	1	1	2	2	1	43
8	1	2	1	2	2	1	1	1	1	2	1	1	2	1	2	2	2	44
9	1	2	1	2	2	1	1	1	1	2	1	1	2	1	1	1	1	45
10	1	2	1	2	2	1	1	1	1	2	1	1	2	1	1	1	2	46
11	1	2	1	2	2	1	1	1	1	2	1	1	2	1	1	2	1	47
12	1	2	1	2	2	1	1	1	1	2	1	1	2	1	1	2	2	48
13	1	2	1	2	2	1	1	1	1	2	1	1	2	1	2	1	1	49
14	1	2	1	2	2	1	1	1	1	2	1	1	2	1	2	1	2	50
15	1	2	1	2	2	1	1	1	1	2	1	1	2	1	2	2	1	51
16	1	2	1	2	2	1	1	1	1	2	1	1	1	1	2	2	2	52
17	2	1	1	1	1	1	2	1	1	1	1	1	1	1	1	2	1	53
18	2	1	1	1	1	1	2	1	1	1	1	1	1	1	1	2	2	54
19	2	1	1	1	1	1	2	1	1	1	1	1	1	1	2	2	1	55
20	2	1	1	1	1	1	2	1	1	1	1	1	1	1	2	2	2	56
21	2	2	1	2	2	1	2	1	1	1	1	1	1	1	1	1	1	57
22	2	2	1	2	2	1	2	1	1	1	1	1	1	1	1	1	2	58
23	2	2	1	2	2	1	2	1	1	1	1	1	1	1	1	2	1	59
24	2	2	1	2	2	1	2	1	1	1	1	1	1	1	1	2	2	60
25	2	2	1	2	2	1	2	1	1	1	1	1	1	1	2	1	1	61
26	2	2	1	2	2	1	2	1	1	1	1	1	1	1	2	1	2	62
27	2	2	1	2	2	1	2	1	1	1	1	1	1	1	2	2	1	63
28	2	2	1	2	2	1	2	1	1	2	1	1	2	1	2	2	2	64
29	2	2	1	2	2	1	2	1	1	2	1	1	2	1	1	1	1	65
30	2	2	1	2	2	1	2	1	1	2	1	1	2	1	1	1	2	66
31	2	2	1	2	2	1	2	1	1	2	1	1	2	1	1	2	1	67
32	2	2	1	2	2	1	2	1	1	2	1	1	2	1	1	2	2	68
33	2	2	1	2	2	1	2	1	1	2	1	1	2	1	2	1	1	69
34	2	2	1	2	2	1	2	1	1	2	1	1	2	1	2	1	2	70
35	2	2	1	2	2	1	2	1	1	2	1	1	2	1	2	2	1	71
36	2	2	1	2	2	1	2	1	1	2	1	1	2	1	2	2	2	72

4.4 Main results of the boundary condition sensitivity analysis (preliminary sensitivity analysis)

The results of the preliminary sensitivity analysis show that the lack of data, especially in the area of the southern and eastern limits of the model domain, does not allow for an unequivocal selection or rejection of Fbcs scenarios. The overall analysis of the results displayed in Fig. 4-7 only shows small variations of the calibration criteria calculated for all tested scenarios.

Overall, however, the results of the preliminary sensitivity analysis show that the hydraulic conductivities of the modelled layers, and particularly those of the aquifers, have a higher impact on the hydraulic head distribution than the flow boundary conditions. The differences in terms of correlation coefficients, mean absolute errors and sum of squared errors between the two tested sets of parameters, i.e. the initial parameters ID_S1 and ID_S2, are higher than the variation of the error induced by the Fbcs scenario.

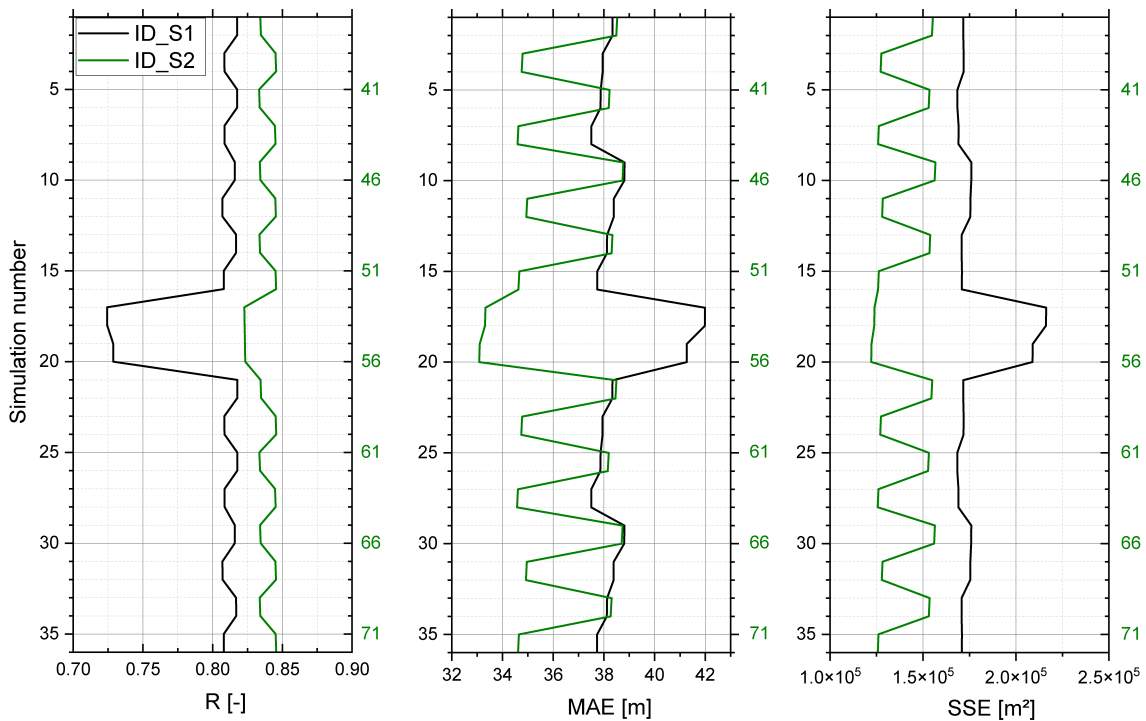


Fig. 4-7: Calculated correlation coefficients R [-], mean absolute errors MAE [m] and sum of squared errors SSE [m^2] for all tested scenarios

The results show that the models 53 to 56 (all utilising parameters from ID_S2) behave differently, i.e. result in lower MAE and SSE , compared to the other models. They share most boundary conditions except for the surface layer and the bottom of the model. They all have high correlation coefficients and the lowest mean absolute as well as squared errors of all performed simulations. However, models 55 and 56 were assigned with homogeneous recharge on the surface layer which does not appear to be plausible given the current meteorological observations in Switzerland, hence these two models were dismissed. The only difference between the remaining models 53 and 54 are the boundary conditions of faults at the model bottom. In model 53, the bottom of the model is assigned with no flow-conditions while in model 54, regional faults transecting the lower boundary are assigned with a constant head mimicking inflow from the basement into the model. These heads were initially extracted from a piezometric map of the Buntsandstein proposed by

(Voborny et al. 1994). However, this piezometric map was based on very few observations and hence carries a very large uncertainty. As the calculated metrics for simulations 53 and 54 are similar (i.e. there is no improvement of simulated heads compared to observations by imposing this additional condition), imposing an additional set of boundary conditions, and uncertain ones at that, would unnecessarily add uncertainties to the model solution. Therefore, the last parameter of the sensitivity analyses (i.e. the boundary conditions of faults at the model bottom) were rejected, making simulation 53 and 54 equivalent.

4.5 Selected model

Overall, the main difficulty encountered during the preliminary sensitivity analysis was to reject some models or validate others based on justified arguments. A major difficulty is related to the lack of data in the southern model domain. The main uncertainties remaining at the end of the preliminary sensitivity analysis are related to both, the type and the strength of Fbcs to assign along this limit. Given the preliminary sensitivity analysis results in conjunction with the least restrictive Fbcs, it seems appropriate to select model 53/54 as a starting point for the calibration to obtain the base case. Applied boundary conditions for model 53/54 are given in Tab. 4-5.

Tab. 4-5: Lateral flow boundary conditions' (Fbcs) definitions for model 53/54

Boundary	BDCode	Definition
Top surface		RSL + prescribed heads on rivers
Bottom of model		no flow (including faults)
Muschelkalk southern limit	MuS	no flow
Muschelkalk eastern limit	MuE	$300 \text{ m} < H < 375 \text{ m}$
Muschelkalk north-eastern limit	MuNE	$H=350 \text{ m}$
Muschelkalk north-western limit	MuNW	no flow
Muschelkalk western limit	MuW	$H=550 \text{ m}$
Muschelkalk surface-water-outcrop intersection	MuO	Fixed head from topography
Malm southern limit	MaS	no flow
Malm eastern limit	MaE	$H = 475 \text{ m}$
Malm north-eastern limit	MaN	no flow
Malm western limit	MaW	no flow
Malm surface-water-outcrop intersection	MaO	Fixed head from topography
OMM southern limit	OMMS	no flow
OMM western limit	OMMW	no flow
OMM surface-water-outcrop intersection	OMMO	no flow

The mean absolute errors of the aquifers implemented in the model are shown in Fig. 4-8. For the Muschelkalk and the Malm aquifers, a reasonable correlation between simulated and measured heads of $R \geq 0.85$ was achieved even without a specific calibration of the model. The other aquifers implemented in the model have not been specifically treated during the initial sensitivity analyses and will be calibrated, together with the Muschelkalk and Malm aquifers, in the next model step.

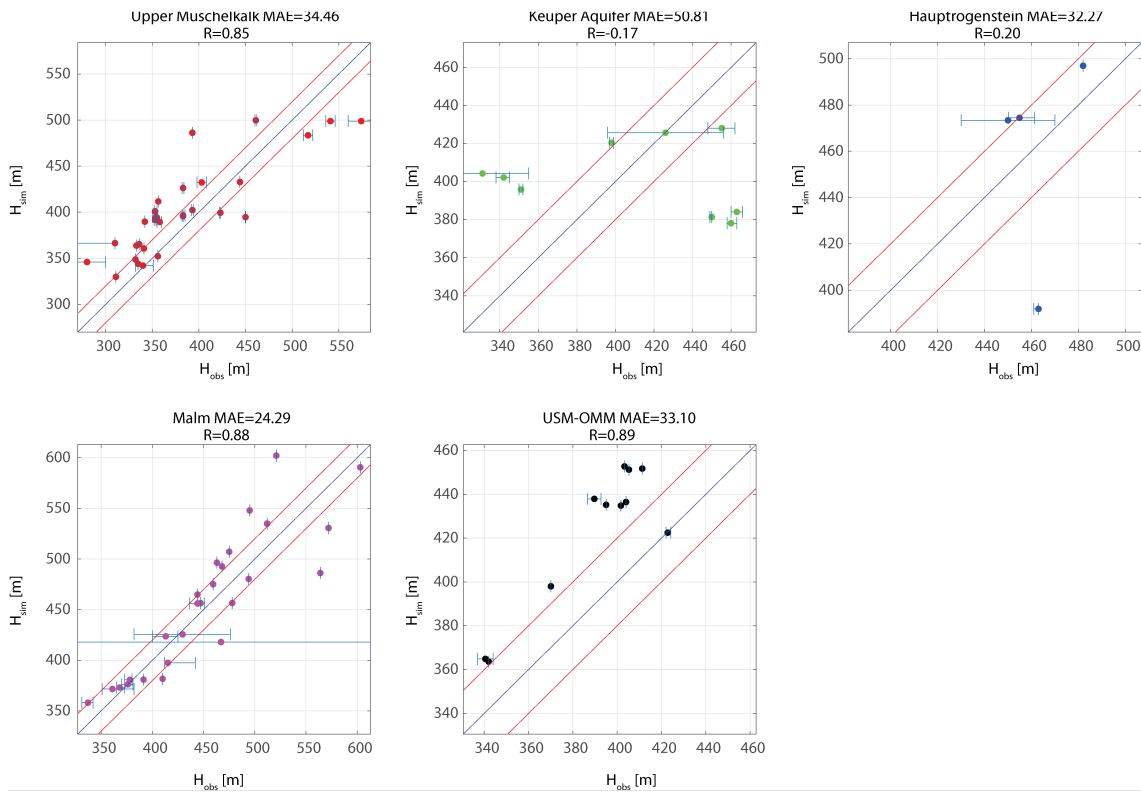


Fig. 4-8: Mean absolute error for the different aquifers (compared to observations) after the sensitivity analyses (but before calibration)

Red lines indicate ± 20 m head difference to the observation.

Faults in the preliminary sensitivity analyses have been parametrised according to the surrounding rocks. This makes faults transparent to the flow in the sense that if the surrounding rocks have high conductivities, the respective layers in the faults also have high conductivities, and vice versa. Only if an offset along the faults interrupts the continuity of a layer, the fault has an impact on the flow field. Though this might be a good representation of the natural setting, a fault sensitivity analysis has been performed to determine the impact of faults with different parameters than the surrounding rocks. This fault sensitivity analysis is detailed in the following chapter.

5 Fault sensitivity analyses

Faults are geological discontinuities that often have complex geometries and can act as conduits, barriers, or semi-permeable barriers to flow (Knott 1993, Fisher et al. 2013). Generally, the hydraulic parameters of faults are controlled by:

- the lithological nature of the formations they cross and their depths
- the orientation and width of the faults in relation to the stress field
- fault connectivity

The amplitude, spatial variability and heterogeneity of properties such as porosity and permeability are highly dependent on the scale of observation. Fig. 5-1 shows several schematic diagrams revealing the distribution of fracture density thereby conditioning the hydraulic conductivity around the fault plane. It also suggests the anisotropy which will influence hydraulic parameters, with higher hydraulic conductivities parallel to the fault plane.

Faults can act as flow drains, connecting adjacent aquifers along their entire length, or as hydraulic barriers separating several flow domains. In a multi-layer aquifer system such as modelled here, faults may already have an impact on the regional flow system simply by the geometric juxtaposition of layers with contrasting lithologies. Some of the faults show large offsets between the hydrogeological units that have been implemented in the hydrogeological model which may result in a flow barrier across the fault.

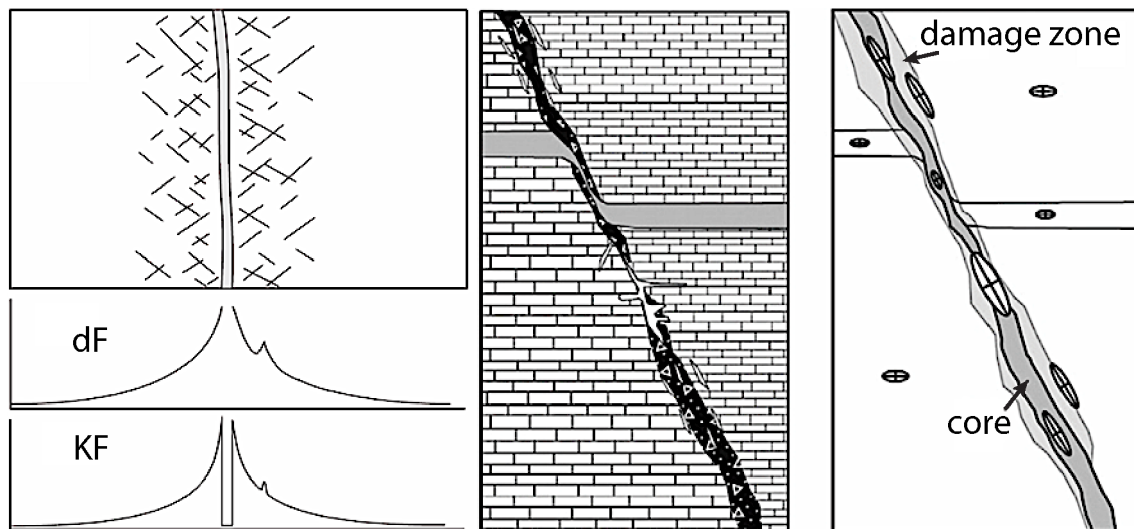


Fig. 5-1: Conceptual fault architecture (centre), 2D representation of the fault zone with the evolution of fracture density (dF) and hydraulic conductivity (KF) with respect to the fault axis (left), anisotropy of fault parameters (modified after Bense et al. 2013) (right)

Next to the offset of aquifers, the parametrisation of faults in the hydrogeological model was based on their orientation relative to the direction of the stress field. It is assumed that faults are more conductive when they are parallel to the maximum horizontal stress magnitude (and in consequence perpendicular to the minimum horizontal stress magnitude) and less conductive when they are perpendicular to it (e.g. Barton et al. 1995, Ishii 2015). The logic of this assumption

is that the “clamping” effect to tighten the fault zone is lowest in the direction of the minimum horizontal stress magnitude. This assumption is used here as a means of performing a parametric sensitivity analysis to qualitatively and quantitatively determine the impacts of regional faults with different parametrisations dependent on the orientation of the fault in relation to the general stress field and to better define their impact on groundwater flow at a regional scale.

In order to avoid parametric bias which may arise from fixed rock parameters, the hydraulic conductivities of the main aquifers (Malm and Muschelkalk) have been calibrated first in order to limit uncertainties of the simulated hydraulic flow field and the resulting heads compared to observations. These calibrations have been performed using the method outlined in Chapter 6.

5.1 Regional faults in the model area

Two fault families with different orientations are most prominent in the hydrogeological model area. The first is oriented SSE – NNW parallel to the maximum horizontal stress magnitude (Nagra 2024g), for example the Neuhausen, Randen and Singen Faults. The second is oriented WSW – ENE, roughly parallel to the Alps and Jura mountains, and hence perpendicular to the maximum horizontal stress magnitude, for example the Mandach and Ruemi Faults or the Baden – Irchel – Herdern Lineament (see Fig. 3-9).

It is worth noting that there are no data to accurately parametrise the regional faults. The modelling of the role of these faults will have to be based on conceptual ideas and scenarios to test their impact. Evidence on the impact of faults comes from the hydrogeochemical investigations of groundwater samples. These data indicate aquifer specific evolution of the groundwaters with a few exceptions. These are the similarities of groundwater samples between Molasse and Malm indicating common genesis and advective-diffusive exchange and local, mostly subordinate cross-formation flow between Muschelkalk- and deeper aquifers, notably in tectonically stronger affected areas (e.g. Nagra 2024f). The aquitards in between these aquifers act as efficient barriers. Notably clay-mineral-rich rocks have a high self-sealing potential, that is faults have low transmissivities and do not act as preferential pathways (Nagra 2024f, Bock et al. 2010). Therefore, faults have variable properties in the vertical dimension.

5.2 Fault parametrisation

5.2.1 Hydromechanical arguments

As mentioned above, the hydraulic parameters of faults are assumed to be conditioned by their orientation relative to the stress field, with the aim of assigning appropriate macroscopic roles and parameters (e.g. Preisig 2013). It is assumed that maximum conductivity develops in the direction parallel to the orientation of the maximum horizontal stress magnitude, and the lowest permeability perpendicular to the maximum horizontal stress magnitude. Using the orientation of faults as a guideline, two different parametrisations have been applied:

- ENE – WSW: these faults are considered as impermeable or as barriers to flow, since they are oriented perpendicular to the maximum horizontal stress magnitude (Nagra 2024g). As prominent examples, the Jura Main Thrust and the Baden – Irchel – Herdern Lineament will be assigned lower hydraulic conductivities than the surrounding rock.
- SSE – NNW: these faults are considered as more transmissive or drains for flow, since they are oriented parallel to the maximum horizontal stress magnitude. As examples, the Neuhausen, Randen and Singen Faults were assigned higher hydraulic conductivities.

Often, the terms 'permeable' and 'impermeable' are used to describe the hydrogeological role of faults. This designation refers to the parameter contrast between the fault and the surrounding rock, but not to specific values. Hence, this terminology describes a macroscopic behaviour, accounting for the fact that the hydraulic properties of tectonic features are not homogeneous throughout the fault plane.

5.2.2 Fault / rock parameter relationships

In the following, fault conductivities are adjusted by the application of multipliers to the adjacent rock conductivities. The fault parameters are thus correlated with those of the surrounding rock. Using different multipliers for faults allows to reduce the contrast or increase it (make them either more or less permeable compared to the surrounding rocks), depending on the faulted rock and the role assigned to the fault itself. In general, the hydraulic conductivities of faulted aquifer elements are higher than those of faulted aquitard elements.

Fig. 5-2 shows an overview of the hydraulic conductivities of the selected large-scale faults according to fault scenario 14 (see Tab. 5-1) and shows that these vary according to the orientation of the fault and also vary vertically according to the faulted geological layer.

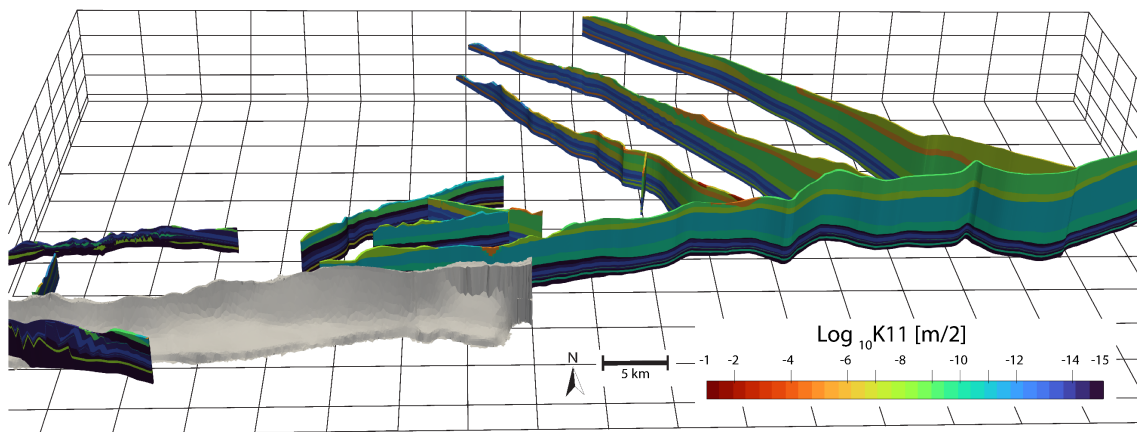


Fig. 5-2: Vertical variability of the hydraulic properties of the regional faults in model scenario 14

The specifically modelled Jura Main Thrust is shown in grey. 3× vertical exaggeration.

5.3 Definition of scenarios for fault sensitivity analysis

Model 53/54, described in Chapter 4, is used to perform fault sensitivity analysis to determine the influence of faults on the regional groundwater flow in Northern Switzerland. Initially, faults inherit the conductivities of the surround rock. These conductivities are adjusted by using a multiplicative factor (F). Conductivities in transmissive faults can be up to three orders of magnitude higher ($F = 1'000$) than those of the surrounding rocks. In contrast, faults with low permeability can be up to three orders of magnitude less permeable ($F = 0.001$) than the surrounding rocks. The fault sensitivity analysis has been performed including several steps:

1. Classification of fault (permeable or impermeable) depending on its orientation
2. Analysis of the hydrogeological role of all impermeable faults simultaneously
3. Analysis of the hydrogeological role of all transmissive faults simultaneously
4. Analysis of the hydrogeological role of all faults, transmissive and impermeable simultaneously.

During each step, an increasingly pronounced contrast, on a logarithmic scale, between the fault elements and the surrounding rocks is applied to the transmissive faults (factors of 10, 100, 1000). The less permeable faults are characterised by decreasing factors (factors of 0.1, 0.01, 0.001). In addition, the following four conceptual scenarios were considered:

1. only fault core elements are considered
2. only fault damage zone (hereafter referred to as “envelop”) elements are considered
3. both fault core and envelop elements are considered transmissive
4. all faults, transmissive and impermeable are activated simultaneously with two contrast factors (factors of: 0.1 and 10, and 0.01 and 100) with respect to the surrounding intact rock
5. Similar to 4, but with different southern boundary conditions.

In total, 19 fault parameter combinations have been defined as presented in Tab. 5-1, leading to 19 scenarios for the fault sensitivity analysis.

Tab. 5-1: Scenario definitions for the fault sensitivity analysis using the base case

Names of the scenarios are indicative for the treatment of faults: C – fault core elements were changed, E – fault envelop elements were changed, CE – both, core and envelop elements were changed.

ID	Scenario Name	Factors for impermeable faults				Factors for transmissive faults			
		1	0.1	0.01	0.001	1	10	100	1'000
0	Model 53/54	×				×			
1	IMPER10		×			×			
2	IMPER100			×		×			
3	IMPER1000				×	×			
4	TRANS10_C	×					×		
5	TRANS100_C	×						×	
6	TRANS1000_C	×							×
7	TRANS10_E	×					×		
8	TRANS100_E	×						×	
9	TRANS1000_E	×							×
10	TRANS10_CE	×					×		
11	TRANS100_CE	×						×	
12	TRANS1000_CE	×							×
13	IT10_C		×				×		
14	IT100_C			×				×	
15	IT10_E		×				×		
16	IT100_E			×				×	
17	IT10_CE		×				×		
18	IT100_CE			×				×	
19	IT10_CE_South		×				×		

5.4 Simulation results

5.4.1 Main results

To assess the hydraulic impact of the faults, the perturbation generated on the head field relative to model 53/54 is mapped for each scenario ($dH \text{ [m]} = H_{\text{Scenario}} - H_{\text{Model53/54}}$). The difference between the hydraulic heads of the model 53/54 and the heads simulated by the tested scenarios is used to assess the sensitivity of the regional groundwater flow model to different parametrisations of major faults. As during the previous sensitivity analysis, the MAE was calculated for each tested scenario to quantify the impacts of variable hydraulic fault properties. The hydraulic head dataset provided in Appendix 1 was used for comparison with the model results. Tab. 5-2 shows these mean absolute errors for all tested scenarios calculated for each aquifer separately.

Tab. 5-2: Difference between mean absolute error [m] of the model 53/54 (ID 0) and all tested scenarios (ID 1 – 19) calculated for each aquifer separately

The column “Model” displays the mean absolute error (MAE), or respective differences, integrated over the whole model domain. Colour bars indicate residuals between the respective scenario and model 53/54. Green colours indicate a decrease of the MAE while orange colours indicate an increase. Names of the scenarios are indicative for the treatment of faults: C – fault core elements were changed, E – fault envelop elements were changed, CE – both, core and envelop elements were changed.

ID	Scenario	Model	Muschelkalk	Keuper	Hauptrogenstein	Malm	USM	OSM
0	Model 53/54	20.61	17.65	33.53	10.00	16.11	32.48	22.27
1	IMPER10	-0.02	-0.20	-0.19	0.00	0.27	-0.25	0.13
2	IMPER100	0.55	1.16	-0.79	0.02	0.74	-1.11	0.03
3	IMPER1000	1.29	3.15	-1.24	0.03	0.99	-1.45	-0.48
4	TRANS10_C	0.00	0.06	0.10	-0.08	0.04	-0.87	-0.10
5	TRANS100_C	0.47	0.68	2.59	-0.34	0.35	-3.34	-0.67
6	TRANS1000_C	4.89	6.85	15.72	-0.50	2.55	-4.81	-2.53
7	TRANS10_E	0.04	0.11	0.38	-0.14	0.09	-1.41	-0.18
8	TRANS100_E	1.11	1.65	4.38	-0.45	0.77	-4.35	-1.09
9	TRANS1000_E	6.11	8.96	18.00	-0.56	3.28	-5.64	-3.29
10	TRANS10_CE	0.08	0.16	0.67	-0.17	0.12	-1.84	-0.26
11	TRANS100_CE	1.78	2.35	6.99	-0.47	1.19	-4.66	-1.41
12	TRANS1000_CE	6.69	9.99	18.98	-0.56	3.55	-5.37	-3.67
13	IT10_C	0.00	-0.13	0.05	-0.07	0.31	-1.16	0.04
14	IT100_C	1.25	2.24	2.04	-0.32	1.15	-4.17	-0.50
15	IT10_E	0.05	-0.07	0.34	-0.13	0.36	-1.69	-0.05
16	IT100_E	2.02	3.36	4.18	-0.43	1.61	-5.03	-0.81
17	IT10_CE	0.09	0.00	0.62	-0.16	0.39	-2.13	-0.12
18	IT100_CE	2.78	4.15	7.16	-0.45	2.03	-5.26	-1.05
19	IT10_CE_South	0.29	0.16	2.34	-0.03	-0.06	-1.03	0.08

The results in Tab. 5-2 indicate that, as expected, the hydraulic behaviour varies from one layer to another. The groundwater flow in the 3D multi-layered system of the hydrogeological model is very complex and depends on several parameters/factors, including the lithology of the rocks and the orientation of faults with respect to flow directions, etc.

Tab. 5-2 shows that, except for scenarios with parametric contrasts higher than 2 orders of magnitude, such as scenario 6, 9 or 12, the alternative parametrisation of the faults increases the error of some layers but at the same time decrease the error of others (compared to model 53/54). The tested scenarios with changes of 2 orders of magnitude or less did not have a significant influence on the main flow directions at the regional scale, despite local hydraulic perturbation of tens of meters. For strong fault contrast scenarios with multiplicative factors of 0.001 or 1'000, a hydraulic perturbation of nearly 100 m was observed e.g. around the Randen Fault with deformed flow directions compared to model 53/54. However, despite considerable change in the flow direction, the overall flow budgets are not significantly changed, and the discharge and recharge areas of the multilayer system remain unchanged.

5.4.2 Analysis of specific scenario: IT100_C (14)

As an example, scenario IT100_C (ID 14 in Tab. 5-2) is described here in more detail because it demonstrates the impact of faults on the groundwater flow when they are not implemented as transparent faults but are parametrised according to their orientation. In this scenario, faults trending WSW – ENE are parametrised with contrast factors (compared to the adjacent, non-damaged rocks) of 0.01 (impermeable faults) and factors of 100 for transmissive faults trending SSE – NNW. This parametrisation is consistent with the concepts and hypotheses presented above: parameters dependent on the orientation of the faults in relation to the current tectonic stress, and on the lithology of the faulted layers.

Fig. 5-3 presents a comparison between simulated (scenario 14) and measured hydraulic heads with uncertainty intervals (compare also Fig. 4-8).

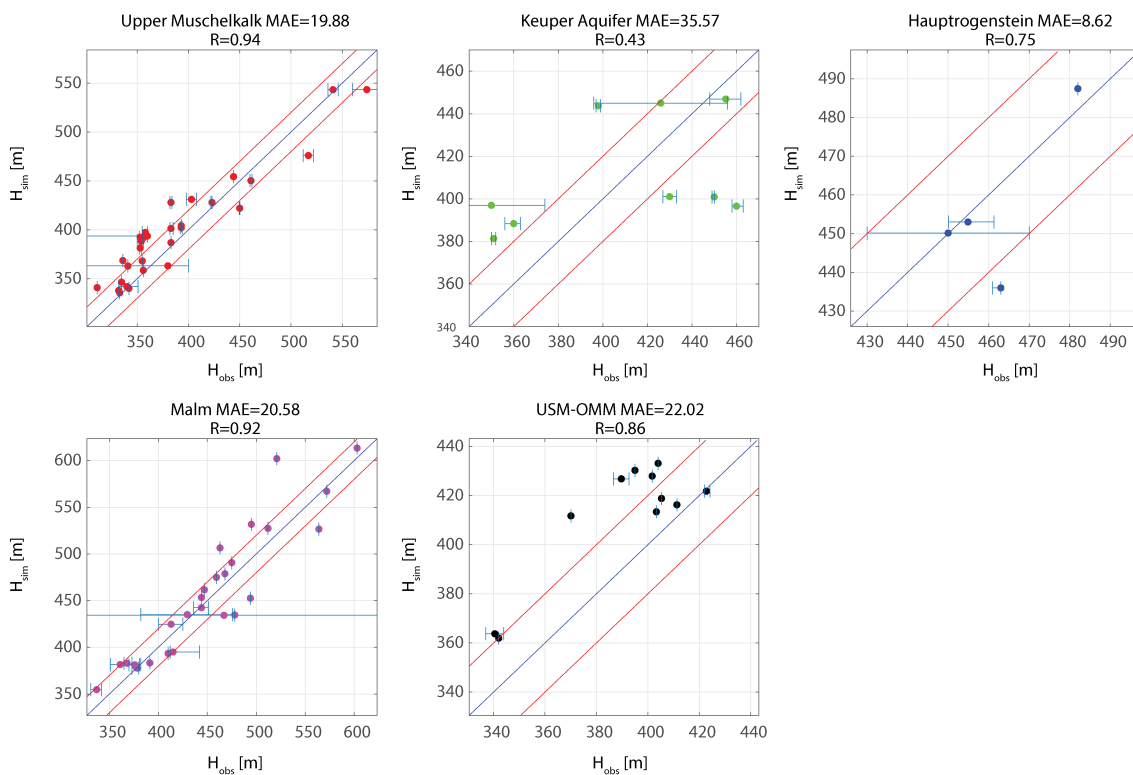


Fig. 5-3: Scenario 14 – Comparison between simulated and measured hydraulic heads

Mean absolute error MAE [m] and correlation coefficient R [-] are shown. Red lines indicate ± 20 m head difference to the observation.

Fig. 5-4 and Fig. 5-5 show the simulated hydraulic heads in the Muschelkalk and Malm aquifers for scenario 14, together with maps of the differences between the hydraulic heads and model 53/54, respectively. The results show that regional flow patterns remain largely unchanged but hydraulic perturbations in the vicinity of faults are higher. The orientation-dependant parameterisation of the faults has induced a compartmentalisation of the flow systems, especially between impermeable faults, such as those surrounding the deep geological repository sites of Jura Ost and Nördlich Lägern.

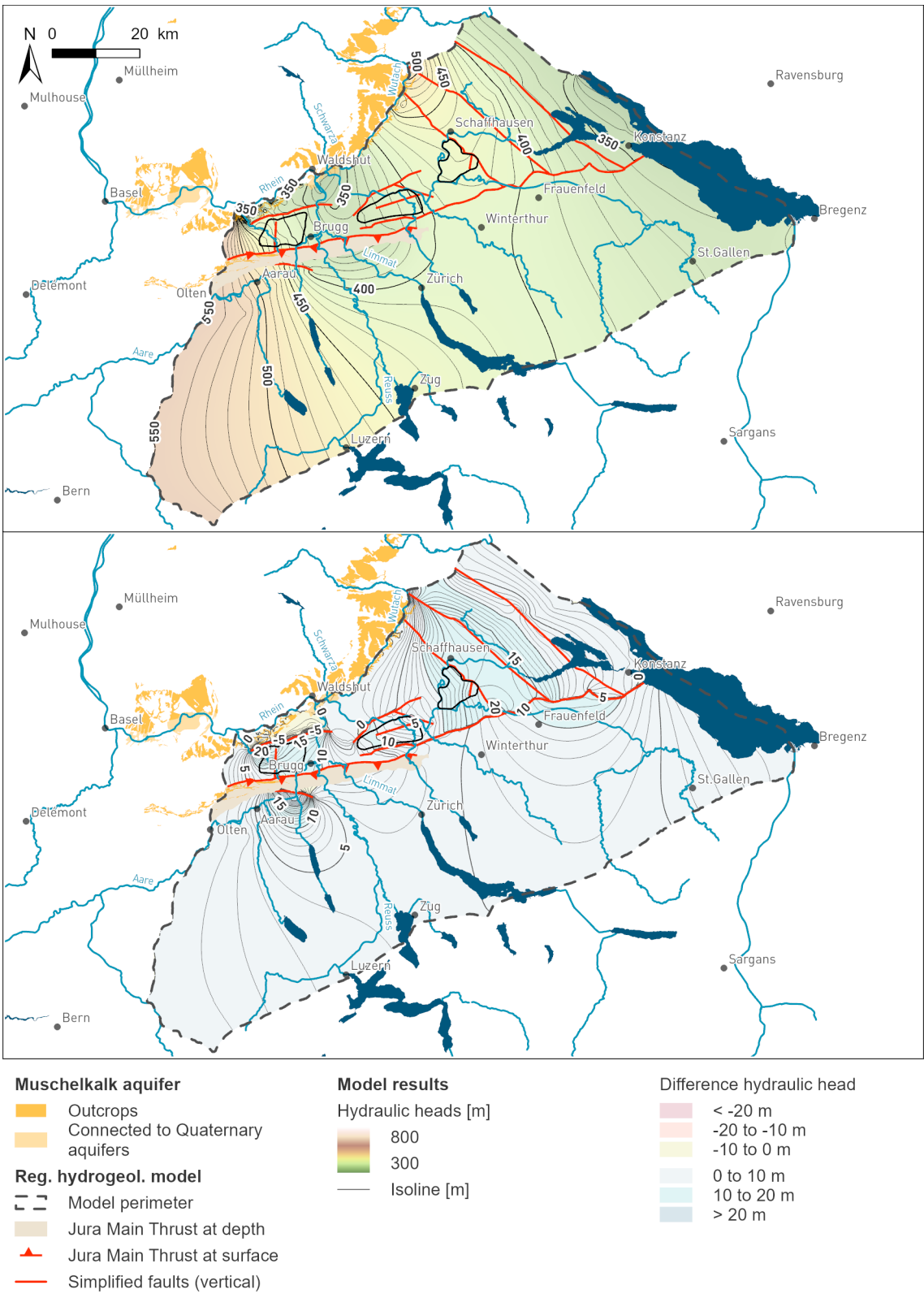


Fig. 5-4: Model results for the Muschelkalk aquifer in Scenario 14 – Top: Simulated hydraulic heads in the Muschelkalk aquifer. Bottom: Differences with model 53/54

Positive values indicate that in the scenario with non-transparent faults (14) the hydraulic heads are higher than in model 53/54 (with transparent faults).

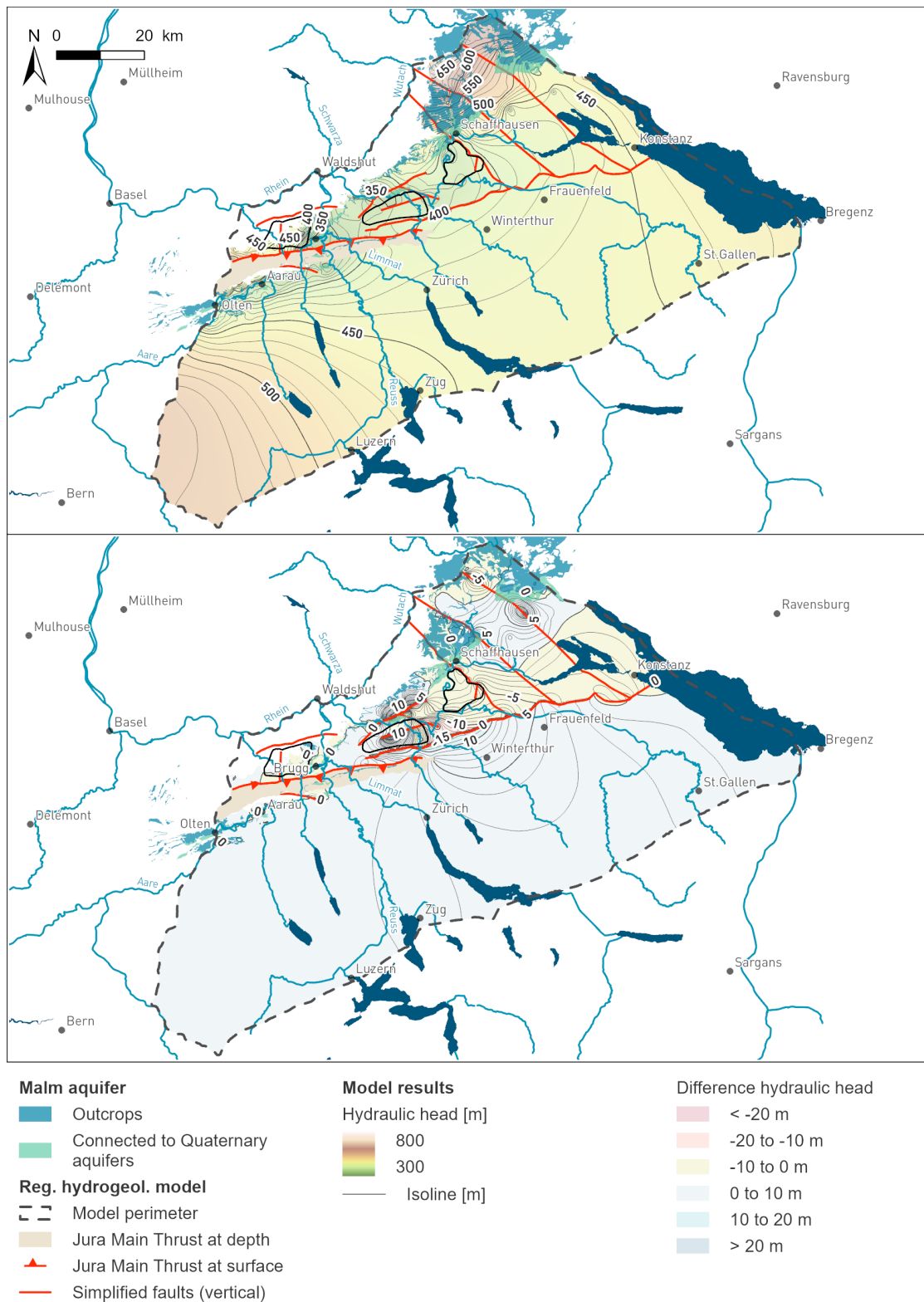


Fig. 5-5: Model results for the Malm aquifer in Scenario 14 – Top: Simulated hydraulic heads in the Muschelkalk aquifer

Bottom: Differences with model 53/54. Positive values indicate that in the scenario with non-transparent faults (14) the hydraulic heads are higher than in model 53/54 (with transparent faults).

Overall, the Randen Fault and Baden – Irchel – Herdern Lineament seem to have the greatest impact on the flow in the Muschelkalk and Malm aquifers. The Baden – Irchel – Herdern Lineament plays the role of a barrier blocking the flow coming from the outcrops in the North towards the south of the modelled domain (Fig. 5-6). The Randen Fault, however, plays the role of a preferential flow path draining surface waters and infiltrations from the outcrops towards the south.

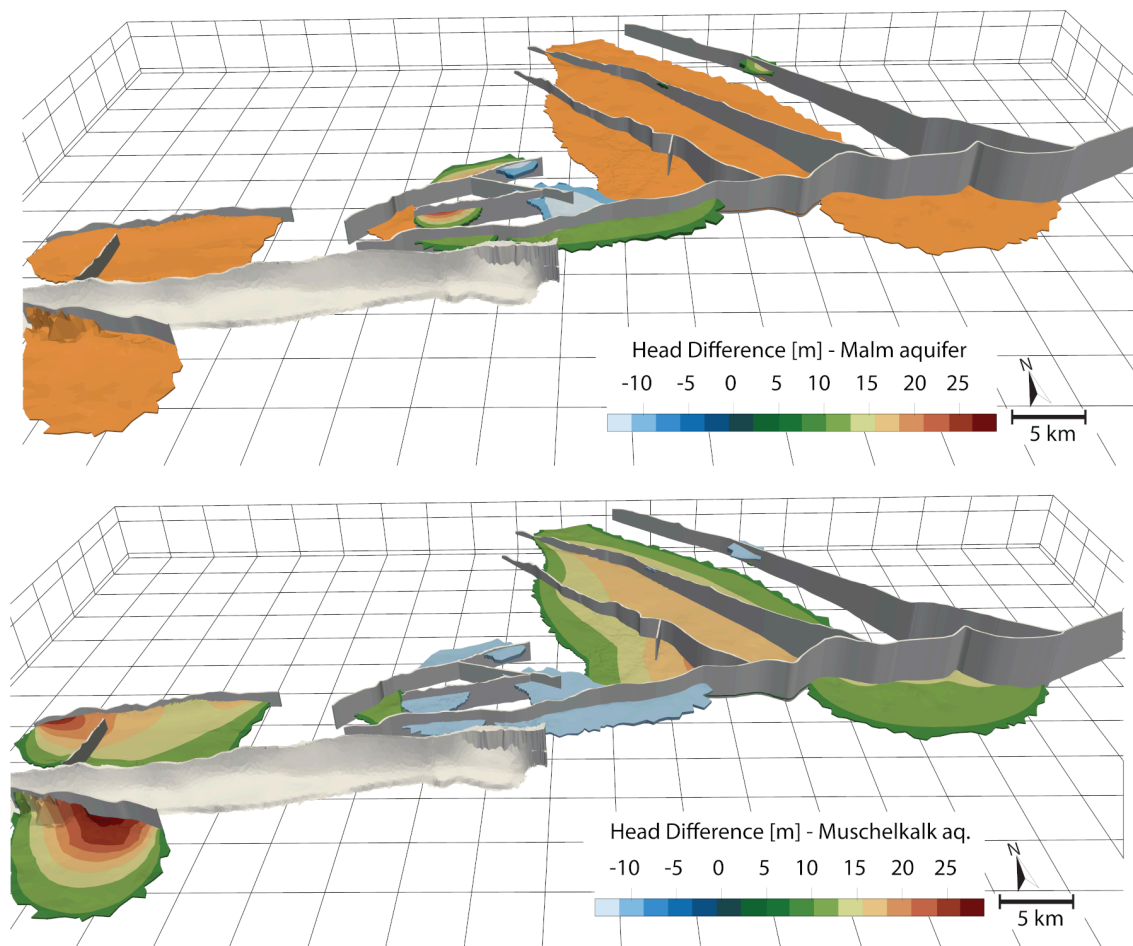


Fig. 5-6: 3D view of the hydraulic perturbation in the Malm and Muschelkalk aquifers compared to model 53/54 (only where difference is < -10 m or > 10 m)

For reference, the Muschelkalk aquifer (top, orange) and the Malm aquifer (bottom, blueish) are included with solid colours. 2× vertical exaggeration. Implemented regional-scale faults are displayed in grey.

5.4.3 General observations from fault hydraulics

Generally, the effects of fault hydraulic parametrisation are more pronounced in deeper units. More specifically, hydraulic head perturbations in the Muschelkalk aquifer are more pronounced than in the Malm aquifer where they gradually diminish in the overlying formations until they become negligible near the surface.

The recurrent observed impacts of the fault parametrisation sensitivity study through the tested scenarios are the following:

- For transmissive faults: they generally may have a much larger effect when they are parallel to the regional flow direction. The draining effect is even more pronounced when the fault is connected to outcropping aquifer units in the recharge areas. In addition, draining faults generally cause a piezometric dome downstream due to the inflow-drainage of larger volumes of water from the recharge areas to depths. This behaviour was for instance observed when parametrising the Randen Fault in the hydrogeological model with increased conductivities.
- For impermeable faults: in general, their effects may be larger when they are perpendicular to the flow lines, thus being flow barriers. Impermeable faults parallel to the main flow direction have no visible effect. The barrier role played by impermeable faults generally results in an increase of heads upstream of the flow and development of a depression in the downstream area. This behaviour was for instance observed after assigning the Baden – Irchel – Herdern Lineament and the Mandach Fault in the hydrological model with decreased conductivities.

Based on the results of the fault sensitivity study, the Randen Fault and the Baden – Irchel – Herdern Lineament may have the greatest impact on the flow field and hydraulic heads because they prevent N-S directed flow (Baden – Irchel – Herdern Lineament) or act as a conduit channelling water from the recharge areas (Randen Fault). Therefore, these two faults were included in model 53/54 and used in the calibration and subsequent modelling. Other faults were considered transparent (i.e. they have the same hydraulic conductivities as the surrounding rock).

6 Model calibration

The preliminary sensitivity analyses (Chapter 4) and subsequent fault sensitivity analyses (Chapter 5) lead to the definition of the initial base case. The initial base case has defined boundary conditions, includes two regional faults, the Randen Fault and Baden – Irchel – Herdern Lineament, with a special parametrisation (the other faults are considered transparent) and preliminary, depth dependent conductivities assigned based on conceptual models and observations. However, the model itself has not, or only rudimentary, been calibrated.

Starting from the initial base case defined in Chapter 4 and including results of the fault sensitivity analysis described in Chapter 5, the influence of possible karstification must also be taken into account, at least for the Malm and Muschelkalk aquifers, as Karst may increase their respective conductivities. To include this effect, based on conceptual considerations, three calibration zones have been defined similar to Gmünder et al. (2014) see Fig. 6-1):

- Zone A is south of the Jura Main Thrust and Baden – Irchel – Herdern Lineament where aquifers are below an increasingly thick overburden towards the south.
- Zone B roughly covers the Internal and western part of the External Jura. Units may strongly be affected by tectonic overprint; active Karst may occur in the outcrop zones.
- Zone C includes the area North of the Baden – Irchel – Herdern Lineament covering the area with only minor tectonic overprint. Active Karst may occur in the outcrop zones.

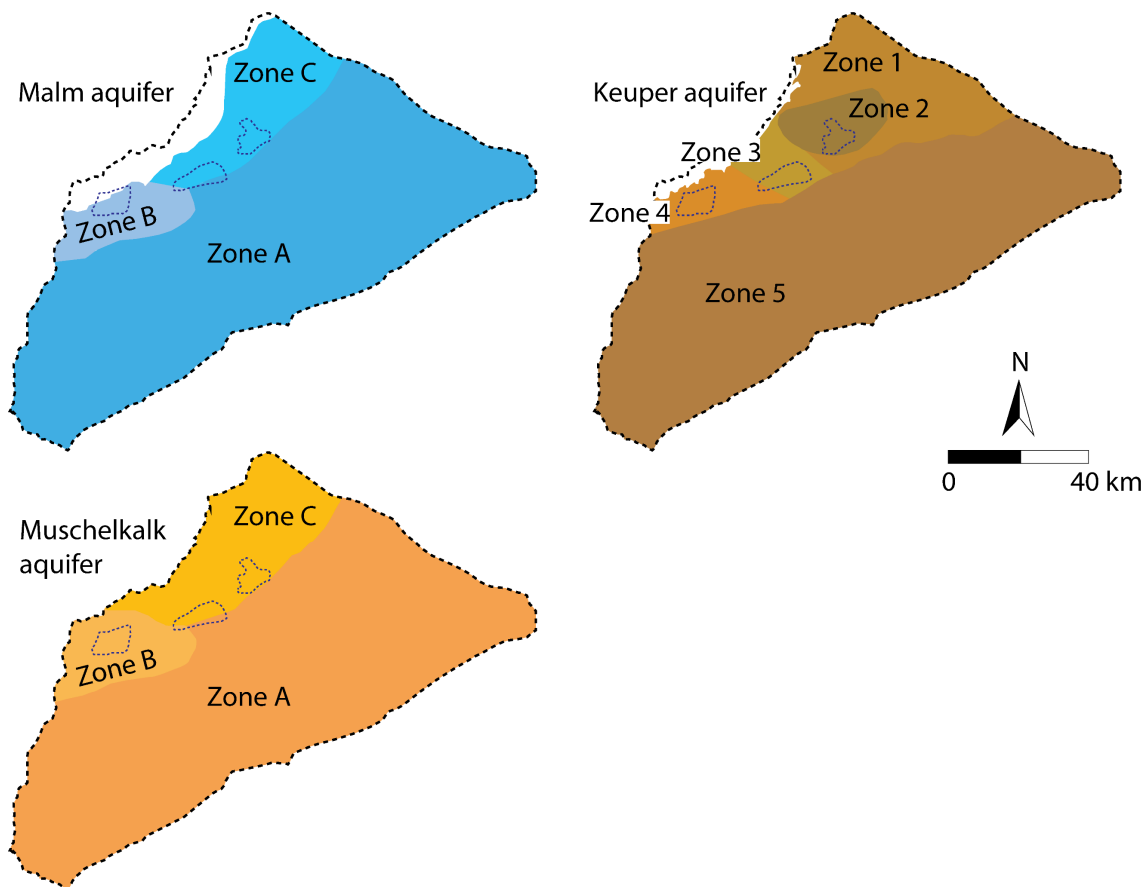


Fig. 6-1: Conceptual zones in the Malm, Keuper and Muschelkalk aquifers

Different zones are determined by different colours, see text for the rationales for each zone.

The hydraulic conductivities in the different zones were calibrated using PEST. Note that the hydraulic conductivities parallel to the west-east and north-south axis were calibrated independently allowing a horizontal anisotropy. The PEST algorithm uses inverse modelling (Doherty 2004) based on the Gauss-Marquardt-Levenberg algorithm and aims to minimise a global error function that compares measured (see Appendix 1) and simulated hydraulic heads through an iterative process. The best fit achieved by successively changing the hydraulic conductivity of the targeted zones is recorded.

Once the zones in the Malm and Muschelkalk had been calibrated, the remaining aquifers were also calibrated using PEST, including anisotropic K values. Of note is also the Keuper aquifer, the next aquifer below the Opalinus Clay. The Keuper aquifer is characterised by strong lateral, and also vertical, variations of its lithology, and hence hydrogeological properties, due to its depositional history (see Nagra 2024f).

To account for these different properties during the calibration and hydrogeological modelling, the Keuper aquifer layer has been divided into 5 zones (see Fig. 6-1). The area south of the Jura Main Thrust and the Baden – Irchel – Herdern Lineament was treated as one large zone (Zone 5 in Fig. 6-1). The area north of this imaginary line was subdivided into 4 different zones based on facies maps, tectonic overprint and hydrogeological observations. The westernmost zone (Zone 4) covers the siting region Jura Ost and approximates the extension of a transmissive facies of the Gansingen Member; the central zone around the siting region Nördlich Lägern (Zone 3) outlines an area where the hydrogeological situation of the Keuper aquifer is dominated by fluvial channels in the Ergolz Member; the easternmost zone (Zone 1) represents the equivalent of the Belchen Member and Seebi Member, while the zone including the Zürich Nordost siting region (Zone 2) is related to the occurrence of the brecciated, cavernous lithofacies of the Seebi Member. As before, the hydraulic conductivities of each zone were calibrated using the algorithms provided by PEST.

Note that a homogeneous isotropic case of the Keuper aquifer was also tested as an alternative to the base case (see Section 8.2). It aims to evaluate the impact of a less compartmentalised model on the groundwater flow system in the Keuper aquifer. Furthermore, two additional cases were considered to investigate the regional impact of a channel system on the large-scale groundwater flow pattern in the Ergolz Member (Section 8.3).

As a metric to characterise the outcome and improvements of the calibration, again the already mentioned criteria of MAE, SSE and R were calculated. In total, 77 hydraulic head observations in the Molasse (i.e. OMM and USM) and Mesozoic aquifers (see Appendix 1) were available. However, most of the available observations are located north of the line defined by the Jura Main Thrust and Baden – Irchel – Herdern Lineament. In the area south of this theoretical line, only very few observation points exist.

The final calibration resulted in much improved MAE and correlation coefficients for all aquifers compared to the original model 53/54 (compare Fig. 6-2 and Fig. 4-8).

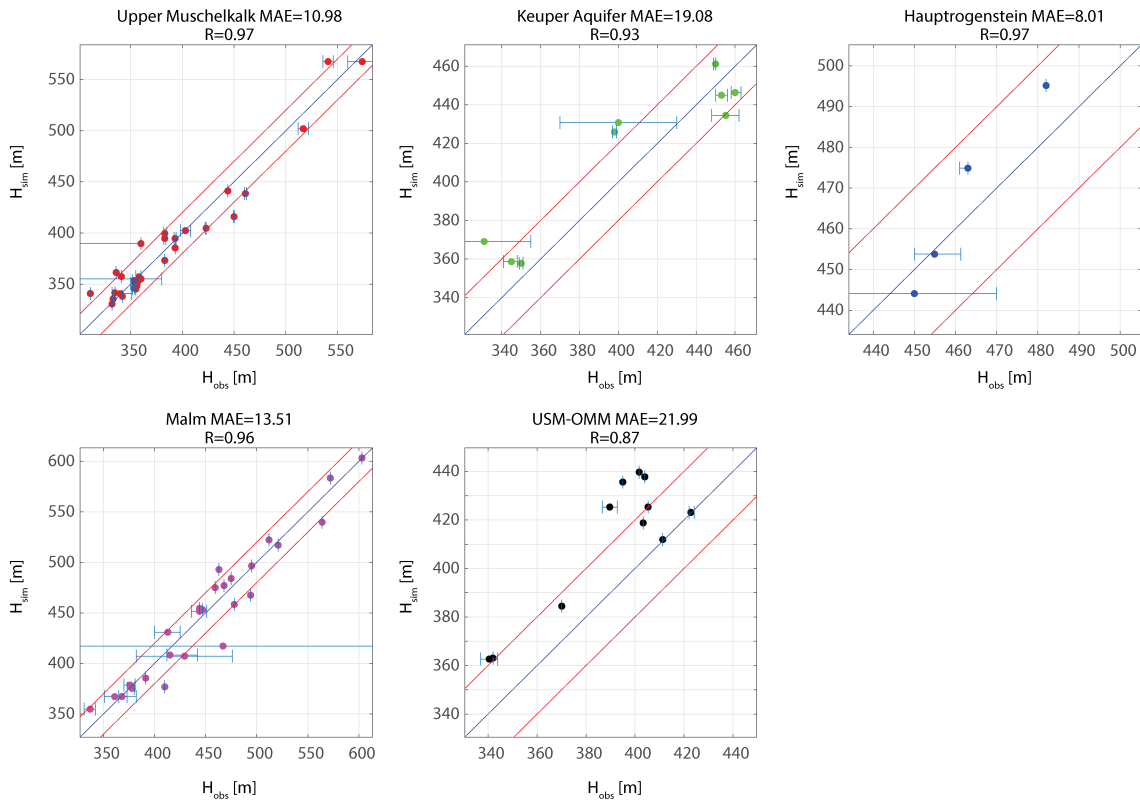


Fig. 6-2: Comparison between simulated and measured hydraulic heads with uncertainty intervals

Observation points are sorted in five layers. Mean absolute error MAE [m] and correlation coefficient R [-] are shown for each unit. Red lines indicate differences of ± 20 m.

The groundwater flow calibration was carried out in conjunction with water budget constraints and cross-validation against estimated values of mainly surface recharge.

Fig. 6-3 shows the flow budget calculated along all flow boundary segments of the model. The surface input budget remains consistent with the water budget estimations. i.e. with groundwater recharge from surface infiltration equal to $2.40 \times 10^9 \text{ m}^3/\text{yr}$ ($\sim 0.30 \text{ m/yr}$ integrated over the model domain of $8'000 \text{ km}^2$). Inflow from rivers equal $2.85 \times 10^9 \text{ m}^3/\text{yr}$, and outflow to rivers and lakes equals $-5.250 \times 10^9 \text{ m}^3/\text{yr}$. The flow budget from lateral boundary is also in agreement with the conceptual definition.

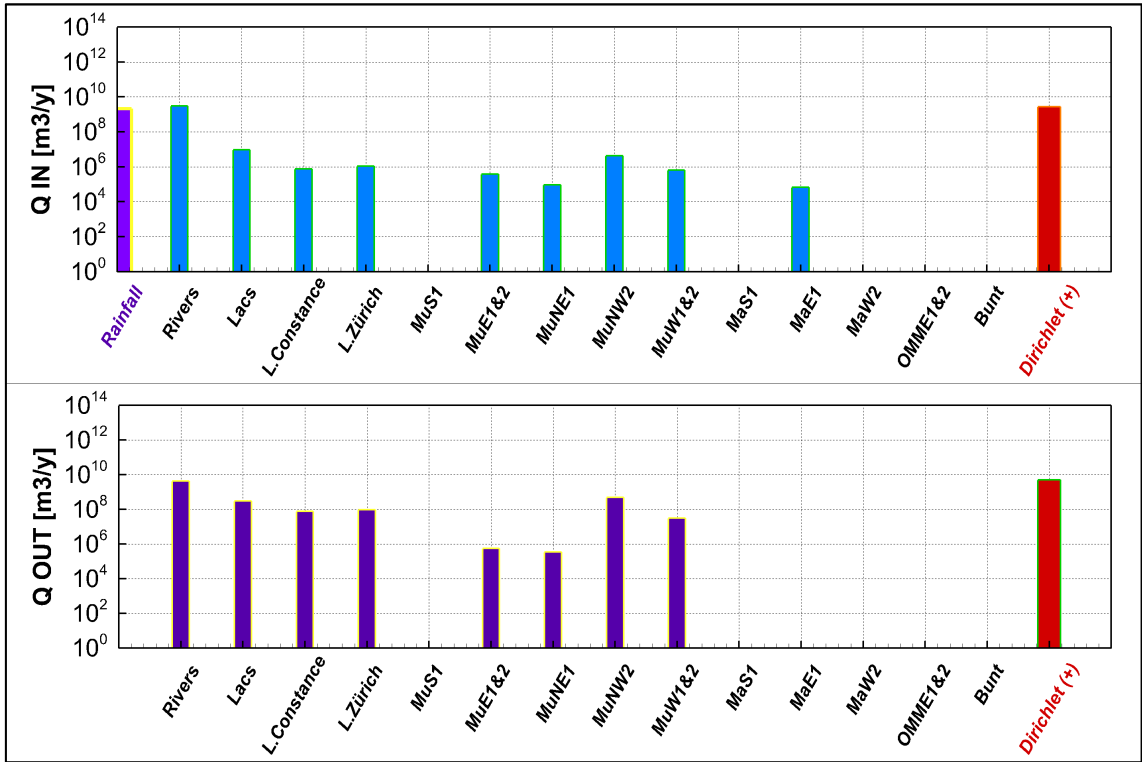


Fig. 6-3: Groundwater flow budgets (Log10 Inflows and Outflows [m³/yr]) at different model boundaries

Section 3.1 shows the location of the different boundaries.

7 Base case

Once the calibration was successfully performed, the resulting flow field was investigated by means of potentiometric maps of hydraulic heads (Sections 7.1 to 7.4), vertical hydraulic gradients across the host rock (Section 7.5), and path lines from particle tracking (Section 7.6). Aquifers are presented from bottom to top in the following sections.

7.1 Muschelkalk aquifer

The hydraulic conductivities in the three zones presented in Fig. 6-1 and in the siting regions resulting from the calibration are presented in Tab. 7-1 and Fig. 7-1.

Tab. 7-1: Hydraulic conductivities and horizontal anisotropy ratio in the Muschelkalk aquifer

The range of hydraulic conductivities K_{xx} parallel to the east – west axis is provided. Note that the hydraulic conductivities of the Muschelkalk aquifer in the model are depth dependent. The horizontal anisotropy ratio is defined as the ratio between the hydraulic conductivity parallel to the east-west axis and the one parallel to the north – south axis (K_{xx}/K_{yy}). Note that the outcrops were considered isotropic in all the three zones A, B and C. The range of hydraulic conductivities derived from hydraulic packer testing in the Muschelkalk aquifer in the siting regions JO, NL and ZNO are indicated in parentheses.

Zone / siting region	Range of hydraulic conductivity (K_{xx})	Horizontal anisotropy ratio (K_{xx}/K_{yy})
A	10^{-11} to 10^{-3} m/s	1.0
B	10^{-7} to 10^{-3} m/s	0.5
C	10^{-7} to 10^{-3} m/s	2.7
JO (in Zone B)	3×10^{-7} to 3×10^{-6} m/s (7×10^{-7} to 2×10^{-6} m/s)	0.5
NL (mainly in Zone C)	7×10^{-8} to 2×10^{-6} m/s (3×10^{-8} to 1×10^{-6} m/s)	0.5 to 2.7
ZNO (mainly in Zone C)	1×10^{-7} to 2×10^{-6} m/s (5×10^{-8} to 1×10^{-6} m/s)	1.0 to 2.7

The widest spectrum of the hydraulic conductivities is found in the southern part of the model (Zone A). This reflects the large range of depth in this part of the model (Tab. 7-1, Fig. 7-1). The lowest values are found near the southern model boundary where the Muschelkalk aquifer horizon lies at great depths. Zones B and C display a narrower range of hydraulic conductivities with values between 10^{-7} and 10^{-3} m/s. In general, the highest hydraulic conductivities are occurring close to outcrops, which are located along the northern limit of the model as well as along the Internal Jura (Folded Jura). Note that the model calibration led to a slight anisotropy of the horizontal hydraulic conductivities in Zones B and C (i.e. in the northern part of the model).

Overall, the hydraulic conductivities in the siting region resulting from the model calibration agree with the ones derived from the hydraulic packer tests (Tab. 7-1).

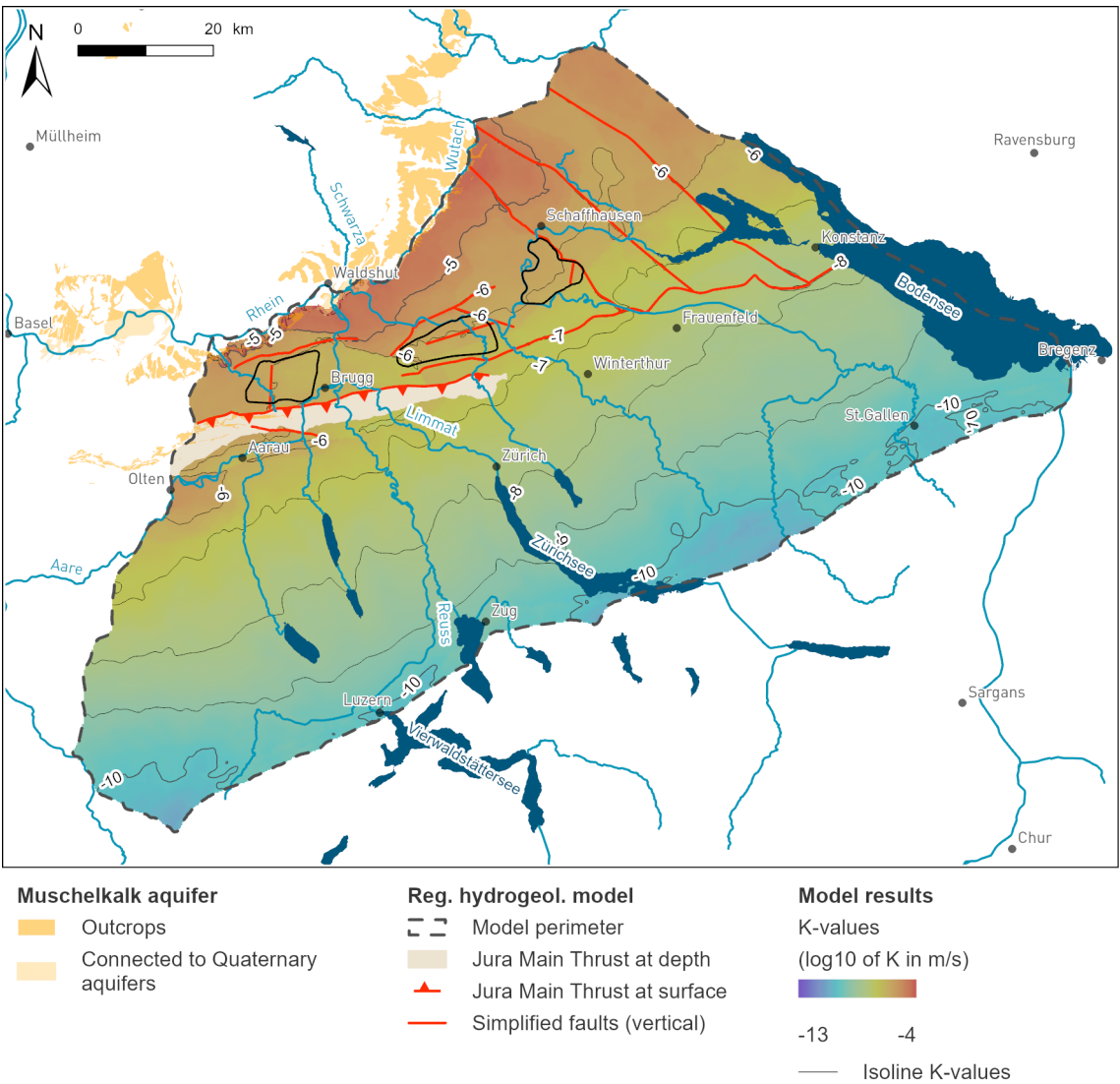


Fig. 7-1: Calibrated hydraulic conductivities in the Muschelkalk aquifer horizon

The distribution of the hydraulic conductivity K_{xx} (i.e. K parallel to the east-west axis) is shown in the figure. The horizontal anisotropy ratio K_{xx}/K_{yy} of the different zones is provided in Tab. 7-1 and varies between 0.5 and 2.7. The map shows the outcrops and the simplified regional fault pattern used in the model. Note the decrease in hydraulic conductivity towards the southeast in response to increasing depths of the Muschelkalk aquifer horizon.

A relatively low MAE value of 10.98 m is obtained for the Muschelkalk aquifer (Fig. 7-2), which represents only 4 – 5% of the total head difference (simulated hydraulic heads vary between approximately 300 m and 600 m). Furthermore, a correlation coefficient of 0.97 indicates a very good agreement between simulated and observed hydraulic heads (Fig. 7-2).

Concerning the spatial distribution of the residuals, the model tends to slightly underestimate the hydraulic heads in Zone C, which contains the NL and ZNO siting regions (Fig. 7-2). This is especially the case in the area north of NL (Fig. 7-3). The calibration led to an especially good agreement between simulated and observed hydraulic heads in the NL siting region. In the ZNO siting region, the difference between the model results and observations are in the range of approximately ± 20 m (over- and underestimation of the hydraulic heads in the MAR1 and TRU1 boreholes, respectively).

In the northwestern zone, the hydraulic heads tend to be slightly overestimated by the model. In the JO siting region, the difference between the model results and observations lies between ± 20 m.

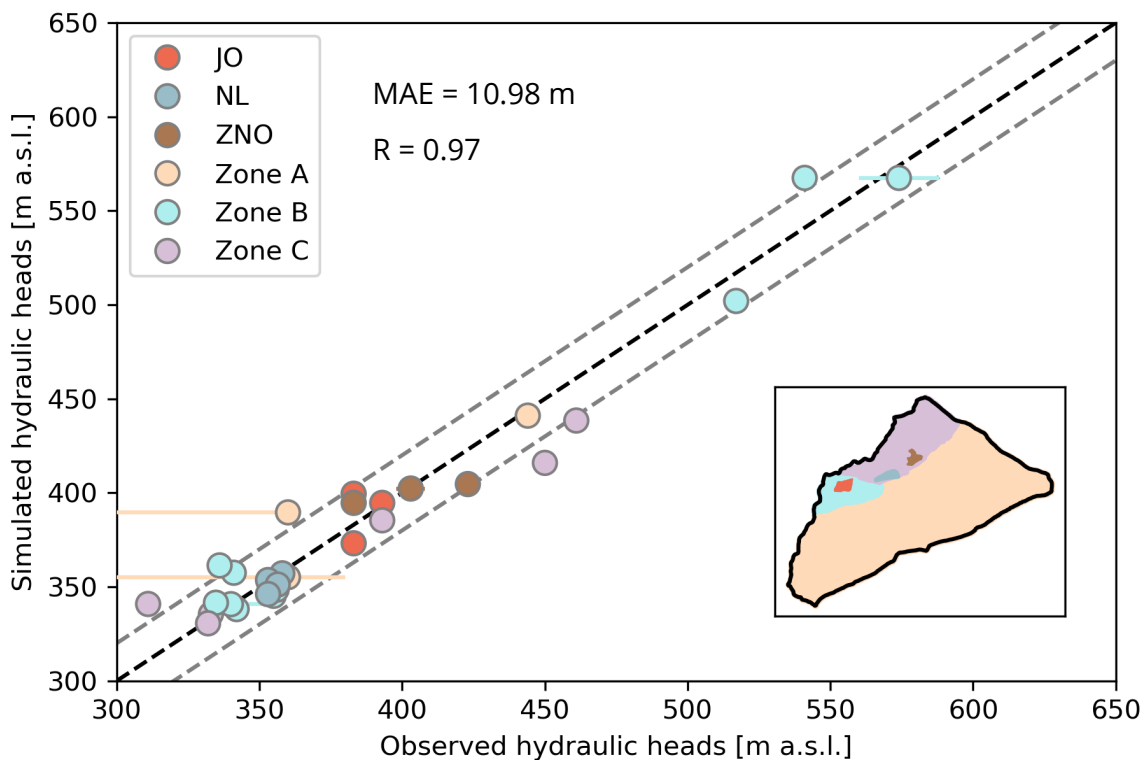


Fig. 7-2: Observed versus simulated hydraulic heads in the Muschelkalk aquifer

The colour of the points refers to the different zones in the Muschelkalk aquifer horizon (Chapter 6) or to the siting regions in which the observations are located. The bandwidth of the observed hydraulic heads is displayed with horizontal error bars. Note that bandwidth may be hidden behind the symbol or may be not available (Enclosure A). The black dashed line represents a perfect fit between observed and simulated hydraulic heads. The above and underlying grey dashed lines represent a difference of ± 20 m between simulated and observed hydraulic heads.

The potentiometric map in Fig. 7-3 highlights the existence of two regional flow domains in the Muschelkalk aquifer. The first domain, located north of the Baden – Irchel – Herdern Lineament and Jura Main Thrust, is controlled by the topography and the outcrop situation and is well constrained by borehole data. The second area is situated south of these regional tectonic features. Comparatively poorly characterised, the latter zone mainly depends on the boundary condition along the southern and western model limits as well as on the low hydraulic conductivities found at greater depths.

In the western part of the model, the northern and southern domains are hydraulically disconnected by the Jura Main Thrust and outcropping low permeability anhydrite below the Muschelkalk aquifer (Fig. 7-3).

The recharge of the Muschelkalk aquifer mainly occurs in the northern part of the model domain along the Wutach Valley (Fig. 7-3). This results in a prominent piezometric dome (hydraulic heads > 600 m a.s.l.) extending toward the south-southeast. The latter acts as a groundwater flow divide as previously described in earlier works (e.g. see Nagra 2002). To the east, groundwater is flowing through the Bodensee area and leaves the model via its eastern boundary. To the west, groundwater flow is directed towards the regional discharge area in the Lower Aare. The latter area constitutes a piezometric low that also drains groundwater coming from the northwestern part of the model (i.e. the JO area).

The northwestern part of the model (i.e. the JO area) displays a groundwater flow that is mainly directed towards the east, with tightly spaced isolines of hydraulic heads (Fig. 7-3). Recharge is occurring at Muschelkalk outcrops to the north and south of the JO siting region. From here, the groundwater flow is directed towards the discharge areas in the lower Aare Valley to the east, and in the Sissle Valley to the west.

In the southern model domain, the Muschelkalk aquifer is recharging in outcrops located on the Internal Jura (Folded Jura) as well as along the western border. Groundwater discharges into the lower Reuss and Aare Valleys, as well as in the Limmat Valley in the Baden area, where the associated rivers cut through the Jura Main Thrust (Fig. 7-3).

The groundwater divide, resulting from the northeastern potentiometric dome, is reaching the southern model domain in the Frauenfeld – Winterthur area, extending towards the southern model limit.

The magnitude of the steady-state Darcy fluxes in the Muschelkalk aquifer were assessed in the JO, NL and ZNO siting regions (Fig. 7-4). The groundwater flow is highest in the JO siting region. This is a result from the proximity of the recharge and discharge areas (Fig. 7-3, Fig. 7-18) and the associated hydraulic head differences. Overall, the NL siting region displays the lowest groundwater fluxes, the latter being slightly lower than the one in ZNO. This is due to the slightly lower lateral hydraulic gradients simulated in the former siting region. Note that the modelled Darcy fluxes are generally higher in the Muschelkalk aquifer than in the Malm and Keuper aquifers.

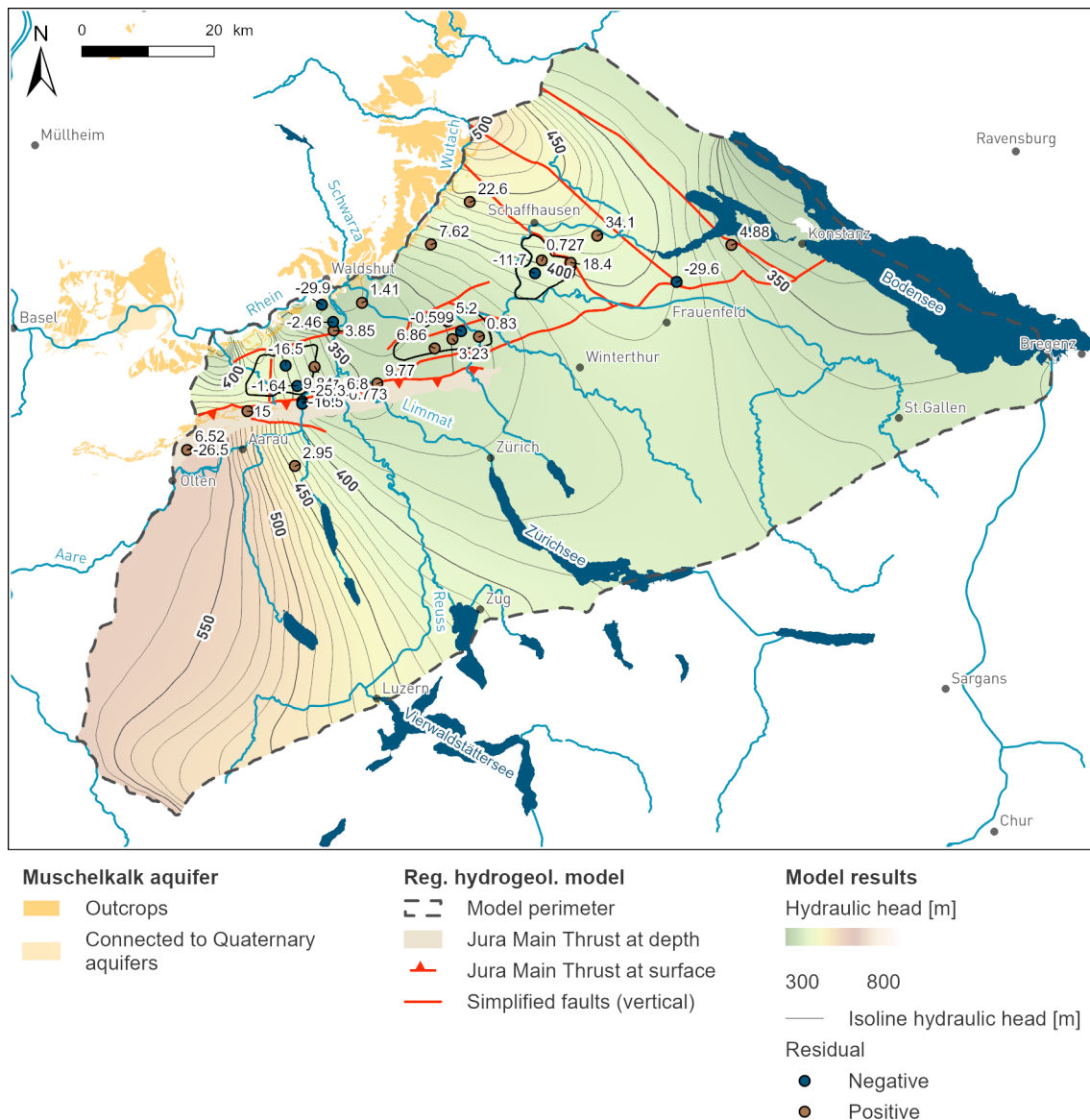


Fig. 7-3: Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Muschelkalk aquifer

Boreholes are displayed with solid circles. Residuals are shown next to the observation locations. Positive residuals indicate underestimated hydraulic heads by the model (i.e. simulated hydraulic heads < observed hydraulic heads). Negative residuals indicate overestimated hydraulic heads by the model (i.e. simulated hydraulic heads > observed hydraulic heads). The siting regions are outlined by black polygons. The map shows the outcrops and the simplified regional fault pattern used in the model. See Fig. 7-18 for a zoom on the northern part of the model. Note the potentiometric dome in the northernmost part of the model that acts as groundwater divide.

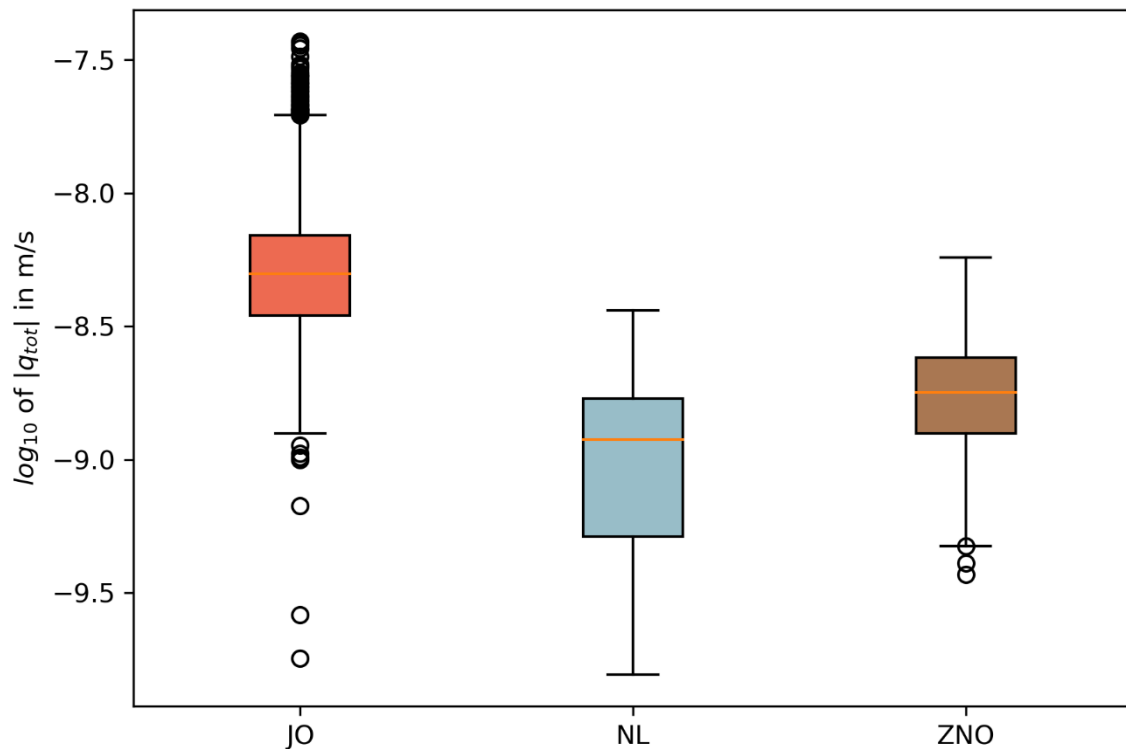


Fig. 7-4: Boxplot of the Darcy fluxes calculated by the model in the Muschelkalk aquifer horizon of the siting regions

The magnitude of the total Darcy fluxes was evaluated at each element within the perimeter of the siting regions in the Muschelkalk aquifer horizon. The logarithmic values of the groundwater flux (in m/s) are displayed. The box of the boxplot extends from the first quartile to the third quartile of the dataset. The whiskers lengthen from the sides of the interquartile range to the utmost observations lying within $1.5 \times$ the interquartile range. The observations falling outside of this interval are displayed with empty black circles. The median of the dataset is shown with a horizontal orange line. Note the comparatively high and low fluxes in the JO and NL siting regions respectively.

7.2 Keuper aquifer

The hydraulic conductivities in the five conceptual zones presented in Fig. 6-1, and in the siting regions, resulting from the calibrations are presented in Tab. 7-2 and Fig. 7-5.

The calibration led to a low hydraulic conductivity zone in the NL area (Tab. 7-2 and Fig. 7-5). In comparison, the zones located to the east and west (Zones 1, 2 and 4) display hydraulic conductivities that are one order of magnitude higher. Only Zone 4 (i.e. JO area) displays a slight horizontal anisotropy of 2.5 (i.e. $K_{xx} > K_{yy}$).

Note that the low hydraulic conductivities in Zone 3 (i.e. NL area) are consistent with the results of the hydraulic packer tests in the NL siting region (Tab. 7-2; Nagra 2024f). The calibrated hydraulic conductivities in the JO and ZNO siting regions do not reflect the higher range of values derived from the packer tests analysis (Nagra 2024f). This could be explained by the fact that the high observed hydraulic conductivities may not dominate at a regional level.

Tab. 7-2: Hydraulic conductivities and horizontal anisotropy ratio in the Keuper aquifer

The range of hydraulic conductivities K_{xx} parallel to the east – west axis is provided. Note that the hydraulic conductivities of the Keuper aquifer in the model are not depth dependent. The horizontal anisotropy ratio is defined as the ratio between the hydraulic conductivity parallel to the east-west axis and the one parallel to the north – south axis. Note that the outcrops were considered isotropic in all zones (1 to 5). The range of hydraulic conductivities derived from hydraulic packer testing in the Klettgau Formation in the JO, NL and ZNO siting regions are indicated in parentheses.

Zone / siting region	Approximate range of hydraulic conductivity (K_{xx})	Horizontal anisotropy (K_{xx}/K_{yy})
Zone 1	2×10^{-9} m/s	1.0
Zone 2	2×10^{-9} m/s	1.0
Zone 3	2×10^{-10} m/s	1.0
Zone 4	2×10^{-9} m/s	2.5
Zone 5	1×10^{-8} m/s	1.0
JO (mainly in Zone 4)	2×10^{-9} m/s (3×10^{-12} to 6×10^{-6})	2.5
NL (mainly in Zone 3)	2×10^{-10} m/s (1×10^{-12} to 2×10^{-6})	1.0
ZNO (mainly in Zone 2)	2×10^{-9} m/s (3×10^{-10} to 2×10^{-6})	1.0

Since no data is available in Zone 5, and because the latter zone has only a limited influence on the northern part of the model, the estimated initial hydraulic conductivity for the Keuper aquifer was maintained (hydraulic conductivity in ID_S2; see Section 4.2).

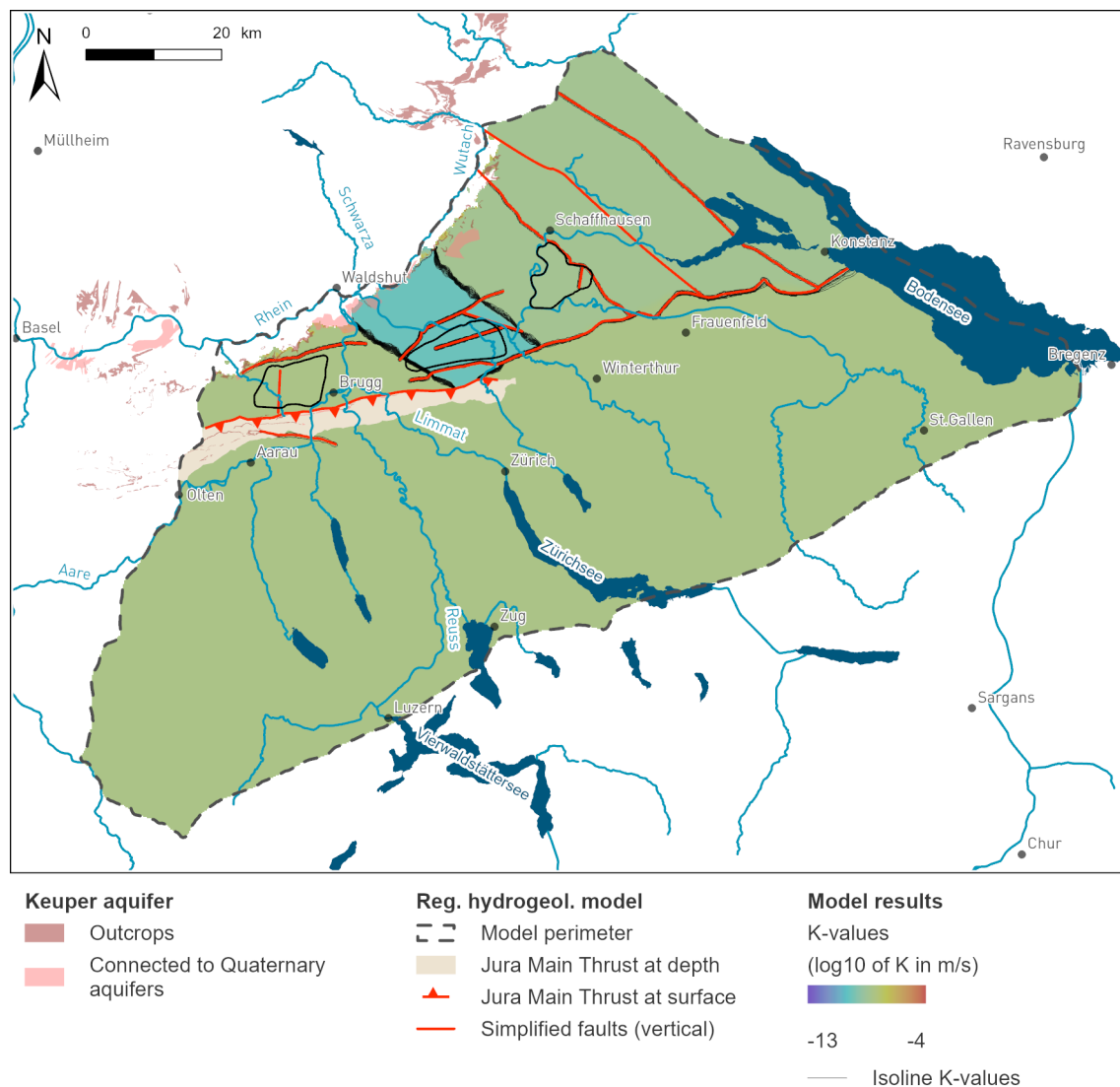


Fig. 7-5: Calibrated hydraulic conductivities in the Keuper aquifer horizon

The distribution of the hydraulic conductivity K_{xx} (i.e. parallel to the east-west axis) is shown in the figure. The hydraulic conductivity K_{xx} in Zone 1, 2 and 4 (i.e. northern part of the model except the NL area; Fig. 6-1) are 2×10^{-9} m/s. The hydraulic conductivity in the southern model area (Zone 5) is 1×10^{-8} m/s. The horizontal anisotropy ratio K_{xx}/K_{yy} used in the different zones is provided in Tab. 7-2. All zones are isotropic except the one in the JO area (Zone 4) that displays an anisotropy ratio of 2.5 ($K_{xx} > K_{yy}$). The map shows the outcrops and the simplified regional fault pattern used in the model. Note the low hydraulic conductivities in the NL area (Zone 3).

For the Keuper aquifer, the MAE of 19.08 m (Fig. 7-6) represents about 5% of the respective total hydraulic head difference (simulated hydraulic heads vary between approximately 300 m and 700 m), with a slightly lower correlation coefficient (0.93) compared to the Muschelkalk and Malm aquifers (Sections 7.1 and 7.4 respectively). Note that the Keuper is less characterised than the two above mentioned regional aquifers and that the observations are all contained within the perimeter of the siting regions.

While the regional model is able to reproduce the large-scale flow patterns in the Keuper aquifer (e.g. in terms of location of the recharge and discharge area), it is not expected to capture the local complex flow patterns resulting from the variable geological setting of the Klettgau Formation (Nagra 2024f). In ZNO, the model struggles to capture the wide range of observed hydraulic heads in the ZNO siting region (i.e. between 398 and 455 m a.s.l.; Fig. 7-6). In particular, the model underestimates the artesian conditions prevailing in the Keuper aquifer of the Benken borehole¹, while it overestimates the hydraulic heads at the location of the TRU1 and MAR1 boreholes.

In the NL siting region, the simulated hydraulic heads at the location of the boreholes STA2 and BAC1 agree well with the observed ones (Fig. 7-6). The model however tends to overestimate the hydraulic head derived from the comparatively low permeability interval in the BUL1 borehole (difference > 20 m). Note that the observed hydraulic head is characterised by a higher uncertainty (Fig. 7-6).

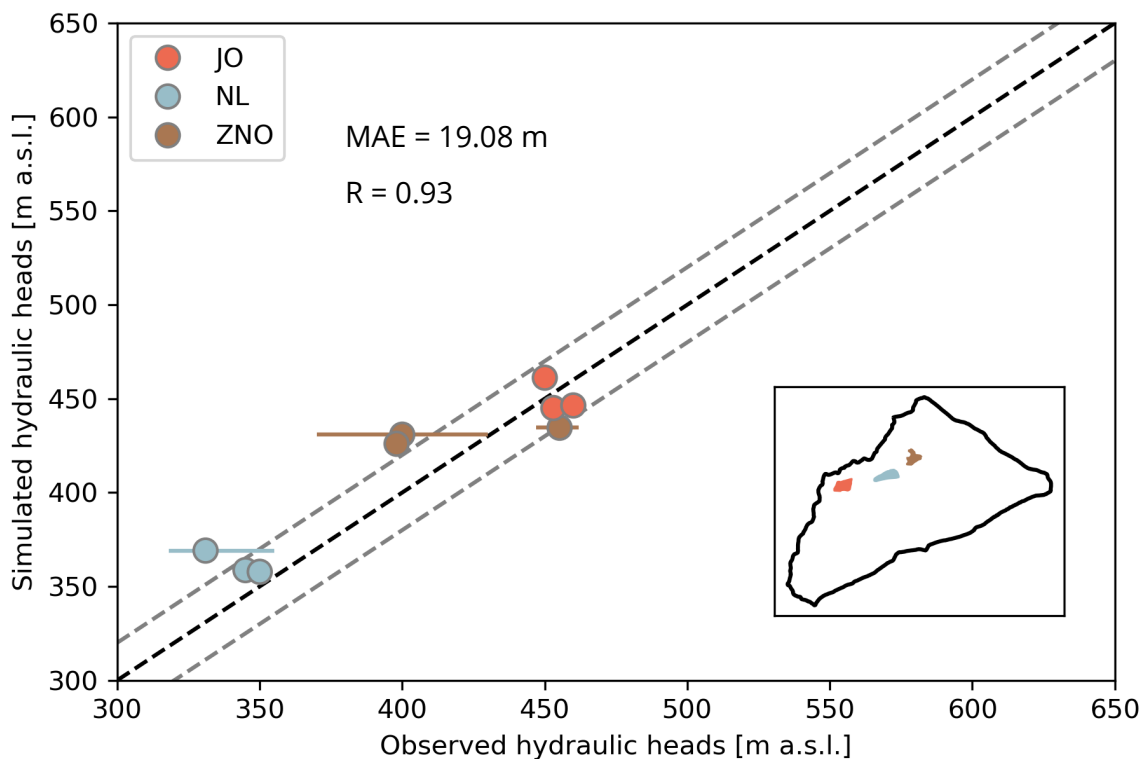


Fig. 7-6: Observed versus simulated hydraulic heads in the Keuper aquifer

The colour of the points refers to the siting regions in which the observations are located. The bandwidth of the observed hydraulic heads is displayed with horizontal error bars. Note that bandwidth may be hidden behind the symbol or may be not available (Enclosure A). The black dashed line represents a perfect fit between observed and simulated hydraulic heads. The above and underlying grey dashed lines represent a difference of ± 20 m between simulated and observed hydraulic heads.

¹ Artesian conditions exist in the Keuper aquifer of the Benken borehole as identified by hydraulic packer testing and later confirmed by long-term monitoring system measurement in the "Stubensandstein" interval (interval 7; period mid-2009 to mid-2020; e.g. Brauchler & Schulte 2019). Since mid. 2020, sub artesian conditions prevail in the monitoring system interval targeting the Klettgau Formation after a drop of the hydraulic head from mid-2018.

Two different regional flow domains stand out from the potentiometric map of the Keuper aquifer (Fig. 7-7). The first one, located north of the Baden – Irchel – Herdern Lineament and Jura Main Thrust, is controlled by the topography and the outcrop situation. All of the available hydraulic head observations were acquired in this area, and more specifically within the siting regions. The domain south of these regional tectonic features display a quieter groundwater flow regime (i.e. with lower lateral hydraulic gradients), though based on a much-reduced set of observations. The hydrogeological situation here is controlled by the boundary condition along the southern limit.

In the western part of the model, the northern and southern domains are hydraulically disconnected by the Jura Main Thrust and the outcropping low-permeable anhydrite below the Muschelkalk (Fig. 7-7).

The recharge into outcrops of the Keuper aquifer in the upper Wutach Valley results in high hydraulic heads (> 600 m a.s.l.). Driven by a steep hydraulic gradient, the groundwater flows radially towards the Bodensee area to the southeast, and towards the regional discharge area in the lower Aare Valley to the west.

In the northwestern part of the model (i.e. in the area of JO), the groundwater flow occurs mainly from the northwest to the southeast. The recharge of the Keuper aquifer occurs in outcrops located north and south of the JO siting region while discharge areas are located in the lower Aare Valley, and locally in the Sissle Valley.

North of the Baden – Irchel – Herdern Lineament and Jura Main Overthrust, the separation of the Keuper aquifer layer in different zones with different hydraulic conductivities (Tab. 7-2, Fig. 7-5) clearly affects the pattern of hydraulic head isolines. In particular, the low hydraulic conductivity zone near NL ($K = 2 \times 10^{-10}$ m/s in Zone 3) acts as a barrier to groundwater flowing from the east and west towards the discharge area in the Lower Aare Valley. This leads to high hydraulic heads upstream of the Zone 3 boundaries (Fig. 7-7). Strong lateral hydraulic gradients also exist at the transition between zones with contrasting hydraulic conductivities. This is notably the case at the eastern and western borders of Zone 3 (i.e. NL area; Fig. 7-7), whereas it is more pronounced between the ZNO and NL areas. This results in a marked piezometric depression in the NL area.

In the southern model domain, the Keuper aquifer is recharging from outcrops located on the Internal Jura (Folded Jura). Groundwater discharges into the Reuss and Aare Valleys, as well as into the Limmat Valley in the Baden area, where the associated rivers cut through the Jura Main Thrust.

The southwestern part of the model, north of the city of Olten, is characterised by high hydraulic heads (> 500 m a.s.l.; Fig. 7-7) as recharge is occurring at Keuper outcrops located to the north in the internal Jura. The hydraulic heads decrease towards the east before reaching a zone with low hydraulic gradients like the Zürichsee and the Thur River further to the east.

The magnitude of the steady-state Darcy fluxes in the Keuper aquifer were assessed in the JO, NL and ZNO siting regions (Fig. 7-8). As for the Muschelkalk aquifer, the groundwater flow is highest in the JO siting region. This is also a result of the proximity of the recharge and discharge areas and the resulting head differences (Fig. 7-7). Overall, the NL siting region displays a wide range of groundwater fluxes in comparison to the other ones. This due to the contrast of lateral hydraulic gradients between the easternmost and westernmost parts, and the central part of the siting region (Fig. 7-7), and the higher hydraulic conductivities in the westernmost part of the siting region (Fig. 7-5). Overall, the NL siting region display lower Darcy fluxes than the other ones. Note that the Keuper aquifer also present the lower fluxes than the Malm and Muschelkalk aquifers.

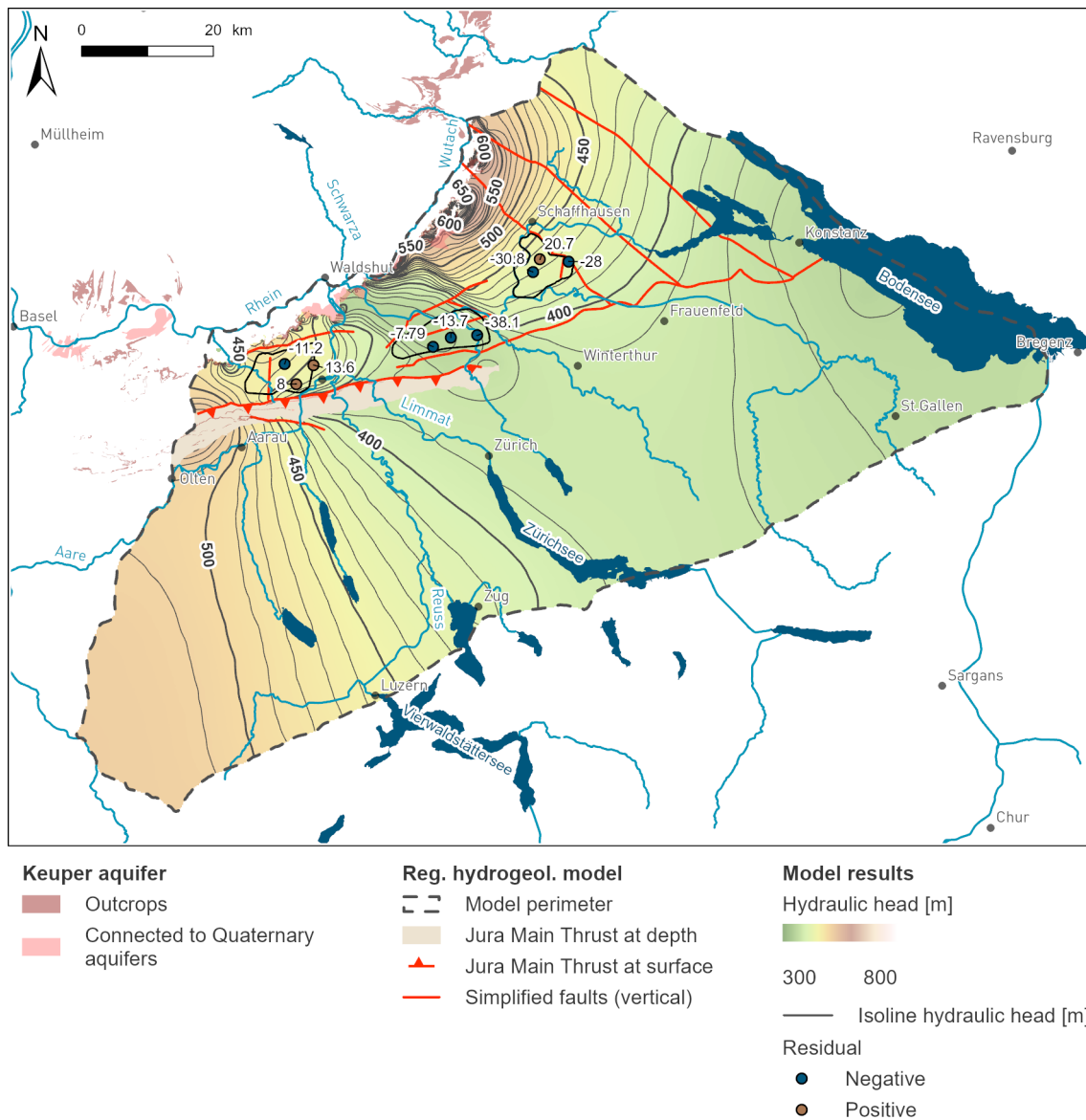


Fig. 7-7: Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Keuper aquifer

Residuals are shown next to the observation locations. Positive residuals indicate underestimated hydraulic heads by the model (i.e. simulated hydraulic heads < observed hydraulic heads). Negative residuals indicate overestimated hydraulic heads by the model (i.e. simulated hydraulic heads > observed hydraulic heads). The siting regions are outline by black polygons. The map shows the outcrops and the simplified regional fault pattern used in the model. See Fig. 7-19 for a zoom on the northern part of the model. Note the high hydraulic heads along the Wutach Valley and the low hydraulic heads in the NL area.

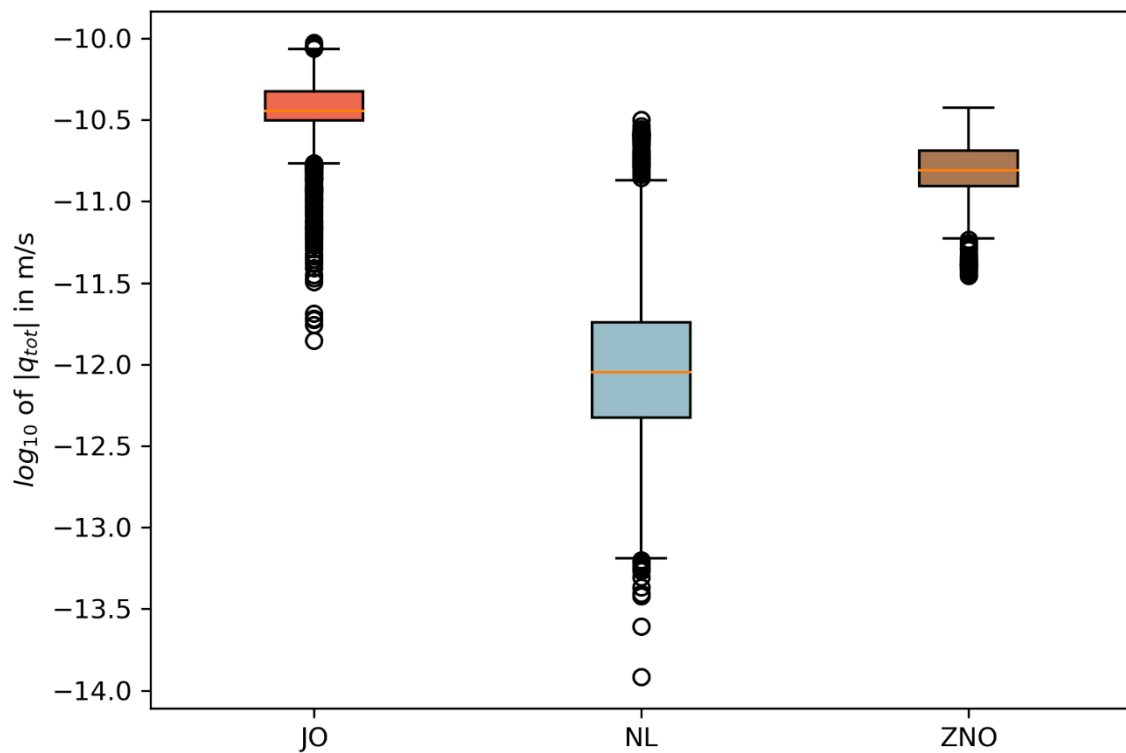


Fig. 7-8: Boxplot of the Darcy fluxes calculated by the model in the Keuper aquifer horizon of the siting regions

The magnitude of the total Darcy fluxes was evaluated at each element within the perimeter of the siting regions in the Keuper aquifer. The logarithmic values of the groundwater flux (in m/s) are displayed. The box of the boxplot extends from the first quartile to the third quartile of the dataset. The whiskers lengthen from the sides of the interquartile range to the utmost observations lying within $1.5\times$ the interquartile range. The observations falling outside of this interval are displayed with empty black circles. The median of the dataset is shown with a horizontal orange line. Note the overall lower groundwater fluxes in the NL siting region.

7.3 Hauptrogenstein aquifer

The hydraulic conductivities in the Hauptrogenstein and in the siting regions resulting from the calibration are presented in Tab. 7-3 and Fig. 7-9.

Tab. 7-3: Hydraulic conductivities and horizontal anisotropy ratio in the Hauptrogenstein aquifer

The range of hydraulic conductivities K_{xx} parallel to the east – west axis is provided. Note that the hydraulic conductivities of the Hauptrogenstein aquifer in the model are depth dependent. The horizontal anisotropy ratio is defined as the ratio between the hydraulic conductivity parallel to the east-west axis and the one parallel to the north – south axis (K_{xx}/K_{yy}). Note that the outcrops were considered isotropic. The hydraulic conductivity derived from the hydraulic test performed in the Hauptrogenstein Formation of borehole BOZ2 is provided in parentheses.

Zone / siting region	Range of hydraulic conductivity (K_{xx})	Horizontal anisotropy (K_{xx}/K_{yy})
Hauptrogenstein horizon	10^{-13} to 10^{-4} m/s	1.0
JO	2×10^{-9} to 5×10^{-7} m/s (1×10^{-8} m/s)	1.0

As for the Muschelkalk and Malm aquifers, the depth dependency of the hydraulic conductivities in the Hauptrogenstein aquifer led to a wide range of values. The lowest hydraulic conductivities are found in the southern part of the model where the depths are largest. The spectrum of hydraulic conductivities is comparatively smaller north of the Jura Main Thrust (between approximately 10^{-9} to 10^{-4} m/s) reflecting the narrower depth range. The hydraulic conductivity estimated from the hydraulic packer tests in the BOZ2 borehole fall in the range of the calibrated hydraulic conductivities in the JO siting region.

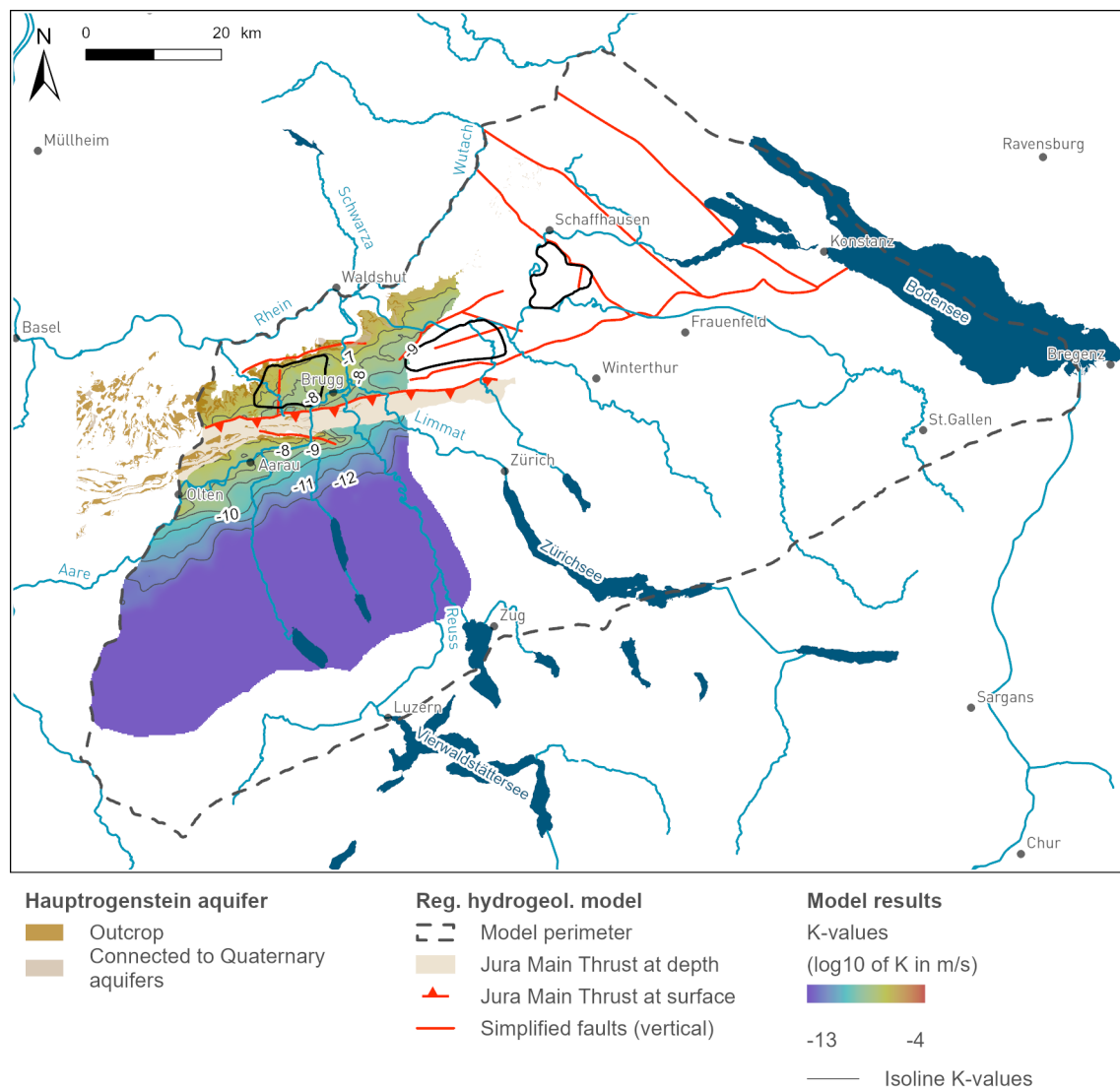


Fig. 7-9: Calibrated hydraulic conductivities in the Hauptrogenstein aquifer horizon

Residuals are shown next to the observation locations. Positive residuals indicate underestimated hydraulic heads by the model (i.e. simulated hydraulic heads < observed hydraulic heads). Negative residuals indicate overestimated hydraulic heads by the model (i.e. simulated hydraulic heads > observed hydraulic heads). The siting regions are outlined by black polygons. The map shows the outcrops and the simplified regional fault pattern used in the model. Note the decrease in hydraulic conductivity towards the southeast in response to increasing depths of the Hauptrogenstein aquifer horizon.

For the Hauptrogenstein aquifer, a MAE of 8.01 m (Fig. 7-10) reflects about 3% of the respective total hydraulic head difference (simulated hydraulic heads vary between approximately 300 m and 600 m), with a correlation coefficient of 0.97. The low MAE and high correlation coefficient must however be put in perspective since:

- The dataset in the Hauptrogenstein aquifer is very limited (four observation points in total).
- Only one observation point is available north of the Jura Main Thrust (i.e. the BOZ2 borehole) against three to the south of this tectonic feature. The available data south of the Jura Main Thrust are located in the same area (Fig. 7-11) close to the western model limit.
- The model areas north and south of the Jura Main Thrust are hydraulically disconnected. A change of the hydraulic conductivities in one of the areas thus does not impact the hydraulic situation in the other.

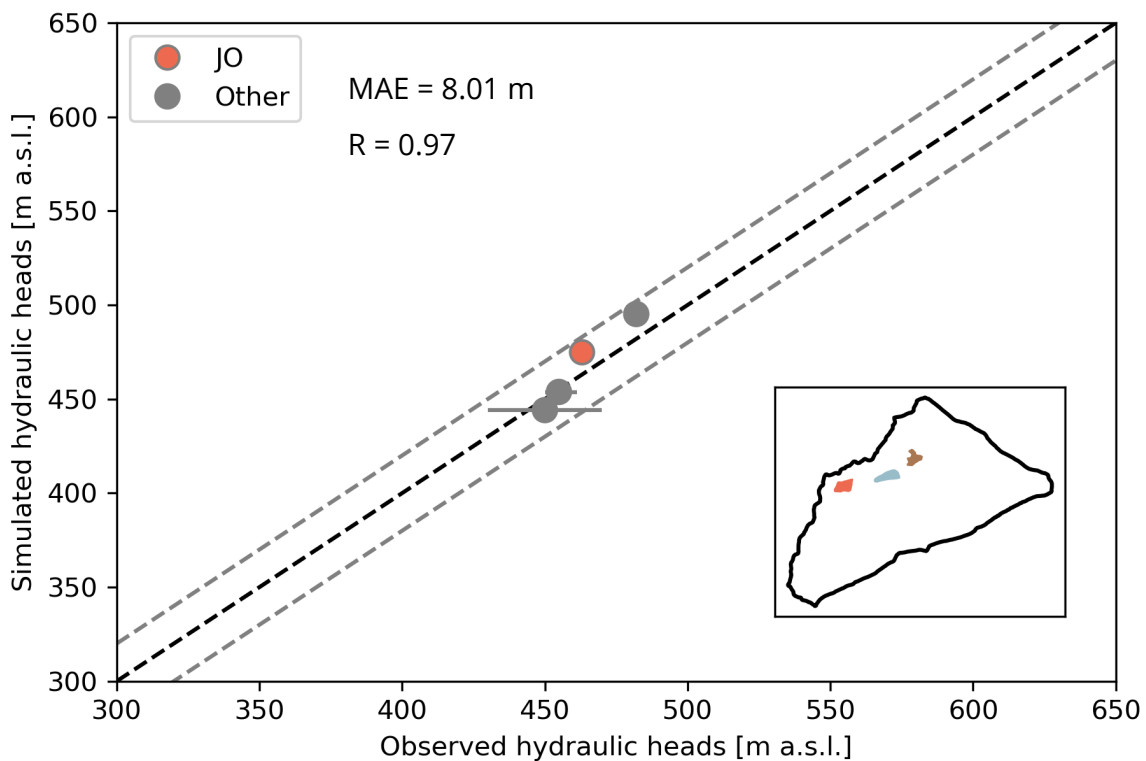


Fig. 7-10: Observed versus simulated hydraulic heads in the Hauptrogenstein aquifer

The colour of the points indicates whether the observation is located inside or outside the perimeter of the JO siting region. The bandwidth of the observed hydraulic heads is displayed with horizontal error bars. Note that bandwidth may be hidden behind the symbol or may be not available (Appendix 1). The black dashed line represents a perfect fit between observed and simulated hydraulic heads. The above and underlying grey dashed lines represent a difference of ± 20 m between simulated and observed hydraulic heads.

The flow system in the Hauptrogenstein aquifer is affected by the local topographic situation and by the facies transition towards clay-rich units in the east (Nagra 2024f). As for the other aquifers, two regional flow domains can be recognised from the potentiometric map (Fig. 7-11), namely north and south of the Jura Main Thrust. The domain north of the Jura Main Thrust is mainly controlled by the tectonic situation, topography and outcrop situation. South of this tectonic feature, a quieter groundwater flow regime exists (i.e. with smaller lateral hydraulic gradients). Here, the groundwater flow is mainly controlled by the boundary conditions at the southern boundary as well as by the low hydraulic conductivities at depth. Note that the northern and southern parts of the model are hydraulically disconnected due to the presence of the Jura Main Thrust.

In the northern part of the domain, the groundwater flow in the Hauptrogenstein aquifer mainly occurs from the west to the east (Fig. 7-11). It is recharging in outcrops located north and west of the JO siting region and is discharging into the Lower Aare Valley to the east. As for the Muschelkalk and Keuper aquifers, the Sissle Valley constitutes a local discharge area west of the JO siting region.

For the southern part of the model, recharge is also occurring in outcrops of the Hauptrogenstein aquifer located on the Internal Jura (Folded Jura), west of the Jura Main Thrust and north of Olten (Fig. 7-11). Overall, the groundwater flow is oriented towards the Brugg area where the Hauptrogenstein aquifer is in contact with the Aare River (or the associated Quaternary aquifer).

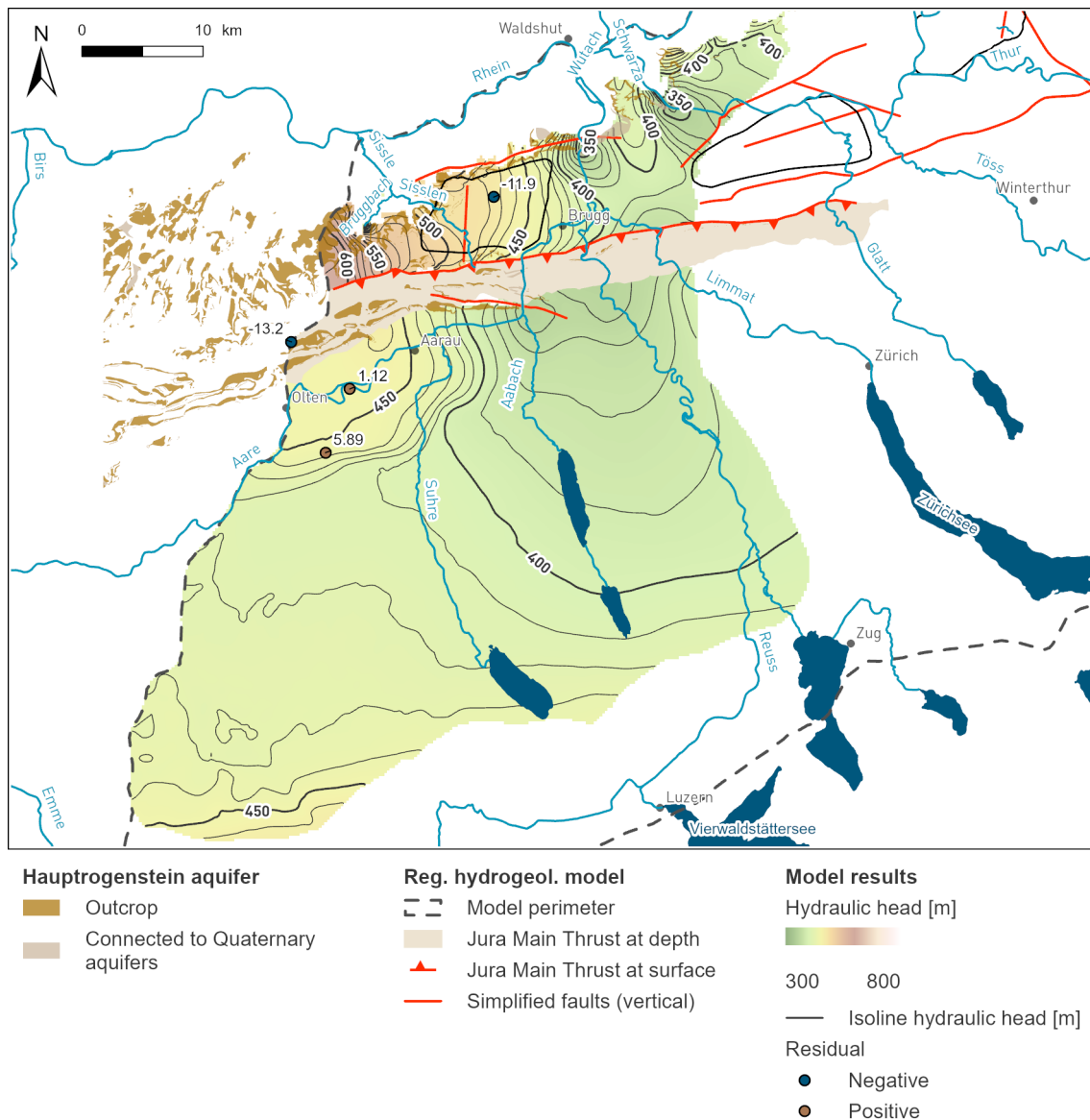


Fig. 7-11: Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Hauptrogenstein aquifer

Residuals are shown next to the observation locations. The siting regions are outlined by black polygons. The map shows the outcrops and the simplified regional fault pattern used in the model. Background map shows the simulated hydraulic heads.

7.4 Malm aquifer

The hydraulic conductivities in the three zones presented in Fig. 6-1 and in the siting regions resulting from the calibration are presented in Tab. 7-4 and Fig. 7-12.

Tab. 7-4: Hydraulic conductivities and horizontal anisotropy ratio in the Malm aquifer

The range of hydraulic conductivities K_{xx} parallel to the east – west axis is provided. Note that the hydraulic conductivities of the Malm aquifer in the model are depth dependent. The horizontal anisotropy ratio is defined as the ratio between the hydraulic conductivity parallel to the east-west axis and the one parallel to the north – south axis (K_{xx}/K_{yy}). Note that the outcrops were considered isotropic in all the three Zones A, B and C. The range of hydraulic conductivities derived from hydraulic packer testing in the Malm aquifer in the siting regions NL and ZNO are indicated in parentheses. Only values from transmissive intervals (i.e. where a groundwater sample could be taken) are considered.

Zone / siting region	Range of hydraulic conductivity (K_{xx})	Horizontal anisotropy (K_{xx}/K_{yy})
A	10^{-13} to 10^{-4} m/s	1.0
B	10^{-8} to 10^{-4} m/s	0.3
C	10^{-8} to 10^{-4} m/s	0.5
NL (mainly in Zone C)	3×10^{-8} to 3×10^{-7} m/s (3×10^{-9} to 1×10^{-7} m/s)	0.3 to 1.0
ZNO (mainly in Zone C)	3×10^{-8} to 4×10^{-7} m/s (1×10^{-8} to 4×10^{-8} m/s)	0.5 to 1.0

The widest spectrum of hydraulic conductivities is found in the southern part of the model, which reflects the range of depth in this part of the model (Tab. 7-4, Fig. 7-12). Zones B and C display a narrower range of hydraulic conductivities with values between 10^{-8} and 10^{-4} m/s. The highest hydraulic conductivities are occurring on outcrops, which are located along the northern limit of the model as well as on the Internal Jura (Folded Jura). Note that the model calibration led to a slight anisotropy of the horizontal hydraulic conductivity in Zones B and C in the northern part of the model (i.e. $K_{xx} < K_{yy}$).

Overall, the hydraulic conductivities in the siting region resulting from the model calibration agree well with hydraulic conductivities at the formation scale derived from the results of the hydraulic packer tests (Tab. 7-4).

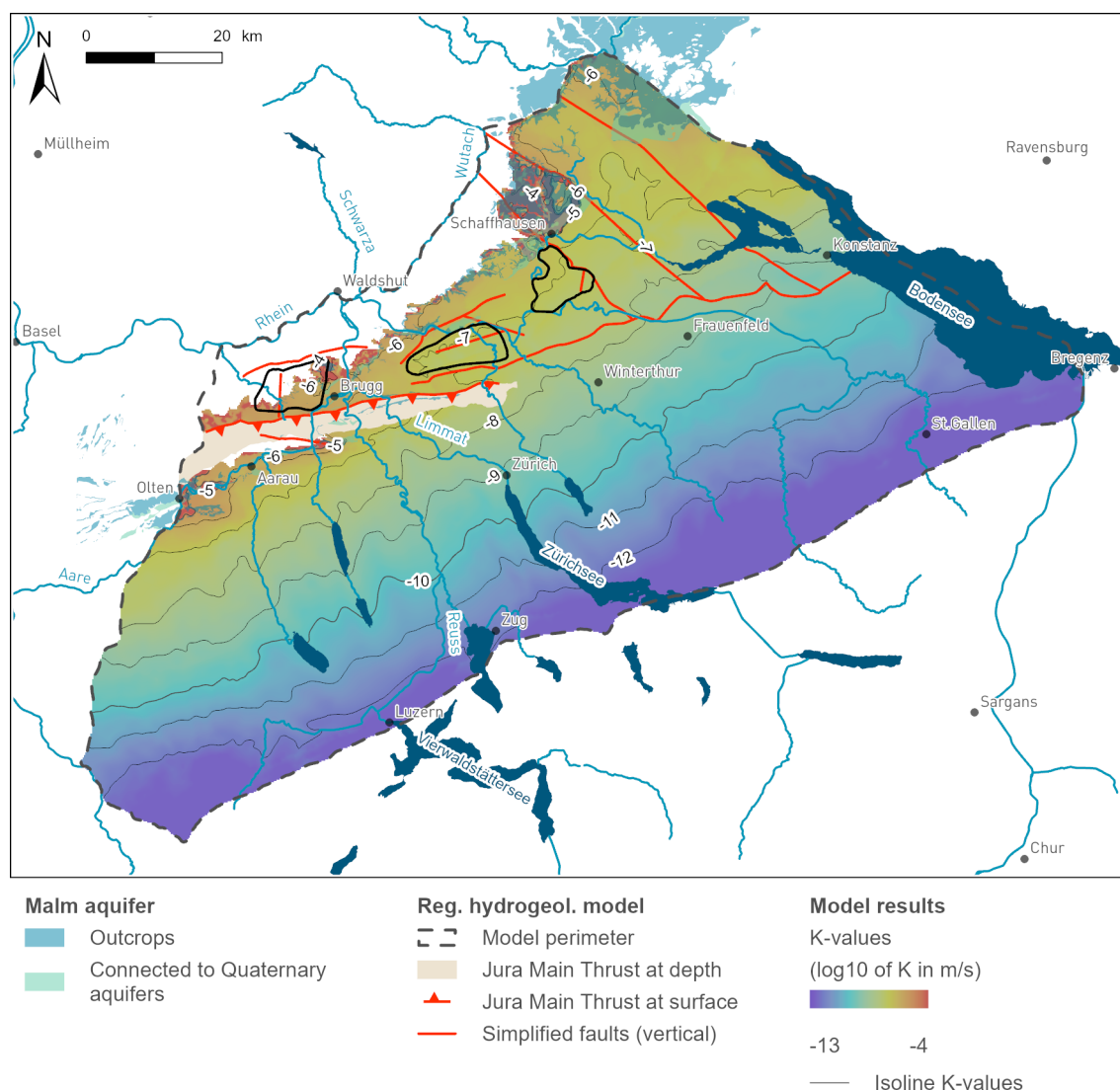


Fig. 7-12: Calibrated hydraulic conductivities in the Malm aquifer horizon

The distribution of the hydraulic conductivity K_{xx} (i.e. K parallel to the east-west axis) is shown in the figure. The horizontal anisotropy ratio K_{xx}/K_{yy} of the different zones is provided in Tab. 7-4 and varies between 0.3 and 1.0. The map shows the outcrops and the simplified regional fault pattern used in the model. Note the decrease in hydraulic conductivity towards the southeast in response to increasing depths of the Malm aquifer horizon.

The calibration of the model resulted in a relatively low MAE of 13.51 m for the Malm aquifer (Fig. 7-13). This represents 4 to 5% of the total head difference (simulated hydraulic heads vary between 350 – 600 m for the Malm aquifer). In addition, the correlation coefficient of 0.96 reflects a very good agreement between simulated and observed hydraulic heads.

The model shows a predominance of overestimated hydraulic heads in the northernmost part of the model (Fig. 7-13; Zone C), especially in the northeastern most corner of the model (Fig. 7-14). Further to the south, the observed hydraulic heads in the siting regions NL and ZNO are generally well reproduced by the model.

In the southern part of the model domain, the model underestimates the hydraulic heads for three of the four observation points located (Fig. 7-13 and Fig. 7-14).

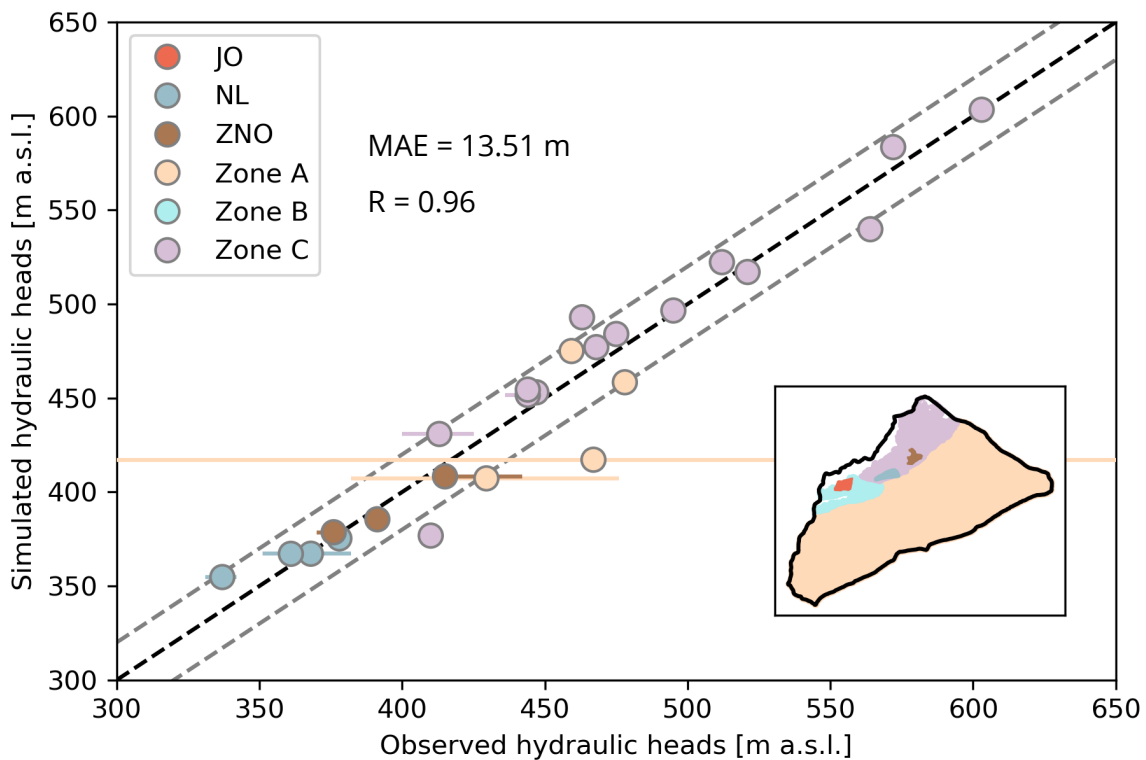


Fig. 7-13: Observed versus simulated hydraulic heads in the Malm aquifer

The colour of the points refers to the different zones defined in the Malm aquifer horizon (Chapter 6) or to the siting regions in which the observations are located. The bandwidth of the observed hydraulic heads is displayed with horizontal error bars. Note that bandwidth may be hidden behind the symbol or may be not available (Appendix 1). The black dashed line represents a perfect fit between observed and simulated hydraulic heads. The above and underlying grey dashed lines represent a difference of ± 20 m between simulated and observed hydraulic heads. The observed hydraulic head with the wide uncertainty bandwidth (about 503 m) was observed in the borehole ZÜR (Zone A; Nusch et al. 2013). This results from the fitting of the test interval transmissivities to the hydraulic head values. Since a quasi-stationary state was reached during the test, the uncertainty can be considered less than 200 m (Nusch et al. 2013).

Two regional flow domains appear from the potentiometric map of the Malm aquifer (Fig. 7-14). In the northern part of the model (i.e. north of the Baden – Irchel – Herdern Lineament and Jura Main Thrust), the hydrogeological situation is mainly affected by the topography and outcrop situation. This part of the model is also well constrained by observations. The zone south of these tectonic features is characterised by a quieter groundwater flow regime (i.e. with overall lower lateral hydraulic gradients) that is mainly influenced by the boundary conditions on the southern limit and by the low hydraulic conductivities at depth.

In the western part of the model, the northern and southern domains are hydraulically disconnected by the Jura Main Thrust and the outcropping low permeability anhydrite below the Muschelkalk (Fig. 7-14).

The most prominent hydrogeological feature in the Malm aquifer consists of a piezometric dome in the northern part of the model. The latter results from the recharge of the Malm aquifer via the outcrops in the Schaffhausen area and the connection with the Danube River in the northernmost corner of the model.

From the north, the groundwater flows toward the south – southeast with a steep hydraulic gradient before converging, along with water entering the model through the eastern boundary, towards the discharge areas along the Rhine River. The latter includes the Rhine Falls and Rheinau areas north of the ZNO siting region, and the region of Kaiserstuhl – Hohentengen north of the NL siting region. Further to the west, the confluence of the Aare, Limmat and Reuss Rivers near the city of Brugg also constitute a regional discharge area.

Similar to the Muschelkalk and Keuper aquifers, additional discharge areas are located along the Jura Main Thrust, where the latter is cut by the Reuss and Aare Valleys (Fig. 7-14). These locations include the Aare River near the cities of Aarburg and Aarau, as well as the Reuss River in the Mellingen area.

In the southern domain, the Malm aquifer is recharging through the outcrops distributed along the Internal Jura (Folded Jura), mainly on the southern side of the Lägern anticline. The resulting piezometric dome extends toward the south and reaches the Zürich area. From this groundwater divide, water is flowing in the direction of two piezometric depressions that approximately follow the trace of the Töss and Reuss Rivers.

The magnitude of the steady-state Darcy fluxes in the Malm aquifer were assessed in the NL and ZNO siting regions (Fig. 7-15). The range of modelled fluxes display differences between the two siting regions, such as the tailing towards higher values in ZNO and the lower values covered in NL. Both siting regions show similar magnitudes, with a slightly higher interquartile range in NL. In both siting regions, the higher fluxes are occurring near the discharge areas along the Rhine River. In the NL siting region, low fluxes are found in the eastern part of the siting region. Low flow in this area is also supported by hydrochemical data in the BUL1, STA2, and STA3 boreholes (Nagra 2024f).

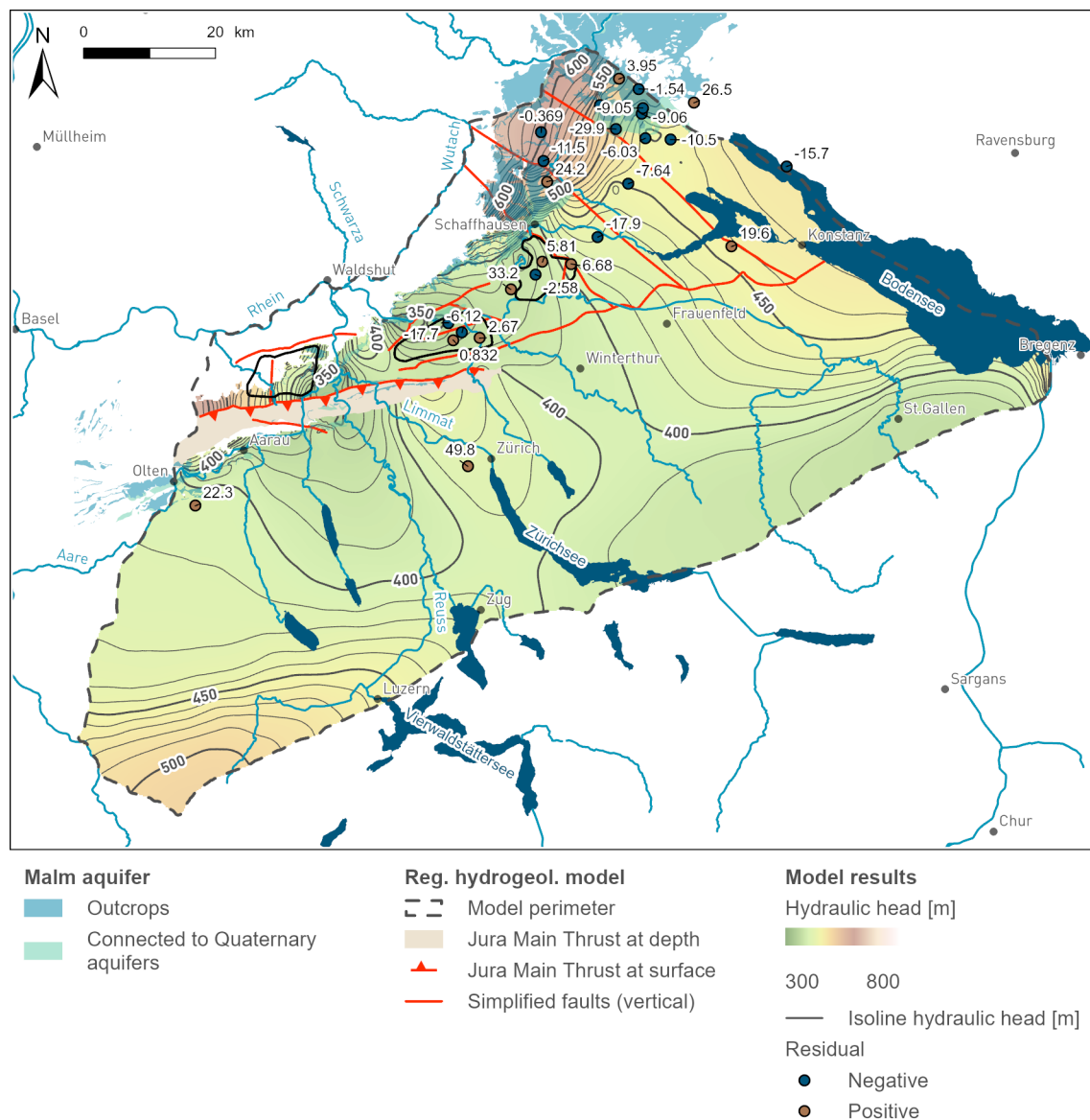


Fig. 7-14: Simulated hydraulic heads and differences between observed and simulated heads (residuals) in the Malm aquifer

Residuals are shown next to the observation locations. Residuals are shown next to the observation locations. Positive residuals indicate underestimated hydraulic heads by the model (i.e. simulated hydraulic heads < observed hydraulic heads). Negative residuals indicate overestimated hydraulic heads by the model (i.e. simulated hydraulic heads > observed hydraulic heads). The siting regions are outlined by black polygons. The map shows the outcrops and the simplified regional fault pattern used in the model. See Fig. 7-22 for a zoom on the northern part of the model. Note the potentiometric dome in the northernmost part of the model.

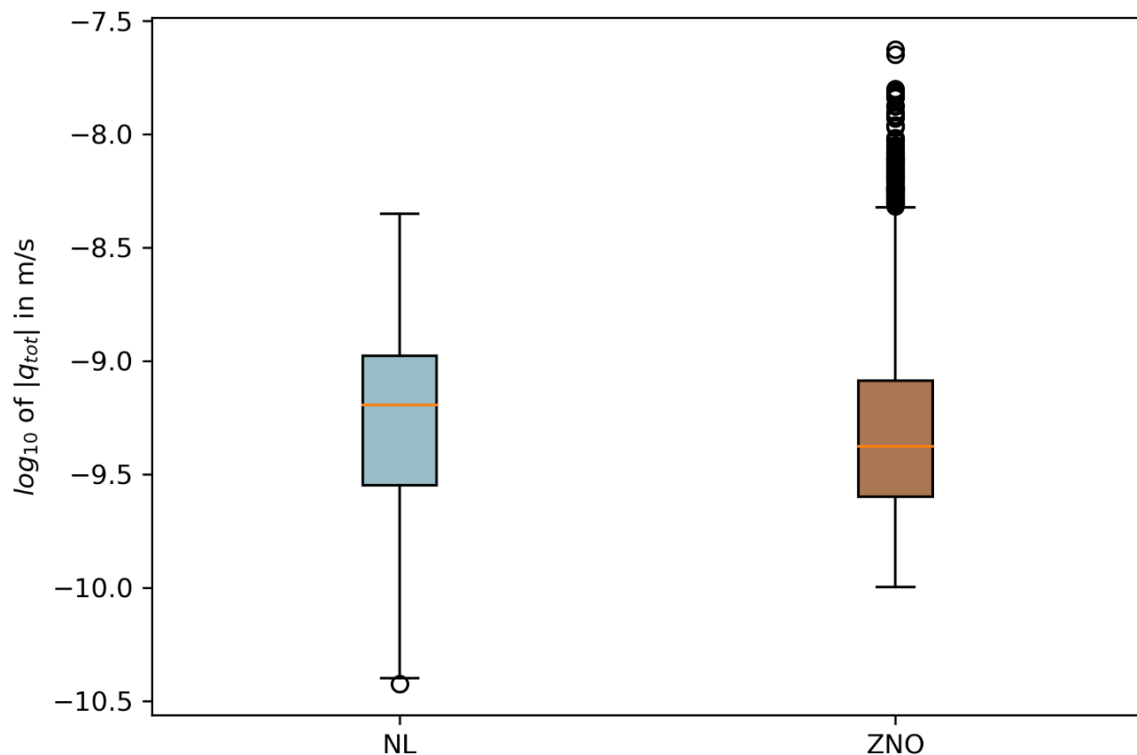


Fig. 7-15: Boxplot of the Darcy fluxes calculated by the model in the Malm aquifer horizon of the siting regions

The magnitude of the total Darcy fluxes was evaluated at each element within the perimeter of the siting regions in the Malm aquifer horizon. The logarithmic values of the groundwater flux (in m/s) are displayed. The box of the boxplot extends from the first quartile to the third quartile of the dataset. The whiskers lengthen from the sides of the interquartile range to the utmost observations lying within $1.5 \times$ the interquartile range. The observations falling outside of this interval are displayed with empty black circles. The median of the dataset is shown with a horizontal orange line. Note the comparable groundwater fluxes in the NL and ZNO siting regions.

7.5 Hydraulic gradients in the Opalinus Clay

Steady-state vertical hydraulic gradients across the Opalinus Clay were regionally evaluated based on the results of the hydrogeological model. The distribution of the simulated vertical hydraulic gradients (Fig. 7-16) is obtained by dividing the differences in hydraulic head between the top and the bottom of the Opalinus Clay by the thickness of this unit. The derived vertical hydraulic gradients give valuable information (i.e. magnitude and direction of the vertical gradients) on transport dynamics under steady-state hydraulic conditions. Note that the vertical gradients across the Opalinus Clay are mainly controlled by the hydraulic head distribution in the over- and underlying aquifers and by the vertical distribution of hydraulic conductivities in the host rock and confining units.

The absolute magnitude of the gradients across the Opalinus Clay is mainly below ca. 0.5 m/m in the area of the siting regions but can be higher close to the aquifer recharge boundaries (up to approximately 0.9 m/m). From a site-specific perspective, downward gradients are calculated for most of the JO siting region (magnitude < 0.3 m/m; Fig. 7-16). Upward hydraulic gradients are however calculated in the northeastern part of the siting region.

Upward gradients are calculated in the ZNO siting region (Fig. 7-16). This agrees with the artesian conditions observed for the Keuper aquifer in the Benken borehole and low hydraulic heads in the Malm aquifer (hydraulic head difference of approximately 60 m). The gradients tend to increase toward the northwest, reaching a value of about 0.5 m/m.

In the NL siting region, the magnitude of the vertical hydraulic gradients is comparably small (Fig. 7-16). This is overall well supported by small hydraulic head differences between overlying and underlying aquifers (< 25 m) in the boreholes STA2, STA3 and BUL1. Upward and downward gradients are found in the northern and southern part of the siting region respectively.

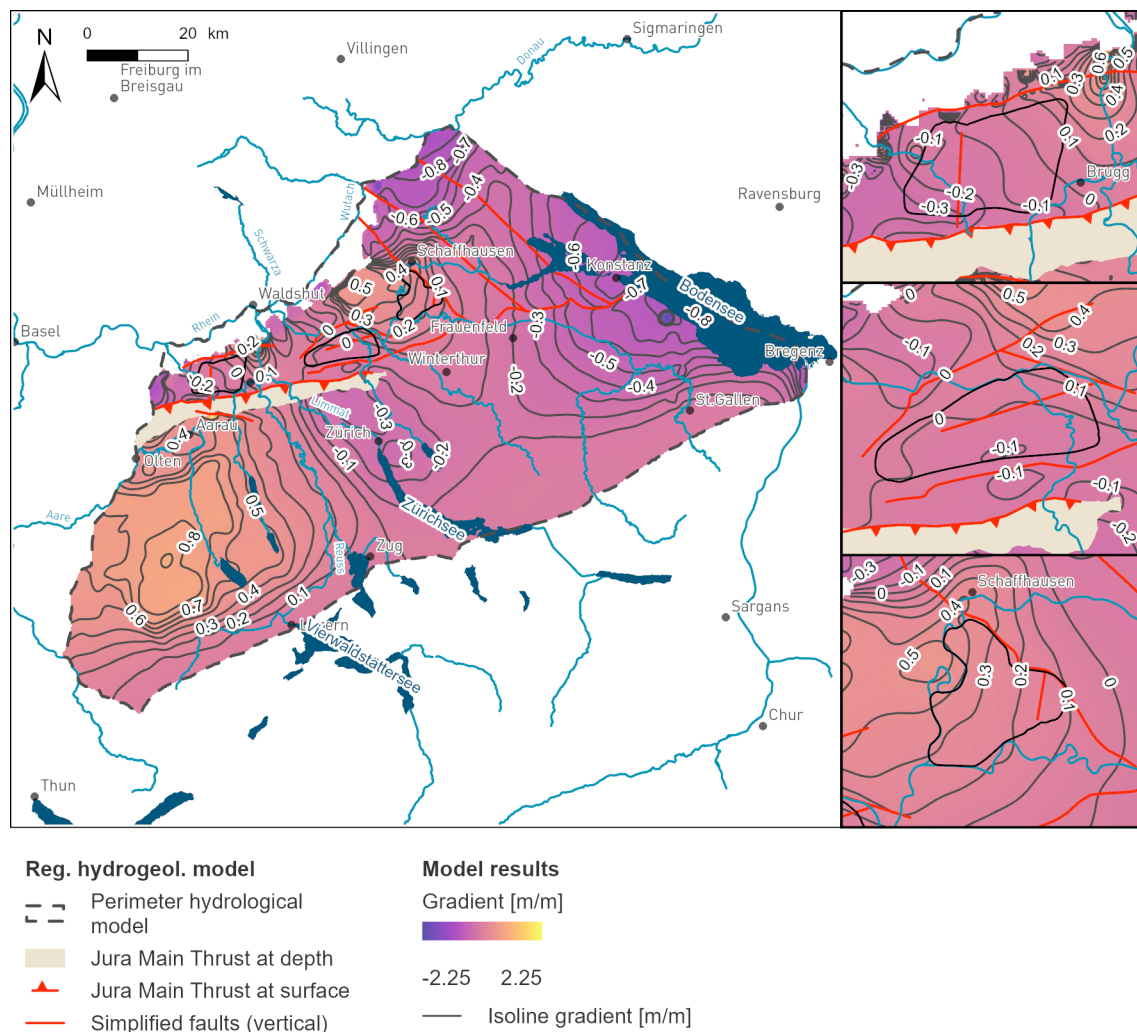


Fig. 7-16: Vertical hydraulic gradient across the Opalinus Clay

The vertical hydraulic gradients across the Opalinus Clay are shown for the entire model on the left and for the siting regions on the right. Positive values represent descending flows and negative values ascending ones. The vertical hydraulic gradients were calculated by dividing the difference in hydraulic heads between the top and bottom of the formation by the thickness of the formation.

The large-scale vertical hydraulic gradients between the aquifers above and below the Opalinus Clay were investigated using hydraulic head difference maps (Fig. 7-17). Note that the Hauptrogenstein and Malm aquifers are the nearest aquifers above the Opalinus Clay west and east of the Aare Valley. Below the Opalinus Clay, the presence or absence of the Keuper aquifer as the nearest aquifer can potentially shorten or increase the thickness of the confining units and impact the vertical hydraulic gradients across the host rock. The hydraulic head difference is thus evaluated considering the possible combinations (i.e. Malm – Keuper, Malm – Muschelkalk, Hauptrogenstein – Keuper and Hauptrogenstein – Muschelkalk). Note that positive and negative values are related to upward and downward hydraulic gradients respectively.

Hydraulic head differences between the Hauptrogenstein and the Keuper aquifers are positive in the lower Aare Valley (values up to about 90 m), and even extend further to the west in the northeastern part of the JO siting region (Fig. 7-17a). This is notably due to the strong hydraulic head decrease towards the discharge area in the lower Aare Valley in the Hauptrogenstein aquifer (Fig. 7-21). In the Keuper aquifer, on the other hand, the lateral hydraulic gradient in the JO area is mainly directed towards the southeast (Fig. 7-19). Negative values occur in the central and western part of the siting region as higher hydraulic heads exist in the Hauptrogenstein aquifer as in the Keuper (values down to about -40 m). This is in part due to the position and altitude of the Hauptrogenstein outcrops to the north of the siting region where recharge occurs (Sections 7.3 and 7.6.3). Hydraulic heads from the Hauptrogenstein and Keuper aquifer in the BOZ2 borehole supports negative differences in the JO siting region.

Hydraulic head differences between the Hauptrogenstein and Muschelkalk aquifers are predominantly negative (values down to about -90 m; Fig. 7-17b) in the area west of the Aare as higher hydraulic heads generally prevail in the Hauptrogenstein aquifer (Fig. 7-21). This is in part due to the location and altitude of the Hauptrogenstein outcrops.

The distribution of the hydraulic head differences east of the Aare is also impacted by whether the Muschelkalk aquifer or the Keuper aquifer are included for the calculation (along with the Malm aquifer). In the case where the Keuper aquifer is considered, positive hydraulic head differences are found in the ZNO area as well in the northern part of the NL siting region up to the Rhine River to the north (Fig. 7-17c). This results from the low hydraulic heads in the Malm aquifer along and near the Rhine River, which serves as a discharge area for the latter aquifer (Sections 7.4 and 7.6.4), and the comparatively higher hydraulic heads occurring in the Keuper aquifer, especially in the ZNO area (Fig. 7-19) as supported by borehole data. This leads to hydraulic differences > 60 m in the Rhine Falls and Rheinau areas. Note that a similar hydraulic head difference exists in the Benken borehole between the Malm and Keuper aquifers. The lower hydraulic heads occurring in the Keuper aquifer around the NL siting regions (see Fig. 7-7 and text of Section 7.2) is reflected by a decrease of the hydraulic head difference towards the west (Fig. 7-17c). The latter siting region is in the area of transition from positive hydraulic head differences in the north (about 20 m) to negative values in the south.

In the case where the Muschelkalk is considered, the zone with positive hydraulic head difference is restricted to the ZNO area (up to about 30 m) whereas the NL area display overall negative values (i.e. down to about -40 m), with the exception of the area of Kaiserstuhl – Hohentengen where low positive values occur (Fig. 7-17c). The prominence of negative differences in the NL area can be explained by the existence of comparatively higher hydraulic heads in the Malm aquifer (Fig. 7-22) that are triggered by the Malm recharge through the Molasse units. Note that hydraulic head data from the STA2, STA3 and BUL1 boreholes support negative hydraulic differences, while a positive difference is observed in the Weiach borehole (located in the north).

Overall, considering the Muschelkalk aquifer for the calculation of the hydraulic head difference leads to a prominence of negative differences in Northern Switzerland that would indicate large-scale downward hydraulic gradients across the Keuper, Dogger and lower Malm formations (Fig. 7-17). On the other hand, considering the Keuper aquifer leads to an extension of the zones with positive hydraulic differences (i.e. indicating large-scale upward gradients across the confining units and the host rock) that predominate in the siting region area. This is highlighting the impact of the presence of the Keuper aquifer on the steady-state advective transport in the aquitards.

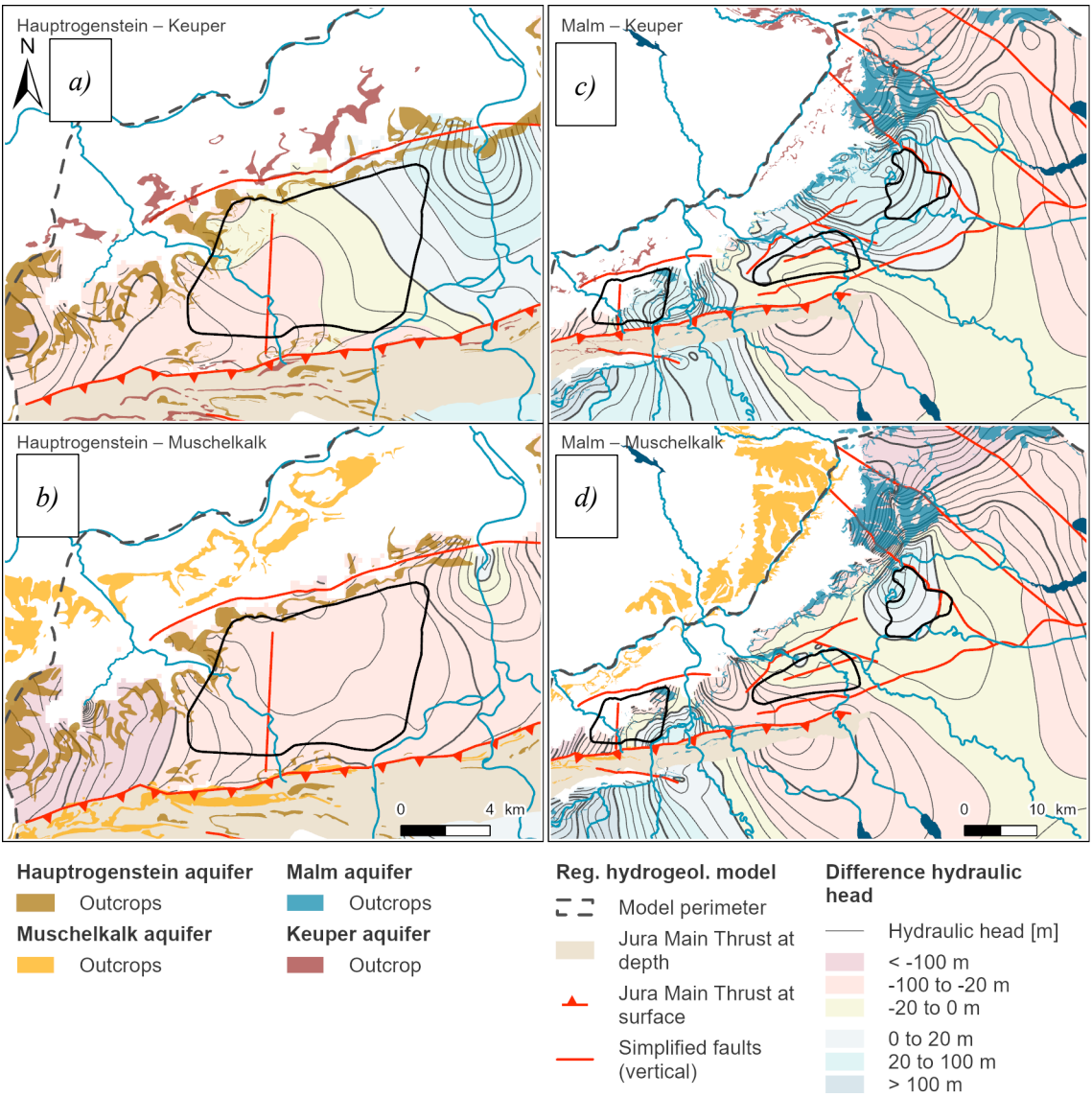


Fig. 7-17: Difference in hydraulic heads between aquifers above and below the Opalinus Clay
Negative and positive values indicate upward and downward gradients, respectively. The maps show the outcrops and the simplified regional fault pattern used in the model.

7.6 Discharge/Recharge from particle tracking

The location of the recharge and discharge areas of the aquifers was assessed using backward and forward particle tracking. The particle pathlines are calculated using the simulated groundwater velocity field (dispersive and diffusive transport is not accounted for) and generic porosities. A timeframe of 5 million years was considered for the calculations with a variable time stepping strategy depending on the elemental velocity and ranging from 1 to 50 years. Note that the validity of the steady-state flow simulation is much shorter than the considered timeframe because of possible changes of the flow boundary conditions. A total of 300 particles were released in each aquifer within the perimeter of the siting regions. This number is sufficiently large to ensure the statistical representativeness of the trajectories.

7.6.1 Muschelkalk aquifer

Pathlines of the backward particles released in the NL and ZNO siting regions show that the groundwater flowing through the sites originates in the Wutach Valley (Fig. 7-18, Section 7.1). From there, the pathlines are oriented toward the south-southeast before turning to the west and crossing the ZNO and NL areas. The forward particle pathlines from both siting regions reach the regional discharge area of the lower Aare Valley further to the northwest. Note that the direction of groundwater flow in the model is in agreement with the one inferred from the borehole data in the NL and ZNO siting regions.

The flow system in the JO siting region is controlled by the local tectonic situation, the topography and the nearby discharge areas. Backward particle tracking indicates that the Muschelkalk aquifer is recharging at outcrops to the north and west of the siting region, as well as on Muschelkalk outcrops located along the Jura Main Thrust to the south (Fig. 7-18). Here, backward particles indicate a downward migration in the Jura Main Thrust before reaching the Muschelkalk aquifer in the northern part of the model.

The discharge areas around the JO siting region identified using forward particle tracking are the lower Aare Valley to the east, and the lower Sissle Valley (to a lesser extent) to the west where Muschelkalk outcrops are in contact with Quaternary aquifers (Fig. 7-18). The groundwater divide that separates the flow towards these two valleys is located near the western border of the siting region. Note that the borehole data (BOZ2, BOZ1 and Riniken) indicates a groundwater flow towards the north, that is approximately towards the lower Aare Valley.

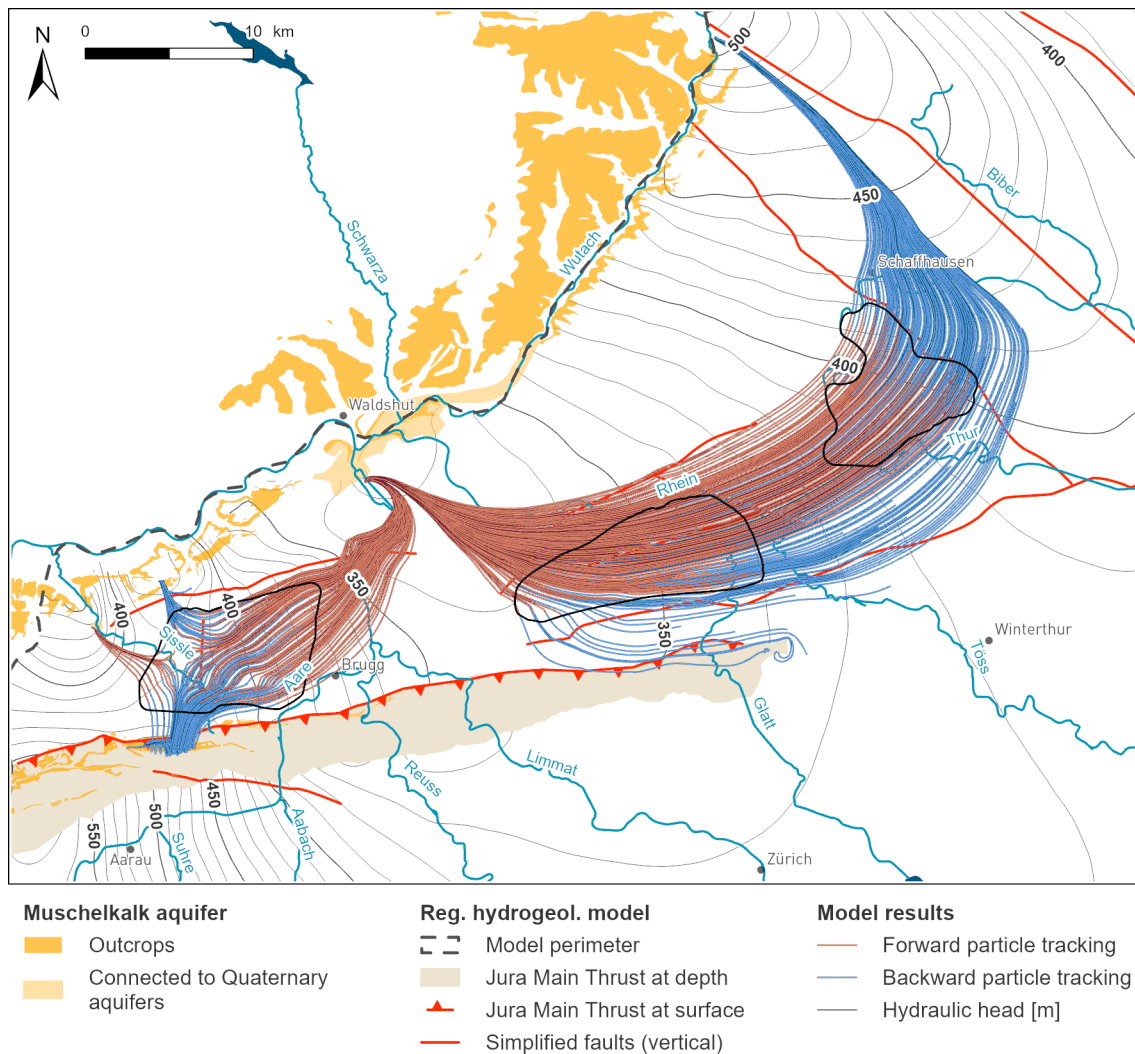


Fig. 7-18: Simulated hydraulic heads and particle tracking identifying recharge and discharge areas in the Muschelkalk aquifer

Hydraulic head situation at the top of the upper Muschelkalk aquifer of the hydrogeological model. The map shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the well-defined regional flow paths of the groundwater flowing through the NL and ZNO siting regions, and the more local groundwater flow system around the JO siting region.

7.6.2 Keuper aquifer

The groundwater flow in the ZNO siting region is largely impacted by the presence of the recharge area in the north (Fig. 7-19). Backward particle pathlines are oriented along an approximately north-south axis, agreeing with the direction of the lateral hydraulic gradient inferred from the borehole data. The groundwater flow then slightly rotates to the south-southwest downstream of the siting region as supported by forward particle tracking. Note that the forward particles do not reach any discharge area during the timeframe considered for the particle tracking (Fig. 7-19). This is due to the relatively low flow velocities but also to the entrapment of particles in the adjacent aquitards.

The low hydraulic conductivities in the NL siting region (2×10^{-10} m/s), in association with low lateral hydraulic gradients (i.e. in comparison to the other siting regions) lead to a very limited particle displacements: particles mainly remain in the perimeter of the siting region (Fig. 7-19) and do not reach any recharge and discharge areas. As an exception, a few backward particles released in the westernmost part of the NL siting region however indicates that recharge is occurring to a small extent at outcrops north of the JO siting region in the model. This results from the higher hydraulic conductivities prevailing in Zone 4 that includes the western part of the siting region (Fig. 6-1 and Fig. 7-5). Note the position of the boundary between Zones 3 and 4 highly uncertain. Isolines of hydraulic heads indicate that the groundwater flow is oriented towards the central part of the siting region where low hydraulic heads prevail. In the eastern part of the site (i.e. where the boreholes BUL1, STA2 and STA3 are located), the model indicates a lateral gradient directed towards the southwest, whereas borehole data indicate a southerly direction.

Based on the isolines of hydraulic heads, the outcrop situation and topography, possible recharge areas for Keuper aquifer in NL are mainly located along the northern boundary of the model, i.e. along the Wutach Valley. As for the ZNO siting region, the likely discharge areas are located in the lower Aare Valley. However, in the current hydrogeological situation particles released into the Keuper in NL do not reach any discharge zones during the time frame considered for the particle tracking.

In JO, the potentiometry is mainly constrained by the outcrops to the north of the siting region, where water is infiltrating, and by the presence of the nearby discharge areas in the lower Aare Valley and in the Sissle Valley to the east and west respectively (Fig. 7-19). The groundwater divide that separates the flow towards these two valleys is located near the western border of the siting region. Note that the borehole data (BOZ2, BOZ1 and Riniken) indicates a groundwater flow direction towards the Sissle Valley suggesting that the groundwater flow divide might be located further to the east. Also, similar to the Muschelkalk aquifer, recharge also occurs to the west along Jura Main Thrust (locally permeable) as supported by backward particle tracking.

The pathlines formed by the forward particles are overall oriented toward the Jura Main Thrust to the southeast where they are significantly slowed down by the low permeability of the Jura Main Thrust. Only one single particle reaches the discharge area in the lower Aare Valley after several million years.

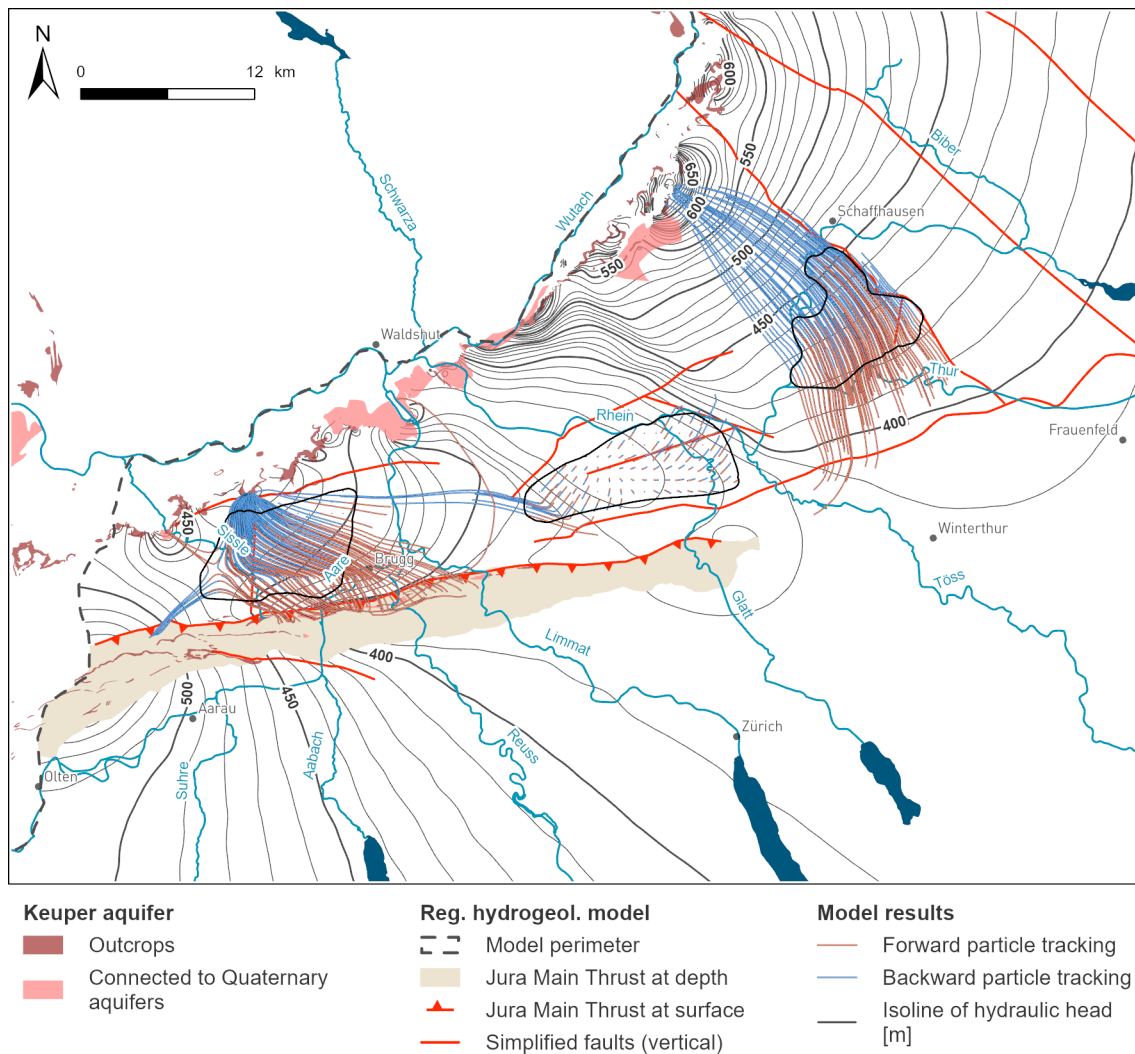


Fig. 7-19: Simulated hydraulic heads and particle tracking identifying recharge and discharge areas in the Keuper aquifer

Hydraulic head situation at the top of the Keuper aquifer horizon of the hydrogeological model. Base case with different domains of hydraulic properties. The map also shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the short distances travelled by the particles released in the NL siting region during the considered timeframe for the particle tracking indicating very slow flow velocities.

The difference in the total distance travelled by the particles is illustrated in Fig. 7-20:

- Most of the backward and forward particles released in the NL siting region typically travel a distance smaller than 1 km. This is due to the comparatively low hydraulic conductivities and the low hydraulic gradients in the NL siting region. The backward particles that travel a longer distance originate from the westernmost part of the siting region as explained earlier in the text.
- The particles released in the JO and ZNO siting regions display a similar median distance (between 4 and 6 km for the backward and forward particle tracking). The left histogram highlights that the recharge area of the Keuper groundwater in ZNO is located further away than the one in JO. The forward particles in JO tend to travel longer distances highlighting the more dynamic flow regime before being trapped in the Jura Main Thrust (also refer to Fig. 7-8 and Fig. 7-19).

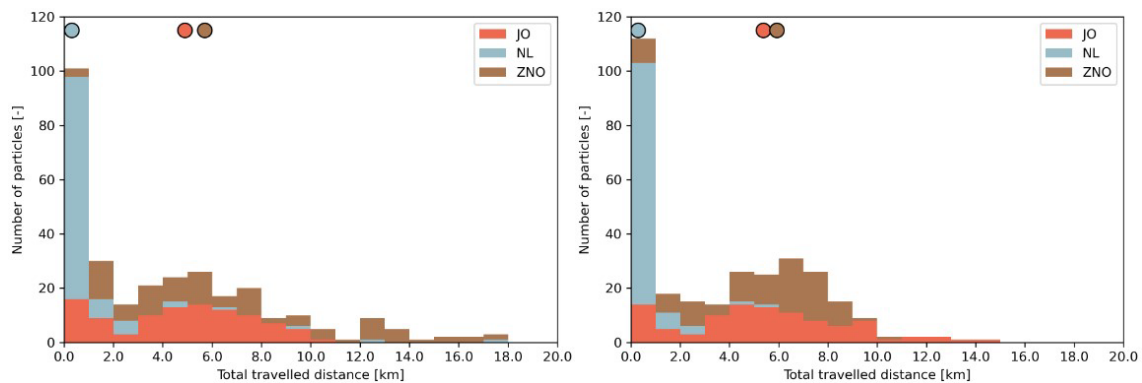


Fig. 7-20: Stacked histogram of the total distance travelled by the backward (left figure) and forward (right figure) particles released in the Keuper aquifer of the JO, NL and ZNO siting regions

The points at the top of the graph illustrate the median of the total travelled distance for the JO, NL and ZNO siting regions (refer to the colour in the legend). A few particles released in JO travelled a distance greater than 20 km.

7.6.3 Hauptrogenstein aquifer

The groundwater flow system in the Hauptrogenstein aquifer mainly occurs parallel to a west – east axis. It is strongly influenced by the topography, the tectonic setting, and the location of the discharge areas.

Recharge mainly occurs at the outcrops to the north of the JO siting region as supported by forward particle tracking (Fig. 7-21). Backward particles released in the siting region also reach outcrops located to the west of the site, along the model boundary.

Assuming that the transmissive facies of the Hauptrogenstein extends further to the east of JO, the lower Aare Valley constitutes the major discharge area for the groundwater flowing in the siting region. The Quaternary aquifers of the Sissle River to the west drain the Hauptrogenstein groundwater flowing in the westernmost part of the siting region. A groundwater divide thus exists in the western part of the siting region diverging the flow to the east and west.

Note that some particles that reach the Jura Main Thrust to the southeast begin a slow upward migration along the Jura Main Thrust in response to the presence of low upward hydraulic gradients. This likely results from the lower hydraulic heads (in comparison to the Hauptrogenstein aquifer) imposed at the surface along the Aare Valley.

Interrupted pathlines correspond to the ones of particles that are trapped in the overlying low permeability units. This is likely due to a decrease in the thickness of the formation towards the east and the local presence of weak upward hydraulic gradients in the aquifer.

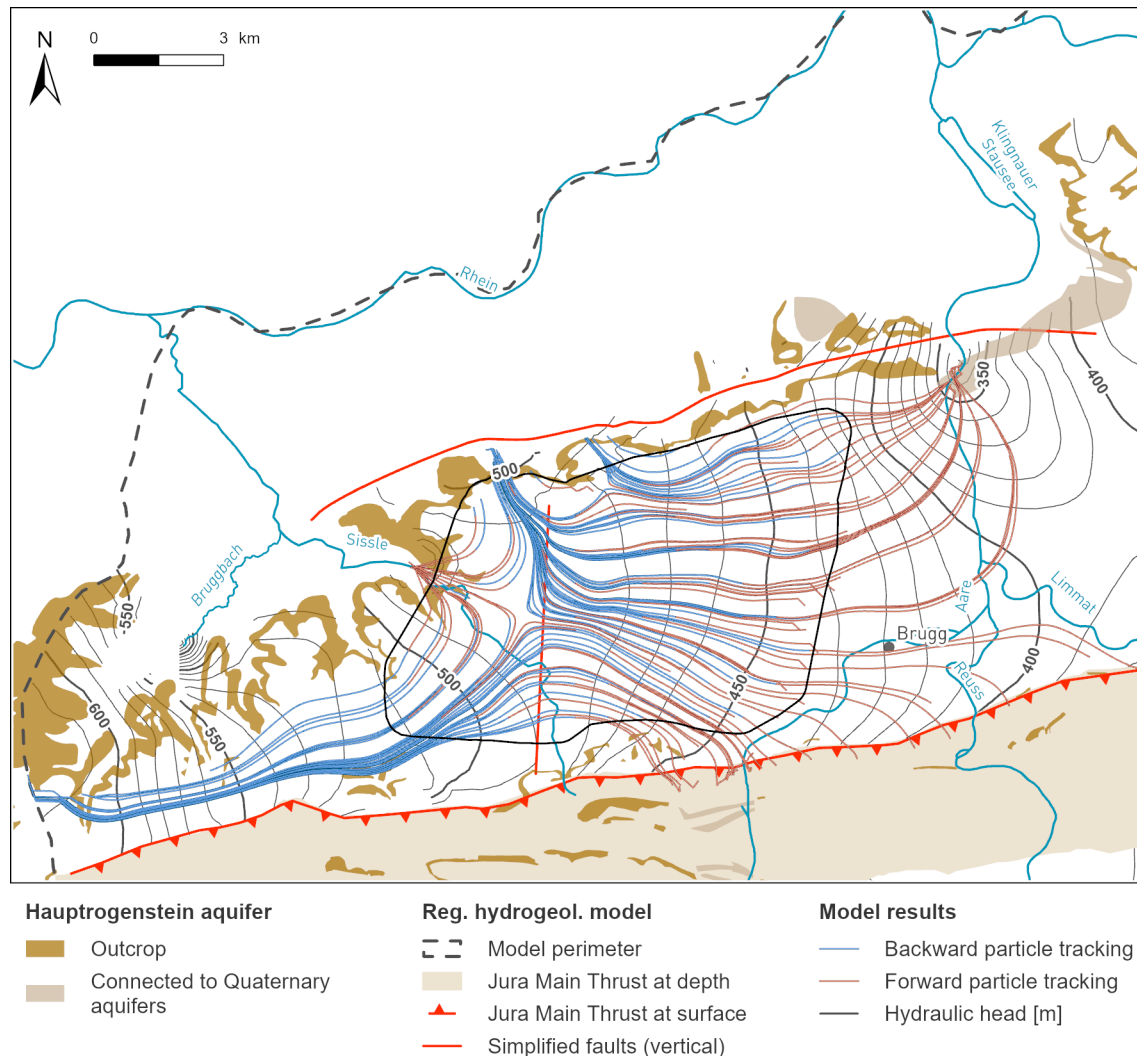


Fig. 7-21: Simulated hydraulic heads and particle paths identifying recharge and discharge areas in the Hauptrogenstein aquifer

Hydraulic head situation at the top of the Hauptrogenstein aquifer of the hydrogeological model. The map shows outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the west to east orientation of the groundwater flow. Particles that stop close to the eastern boundary of the site do not display any further displacement as they are trapped in the overlying low permeability formation.

7.6.4 Malm aquifer

The topography and outcrop locations of the Malm aquifer in the northern part of the model leads to site-specific hydrogeological situations (Fig. 7-22). For the ZNO siting region, backward particle tracking shows that the Canton Schaffhausen and adjacent southern Germany area is an important recharge area for the groundwater flowing through the siting region (outcrops of the Malm aquifer, Malm aquifer connected with the Danube River). Furthermore, it highlights the important role of the suspected highly conductive Randen Fault that tends to channel flow further to the south-southeast. The groundwater flow then converges to the siting region before discharging in the Rhine River at the Rhine Falls and Rheinau area as indicated by forward particle tracking.

A comparatively small number of particles released in the western part of the siting region indicates that the Südranden area consists of a local recharge area. The resulting local groundwater flow systems also exfiltrate at the Rhine Falls and Rheinau area after briefly flowing through the westernmost part of the siting region.

The recharge dynamic of the Malm aquifer in the NL siting region is mainly influenced by the existence of downward hydraulic gradients between the Molasse units and the Malm aquifer along the Lägern heights (illustrated by negative hydraulic head differences on Fig. 7-23): water infiltrates deep into the thick Molasse units and down into the Malm aquifer as supported by particle tracking. This especially the case in the western part of the siting region where the vertical gradients are the strongest. The eastern part of the siting region is characterised by lower vertical hydraulic head differences (Fig. 7-23) leading to less vertical displacement of the particles.

Note that the Jura Main Thrust and the Baden – Irchel – Herdern Lineament do not act as preferential pathways as they were assigned hydraulic conductivities similar to, or lower than, the surrounding rocks. Indeed, faults normal the prevailing stress direction are assumed less permeable than the surrounding rocks (Section 5.2).

Forward particle pathlines are oriented toward the Malm outcrops along the Rhine River to the north where the Malm aquifer is discharging (i.e. area of Kaiserstuhl – Hohentengen in the Rhine Valley north of the NL siting region).

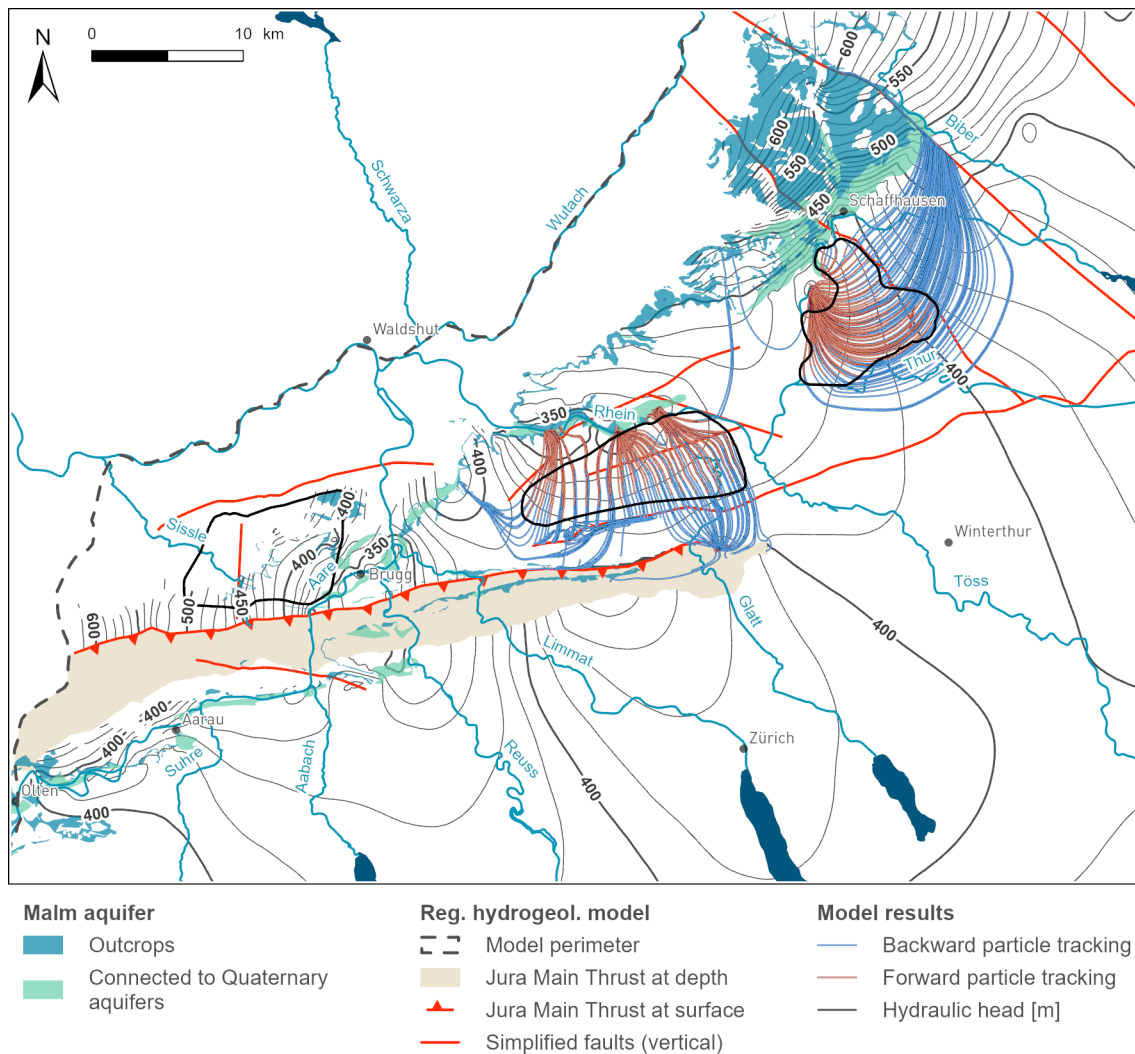


Fig. 7-22: Simulated hydraulic heads and the particle paths identifying recharge and discharge areas of the Malm aquifer

Hydraulic head situation at the top of the Villigen Formation in the hydrogeological model. The map also shows Malm outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the site-specific groundwater flow systems.

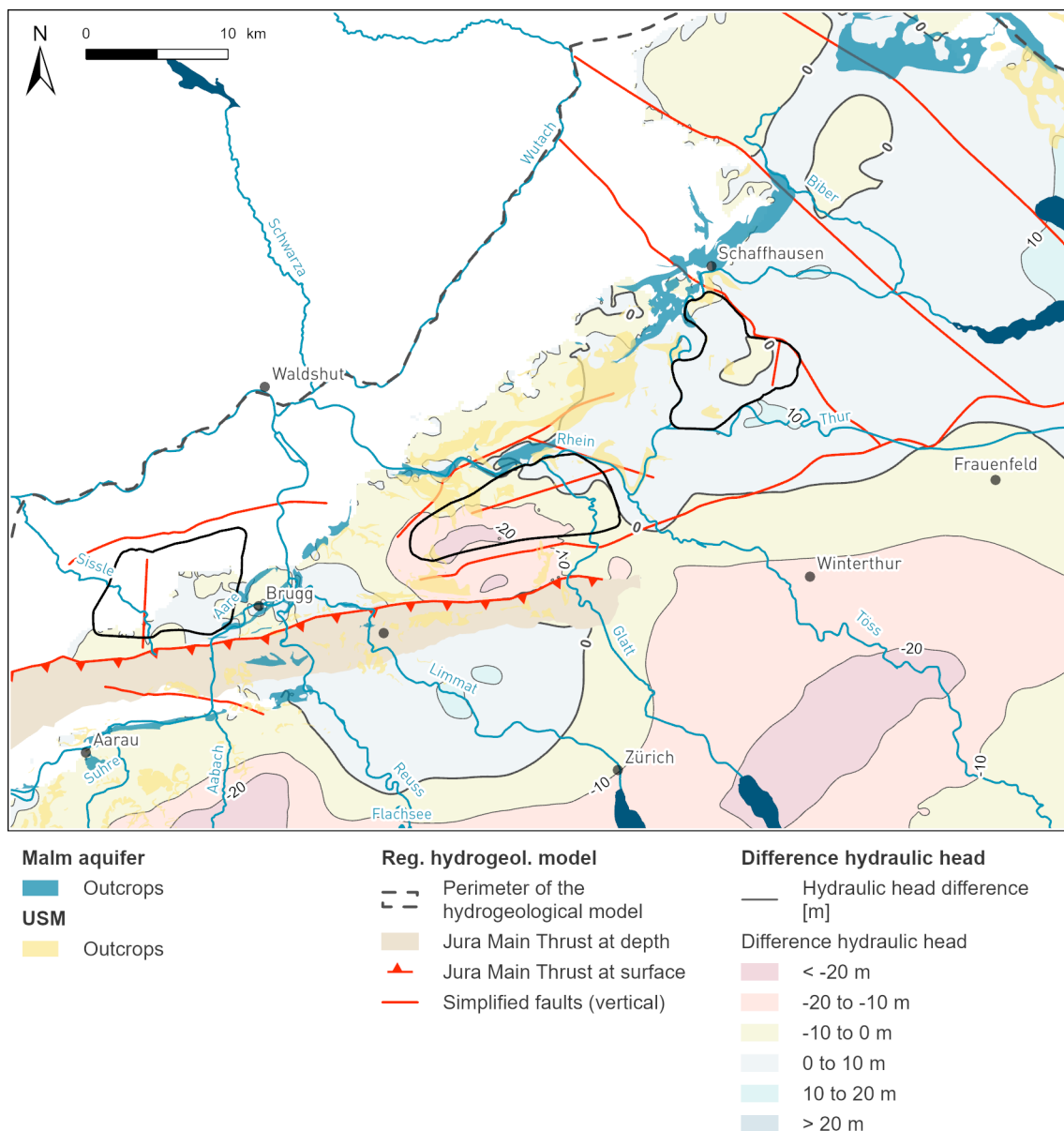


Fig. 7-23: Hydraulic head differences between the Malm aquifer and the Lower Freshwater Molasse (USM)

Positive and negative head differences indicate upward and downward hydraulic gradients respectively. The hydraulic heads at the top of the Villigen Formation and at the top of the lowermost USM horizons of the model were considered. The map also shows outcrops and the simplified regional fault pattern used in the model. Note the negative hydraulic head difference in the NL siting region indicating vertical recharge of the Malm aquifer through the Molasse deposits.

8 Additional cases

8.1 Introduction

The calibration process detailed in Chapter 6 focused on the calibration of the base case while Chapter 7 focused on its analyses. Thereby, well-defined conceptual models were integrated and assessed. However, several additional conceptual models, resulting in additional cases, have also been identified. These are all physically possible cases but are considered less probable based on the available observations. For some cases, the motivation is to explore the sensitivity of the model. To not unnecessarily include these uncertainties in the base case, they have been simulated and analysed separately. The additional cases include:

- Case Keuper aquifer

The Keuper consists of layers of continental and marine sandstones (mainly the Ergolz and Belchen Members) and dolostones (Seebi and Gansingen Members). These are interspersed with low-permeability marls and claystones. Strong spatial facies variation led to the development of local groundwater flow systems. To explore the sensitivity of the model with regard to different conceptualisations of the complex Keuper aquifer, the latter aquifer was further investigated with additional cases. In addition to the base case (Sections 7.2 and 7.6.2), the Keuper aquifer was investigated at the regional scale through the following cases:

- Homogeneous isotropic case (Section 8.2): To evaluate the impact of a less compartmentalised model on the groundwater flow system (in comparison to the base case), a homogeneous and isotropic medium was considered as an alternative to the base case (Sections 7.2 and 7.6.2). Here, the area of the Keuper aquifer north of the Jura Main Thrust and the Baden – Irchel – Herdern Lineament is assigned homogeneous and isotropic hydraulic conductivities.
- Two additional cases (Section 8.3) aiming to explore the regional flow patterns possibly occurring in permeable fluvial deposits of the Ergolz Member (Nagra 2024f) were further considered. These scenarios are based on the concept that the presence of relatively uniformly oriented fluvial channels on a regional scale would result in an anisotropic hydrogeological system, with the maximum and minimum hydraulic conductivities being oriented parallel and perpendicular to the regional orientation of the channels respectively. A north-south and an east-west orientation was considered.

- Case Malm aquifer

In the base case, the Malm has been simulated as a conductive unit. However, hydraulic tests in boreholes showed that, at least in some areas, only the upper part of the Malm («Felsenkalke» and «Massenkalk») are transmissive while the lower part (Schwarzbach Formation and Villigen Formation) are not. The case Malm specifically includes these observations and analyses their impact (Section 8.4).

In these additional models, only the respective model elements to be tested were changed compared to the base case. This has the obvious advantage that the influence of the impact of the changes of the additional cases on the regional flow field and its differences to the base case can easily be determined and analysed.

8.2 Case homogeneous and isotropic Keuper aquifer

8.2.1 Case rational

The Klettgau Formation (upper unit of the Keuper Group) underlies the Staffelegg Formation and includes the local Keuper aquifer. It is of particular importance because it is the nearest aquifer below the Opalinus Clay. The Keuper aquifer consists mostly of sediments deposited in a terrestrial and marine environments (Nagra 2024f). Hence, it is composed of highly variable lithologies with equally highly variable thicknesses which is also reflected in the highly variable hydraulic properties with hydraulic test transmissivities ranging over eight orders of magnitude (Nagra 2024f). This variability is already reflected in the base case where 4 zones were implemented in the Keuper aquifer horizon in the northern part the model (Chapter 7) to reproduce this variability. The calibration of the Keuper aquifer led to a zone-specific parametrisation. This is notably the case between the low hydraulic conductivity zone around the NL siting region and the adjacent zones to the east and west. The sharp changes of hydraulic conductivities occurring at the zone boundaries lead to a compartmentalisation of the model with strong lateral hydraulic gradients. Sudden changes in hydraulic conductivities are however not expected as gradual transition from one facies to another would generally be expected.

A case with a homogeneous and isotropic Keuper aquifer was thus tested as an alternative to the base case. It aims to test the effect of a less compartmentalised model on the groundwater flow system in the Keuper aquifer.

8.2.2 Definition of model

Unlike the base case, the Keuper aquifer was here divided into two distinct zones only: the first is located north of a west-east line formed by the Baden – Irchel – Herdern Lineament and Jura Main Thrust while the second includes the area south of this (i.e. similar to the base case). In both zones, isotropic conditions were imposed for the horizontal hydraulic conductivities (i.e. $K_{xx} = K_{yy}$).

All other model parameters and flow boundary conditions compared to the base case have been kept unchanged (including for the Keuper aquifer in the southern model part).

The Keuper aquifer was then calibrated using the PEST algorithm leading to a zone-specific parametrisation (2×10^{-9} and 1×10^{-8} m/s in the northern and southern part of the model, respectively).

8.2.3 Simulation results

The groundwater flow solution in the Keuper aquifer resulting from the alternative homogeneous isotropic case shares the following similarities with the base case:

- The quality of the fit for the additional case is very similar to the base case, although not quite as good, with a MAE of 23.35 m and a correlation coefficient of 0.91 (Fig. 8-1). Note that the homogeneous isotropic case resulted in higher simulated hydraulic heads in the NL area and lower values in the ZNO area.
- Similar recharge and discharge areas are highlighted by particle tracking (compared to base case). Recharge areas are located in the northern part of the model where the Keuper crops out (i.e. along the Upper Wutach Valley) as well as along Keuper outcrops located north of the JO siting region. Potential discharge areas include the Lower Aare Valley, as well as the Jura Main Overthrust, where it is cut by the Aare, Reuss and Limmat Rivers. In the north-westernmost part of the model, groundwater discharges into the Sissle Valley.
- Forward particles do not reach any discharge area but remain in the Keuper horizon or are entrapped in the adjacent aquitards. Also, while the groundwater flow in the alternative homogeneous isotropic case is higher than in the base case in the NL siting region (as shown by the longer distance travelled by the backward and forward particles on Fig. 8-3, Fig. 8-4 and Fig. 8-5), the travelled distance in the NL siting region is still the lowest for the three siting regions (Fig. 8-5).

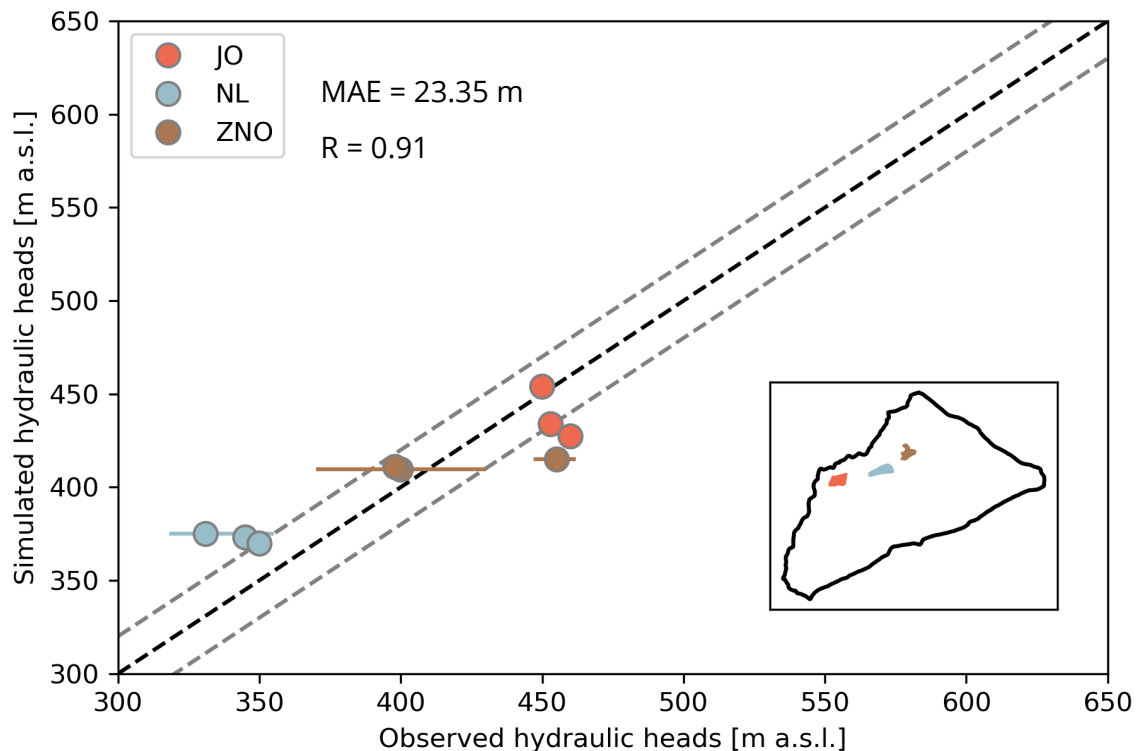


Fig. 8-1: Cross plot of the simulated and observed hydraulic heads for the case of a homogeneous isotropic Keuper aquifer

The colour of the points refers to the siting regions in which the observations are located. The bandwidth of the observed hydraulic heads is displayed with horizontal error bars. Note that bandwidth may be hidden behind the symbol or may be not available (Enclosure A). The black dashed line represents a perfect fit between observed and simulated hydraulic heads.

The alternative homogeneous isotropic case however differs from the base case in the following respects:

- Differences in hydraulic heads exist between the two cases in the northern part of the model, especially in the area between the JO and ZNO siting regions (Fig. 8-2). This is attributed to the absence of a low hydraulic conductivity zone in and around the NL area in the homogeneous isotropic case (unlike in the base case) so groundwater flow towards the discharge area in the Lower Aare Valley is easier. This leads to lower hydraulic heads in the northeastern and northwestern areas of the model and higher hydraulic heads in the NL – Lower Aare Valley area (e.g. Fig. 8-3). This leads to a slight decrease of the model fit in the ZNO and NL siting regions compared to the base case.
- Another direct consequence is the comparatively lower lateral hydraulic gradients prevailing in the alternative homogeneous isotropic case in the northwestern (JO area) and northeastern (ZNO area) parts of the model. The effect is visible from particle tracking in the JO and ZNO siting regions with a lower travelled distance (compare median travelled distances in Fig. 7-20 and Fig. 8-5 for the base case and the homogeneous isotropic case, respectively). As mentioned earlier, the longer distance displayed in NL is due to the higher hydraulic conductivities in the homogeneous alternative case.

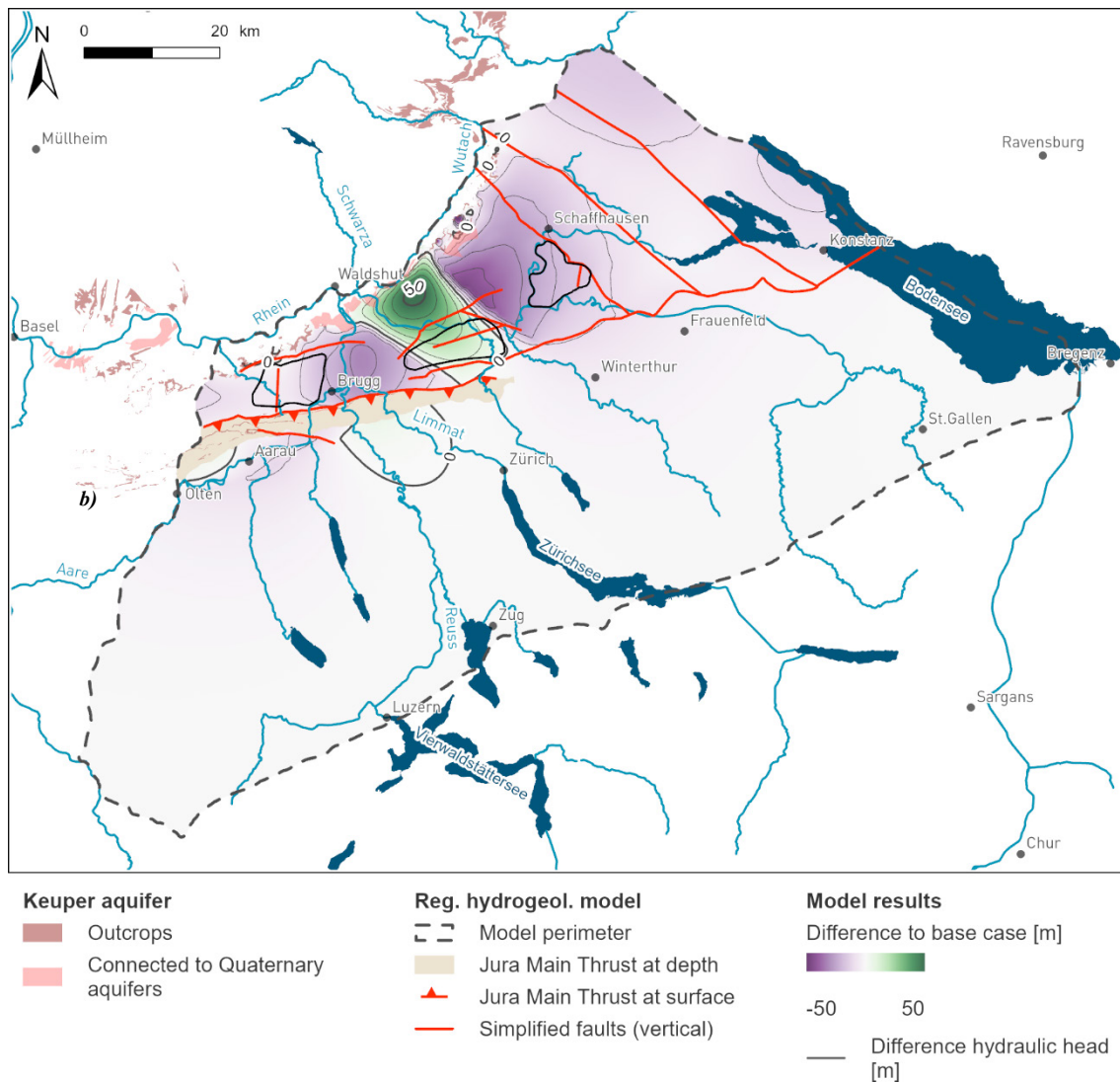


Fig. 8-2: Hydraulic head difference between the homogeneous isotropic case and the base case

The hydraulic head difference is calculated by subtracting the hydraulic heads of the base case to the one of the additional cases ($H_{\text{alt. case}} - H_{\text{base case}}$). A positive indicates that the additional case led to higher hydraulic head than the base, and vice versa.

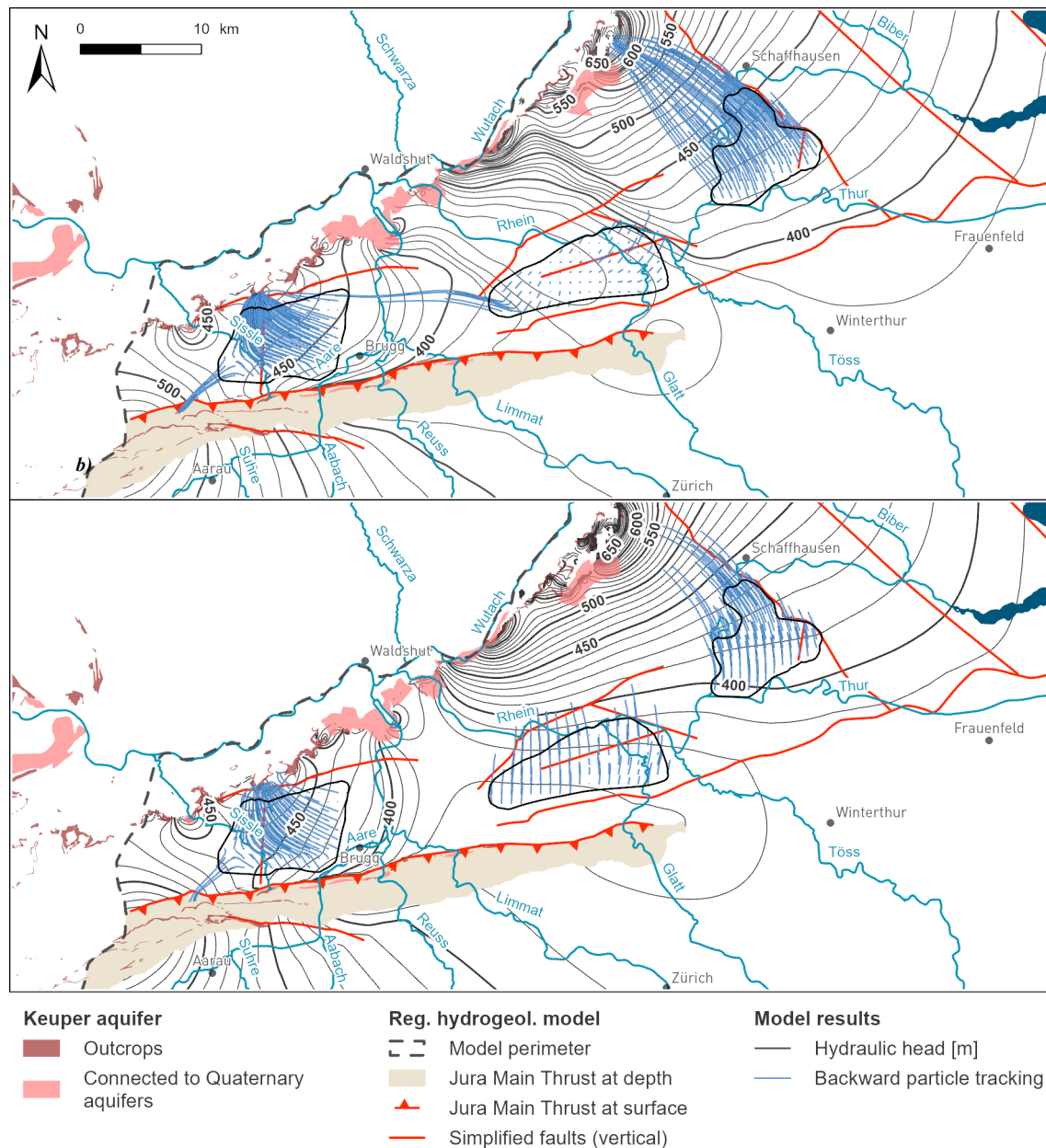


Fig. 8-3: Simulated hydraulic heads and backward particle tracking identifying recharge areas in the Keuper aquifer for the base case (upper figure) and the homogeneous isotropic case (lower figure)

Hydraulic head situation at the top of the Keuper aquifer horizon of the hydrogeological model. Base case with different domains of hydraulic properties (Section 7.2), alternative homogeneous isotropic case assuming uniform properties north of the Jura Main Thrust and the Baden – Irchel – Herdern Lineament. The map also shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the relatively short distances travelled by the particles released in the NL siting region during the considered timeframe for the particle tracking indicating very slow flow velocities, particularly in the base case.

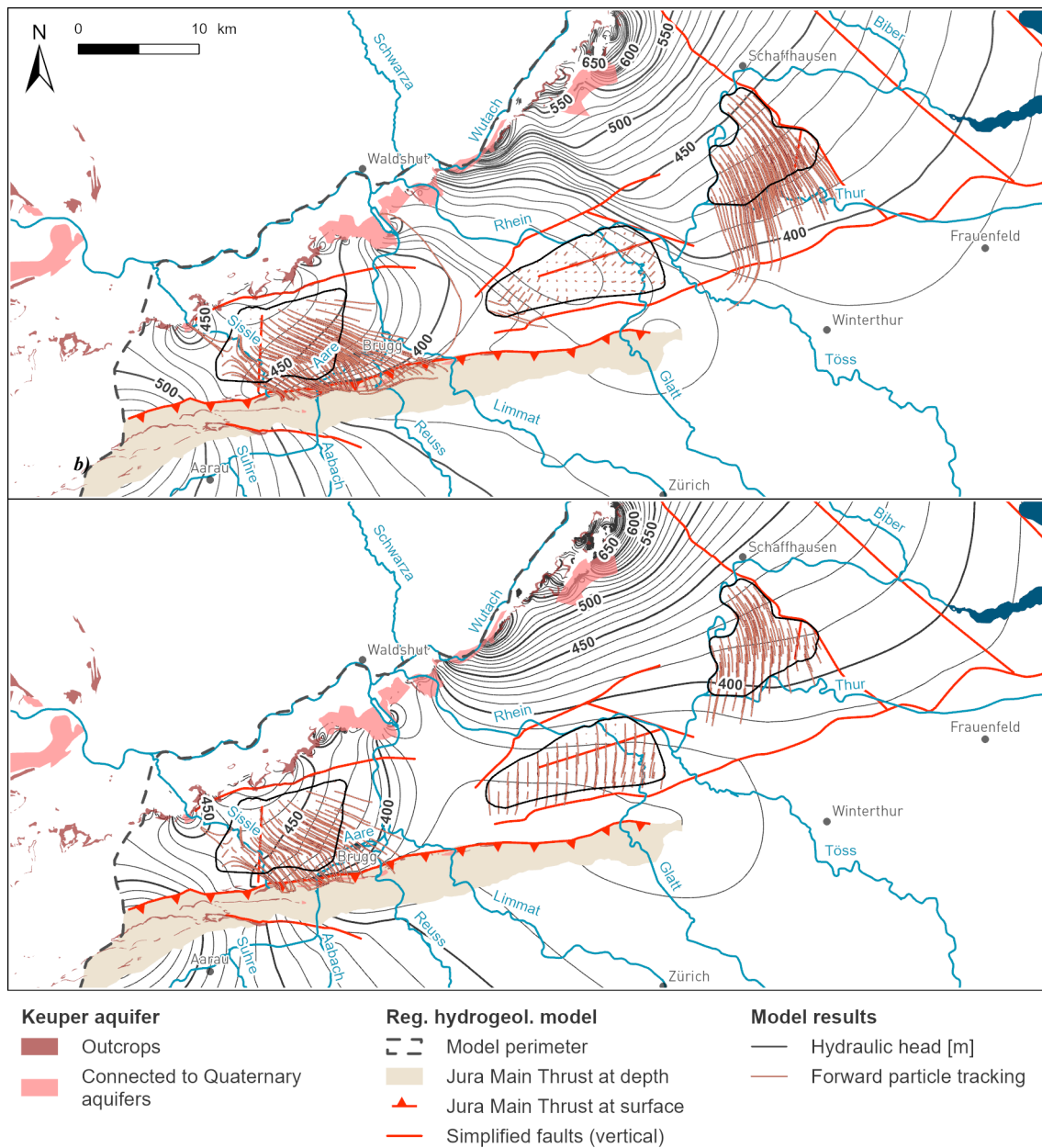


Fig. 8-4: Simulated hydraulic heads and forward particle tracking identifying discharge areas in the Keuper aquifer for the base case (upper figure) and the homogeneous isotropic case (lower figure)

Hydraulic head situation at the top of the Keuper aquifer horizon of the hydrogeological model. Base case with different domains of hydraulic properties (Section 7.2), alternative homogeneous isotropic case assuming uniform properties north of the Jura Main Thrust and the Baden – Irchel – Herdern Lineament. The map also shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the relatively short distances travelled by the particles released in the NL siting region during the considered timeframe for the particle tracking indicating very slow flow velocities, particularly in the base case.

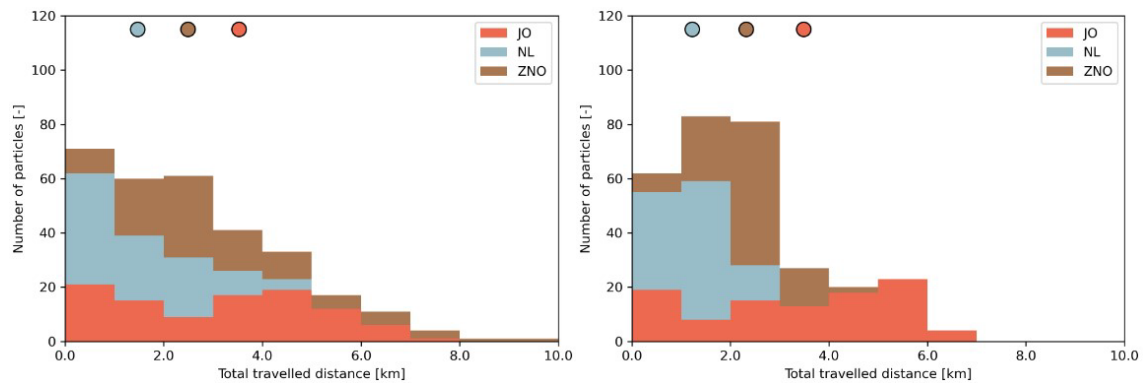


Fig. 8-5: Stacked histogram of the total distance travelled by the backward (left figure) and forward (right figure) particles released in the Keuper aquifer of the JO, NL and ZNO siting regions

The points at the top of the graph illustrate the median of the total travelled distance for the JO, NL and ZNO siting regions (refer to the colour in the legend). The timeframe considered for the particle tracking is 5 million years.

8.2.4 Summary

An additional homogeneous isotropic case for the Keuper aquifer layer was considered as an alternative to the base case presented in Section 7.2. The aim was to assess the effect of a less compartmentalised model on the potentiometry of the Keuper aquifer. Here the Keuper aquifer is divided in two zones: one north of the Baden – Irchel – Herdern Lineament and Jura Main Thrust, and one south of these tectonic features. The two zones were further calibrated using the PEST algorithm. This resulted in a slightly less good fit of the simulated and observed hydraulic heads in comparison to the base case. Both models, however, remain very similar in terms of calibration criteria. The homogeneous isotropic case and the reference case display the same recharge and discharge areas, as well as a similar flow dynamic in the area south of the Baden – Irchel – Herdern Lineament and the Jura Main Thrust. As in the base case, the particles released in the NL siting region are always those that travel the least of all the siting regions.

The main difference between the cases are the hydraulic head differences occurring in the northern part of the model, especially around the NL siting regions. Here, the absence of a low hydraulic conductivity zone around the NL siting region in the homogeneous isotropic case leads to higher hydraulic heads in the considered area and lower hydraulic heads in the northeastern and northwestern part of the model. The absence of hydraulic conductivity contrast in the northern part of the model also induces a smoother potentiometry, i.e. with smoother hydraulic gradients.

8.3 Case anisotropic Keuper aquifer

8.3.1 Case rational

During Nagra's most recent drilling campaign, channel-like features consisting of permeable sandstones were encountered in the Ergolz Member in the NL siting region (Nagra 2024f). Hydrogeochemical data indicates that these features may accommodate an active groundwater flow system (Nagra 2024f) and are considered as part of the Keuper aquifer in NL. It is however unclear how and where these channels are connected to the larger scale groundwater flow systems (i.e. location of the recharge and discharge area).

Note that the channels encountered in the Ergolz Member are likely not restricted to the NL area but may be found, albeit as local features, anywhere across Northern Switzerland (Nagra 2024f). Conceptually, a preferential orientation of these channels is expected to result in a large-scale anisotropy. Two anisotropy orientations were tested: N-S and W-E.

The two above-mentioned orientations were parametrised in two additional test cases aiming to explore the regional flow patterns occurring in the permeable fluvial deposits of the Ergolz Member. These cases are based on the concept that the presence of multiple relatively thin channels with a uniform orientation could result in an anisotropic hydrogeological system at the regional scale.

8.3.2 Definition of model

In order to identify changes of an anisotropic Keuper aquifer compared to the base case, two generally possible channel orientations have been simulated. Hence, the anisotropy considered for both cases was only implemented north of a line defined by the Baden-Irchel-Herdern Lineament and the Jura Main Thrust. The southern area of the model, where no information is available, was considered isotropic. Note that a calibration of these two cases was not performed.

The parametrisation of the two test cases is:

- Anisotropic K W-E: A homogeneous but anisotropic hydraulic conductivity was assigned to the entire northern zone with maximum hydraulic conductivity in the West-East direction ($K_{\max} = 5 \times 10^{-8}$ m/s, $K_{\min} = 5 \times 10^{-9}$ m/s)
- Anisotropic K N-S: A homogeneous but anisotropic hydraulic conductivity was assigned to the entire northern zone with a maximum hydraulic conductivity in the North-South direction ($K_{\max} = 5 \times 10^{-8}$ m/s, $K_{\min} = 5 \times 10^{-9}$ m/s).

Note that the term W-E and N-S refer to the orientation of the highest horizontal hydraulic conductivity. The latter is based on the results of hydraulic packer tests performed in the Ergolz Member. The horizontal anisotropy ratio was fixed to 10 as higher ratios overall lead to groundwater flow field that are strongly constrained by the anisotropy: the isolines of hydraulic head developing almost only perpendicular to the orientation of the lowest horizontal hydraulic conductivities.

For the two cases, all other model parameters and flow boundary conditions compared to the base case have been kept unchanged (including for the Keuper aquifer in the southern model part).

8.3.3 Simulation results

The discussion below focuses on the northern area of the model (i.e. north of the Baden – Irchel – Herdern Lineament and Jura Main Thrust) as most of the changes occur in the northern model area compared to the base case and the homogeneous isotropic case. The southern model area is only slightly affected by the changed model parametrisation of the Keuper aquifer in the northern part.

As expected, the implementation of an anisotropy resulted in a distortion of the hydraulic head isolines e.g. in comparison to the alternative homogeneous isotropic case (Section 8.2). As expected, potentiometric maps of the anisotropic cases (e.g. Fig. 8-6) display hydraulic head isolines oriented perpendicular to the orientation of the lowest hydraulic conductivity.

In the NL siting region, the hydraulic heads derived from hydraulic packer tests indicate a lateral hydraulic gradient oriented towards the south. This is consistent with the potentiometric situation in the NL area simulated as part of the W-E case (e.g. Fig. 8-6). On the contrary, the N-S case shows a lateral hydraulic gradient oriented towards the southwest. Furthermore, the W-E case results in lower hydraulic heads in the NL area (between approx. 390 and 420 m a.s.l.) compared to its N-S counterpart (between appr. 430 and 500 m a.s.l.). The former case is thus more consistent with the low observed hydraulic heads in the NL boreholes (between approx. 330 and 390 m a.s.l.).

Because of the considered anisotropy, the particles path lines do not cross the isolines perpendicularly (e.g. as in the homogeneous isotropic case) but tend to be aligned in the direction of the highest horizontal hydraulic conductivity (i.e. the assumed direction of the channel system) (Fig. 8-6 and Fig. 8-7). For the N-S and W-E cases, the particles released in the siting regions roughly follow a N-S and W-E axis orientation, respectively.

While the path lines display a different trace between both cases, they however point consistently towards similar recharge areas in the north as shown by backward particle tracking (Fig. 8-6). Recharge mainly occurs in outcrops near the northern limit of the model, and, to a minor extent in outcrops located in the Internal Jura (Folded Jura) west of the JO siting regions for the W-E case. In the latter case, the anisotropy also leads some backward particles originating from the NL siting region to reach outcrops located to the north of JO.

As for the base case and the homogeneous isotropic case, the identification of discharge areas for the Keuper aquifer is not evident based on forward particle tracking (Fig. 8-7). In both cases, forward particle released in the JO and NL siting regions flow towards the south (N-S case) or south-east (W-E case) where they tend to migrate in the underlying aquitard. This downward flow is triggered by lower hydraulic heads in the Muschelkalk aquifer.

In the siting region ZNO, the particles flow toward the south without reaching the model surface during the timeframe considered for the particle tracking (Fig. 8-7).

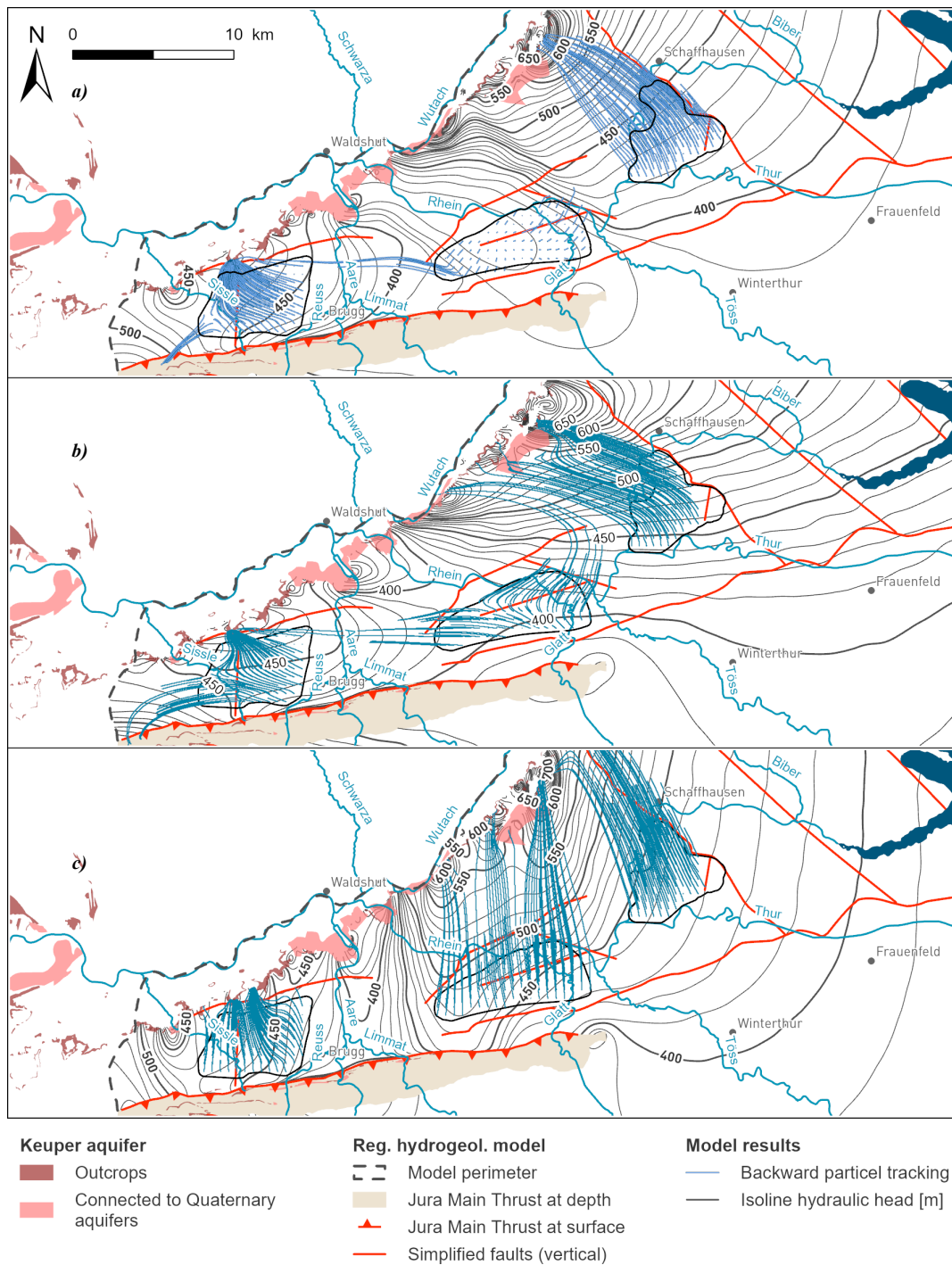


Fig. 8-6: Simulated hydraulic heads and backward particle tracking identifying recharge areas in the Keuper aquifer for the base case (figure a), the anisotropic K W-E case (figure b), and the anisotropic K N-S case (figure c)

Hydraulic head situation at the top of the Keuper aquifer horizon of the hydrogeological model. Base case with different domains of hydraulic properties (Section 7.2), alternative cases with an anisotropy of the horizontal hydraulic conductivities. The highest horizontal hydraulic conductivity was implemented parallel to the east-west and north-south axis in the W-E and N-S cases respectively. The map also shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces.

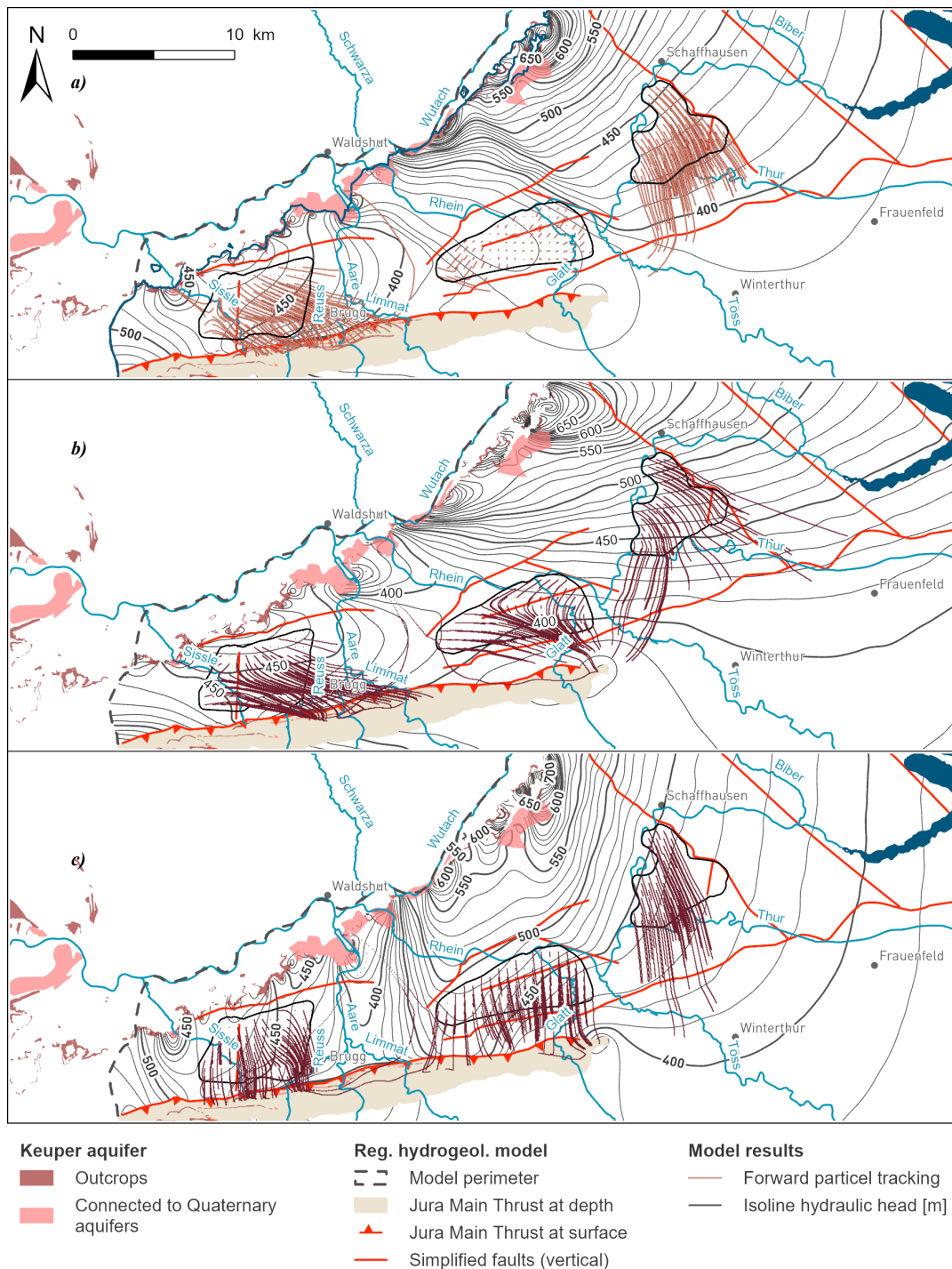


Fig. 8-7: Simulated hydraulic heads and forward particle tracking identifying recharge areas in the Keuper aquifer for the base case (fig. a), the anisotropic K W-E case (fig. b), and the anisotropic K N-S case (fig. c)

Hydraulic head situation at the top of the Keuper aquifer horizon of the hydrogeological model. Base case with different domains of hydraulic properties (Section 7.2), alternative cases with an anisotropy of the horizontal hydraulic conductivities. The highest horizontal hydraulic conductivity was implemented parallel to the west-east and north-south axis in the W-E and N-S cases, respectively. The map also shows the outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces.

8.3.4 Summary

Located at the base of the Klettgau Formation, the Ergolz Member contains permeable sandstone channels embedded in clay-rich and low permeable rocks. Available hydrogeochemical and hydraulic packer test investigations support the existence of local active groundwater flow systems in these features in the NL siting regions (Nagra 2024f). Observations outside of the siting regions however indicate that similar channels are not only NL related but could locally be found elsewhere in Northern Switzerland.

Since the exact orientation of these channels is not known, and hence no precise, channel-parallel anisotropy can be implemented, the impact of these channels has been studied by implementing two cases with a pronounced WE or NS-anisotropy in the northern part of the model.

The goal of these two cases was to study the large scale potentiometry of the Ergolz Member, to identify the most likely associated recharge and discharge areas and assess the most likely direction of the regional anisotropy caused by a preferential orientation of channels in the Ergolz Member. These cases are thus meant as test cases and not as an alternative to the base case.

Both cases show lateral hydraulic gradients preferentially oriented in the direction of the lowest hydraulic conductivity. While the two models were not calibrated, the W-E model led to a more consistent hydrogeological situation when compared with observations acquired in the NL siting region:

- The W-E model displays a lateral hydraulic gradient directed towards the south as supported by the available observations.
- The simulated hydraulic heads of the W-E model are more consistent with the observations (although slightly higher) in comparison to the N-S model.

While both models resulted in contrasting particle pathlines, they give a consistent picture regarding the location of recharge and discharge areas. The latter is also similar to the one presented for the base case (Section 7.2) and the alternative homogeneous isotropic case (Section 8.2). Note that the forward particles do not highlight a path toward a discharge area. Instead, particles flow to the south and remain in the model after the timeframe considered for the particle tracking.

8.4 Case Malm

8.4.1 Case rational

In general, the Malm aquifer relates to the thick limestone units above the Wildegg Formation, that is the «Felsenkalke» and «Massenkalk» and the Villigen Formation to the bottom of the Molasse units. The «Felsenkalke» and «Massenkalk» and the Villigen Formation are separated by the thinner, marly Schwarzbach Formation. In the base case, the Malm Aquifer includes all 3 aforementioned units and formations (i.e. disregarding the Schwarzbach Formation as a possible aquitard due to its higher clay content). This definition mainly comes from observations in outcrops in the Internal Jura (Folded Jura), the canton Schaffhausen and the Swabian Alb area of Southern Germany. However, during Nagra's most recent borehole campaign, the most transmissive zone were found in the Malm above the Schwarzbach Formation (Nagra 2024f). The case Malm therefore evaluates the impact of only the upper part of the Malm aquifer being transmissive on the field of hydraulic heads in this aquifer, the location of the discharge and recharge areas, and vertical gradient across the host rock.

8.4.2 Definition of model

To adjust the parametrisation to reflect the changed transmissivities, the hydraulic conductivity of the «Felsenkalk» and «Massenkalk» has been increased proportionally to conserve the total transmissivity of the Malm aquifer as estimated in the base case. The hydraulic conductivity of the Villigen and Schwarzbach Formations have been reduced to 10^{-12} m/s.

Again, all other model parameters, as well as the flow boundary conditions, were kept unchanged with respect to the base case.

8.4.3 Simulation results

Comparing the simulated hydraulic heads as well as the vertical hydraulic gradients resulting from this case with distributions in the base case only showed very minor differences. When analysing particle path lines (Fig. 8-8), the location of the recharge areas calculated in the base case moved slightly to the south from the outcrops of the Villigen Formation to the outcrops of the «Felsenkalk» and «Massenkalk» (compare Fig. 8-8a and c). This simply is a reaction to the increased hydraulic conductivity in the «Felsenkalk» and «Massenkalk» and the reduced hydraulic conductivity of the Villigen and Schwarzbach Formations. Analysing the discharge areas show no marked changes (compare Fig. 8-8b and d). The increase of the hydraulic conductivity in the «Felsenkalk» and «Massenkalk» also lead to higher Darcy fluxes. Note that the low hydraulic conductivities implemented in the Schwarzbach and Villigen Formations in the model increases the distance between the aquifers above and below the Opalinus Clay east of the Aare River. Interestingly, this has only a limited impact on the vertical hydraulic gradients across the Opalinus Clay.

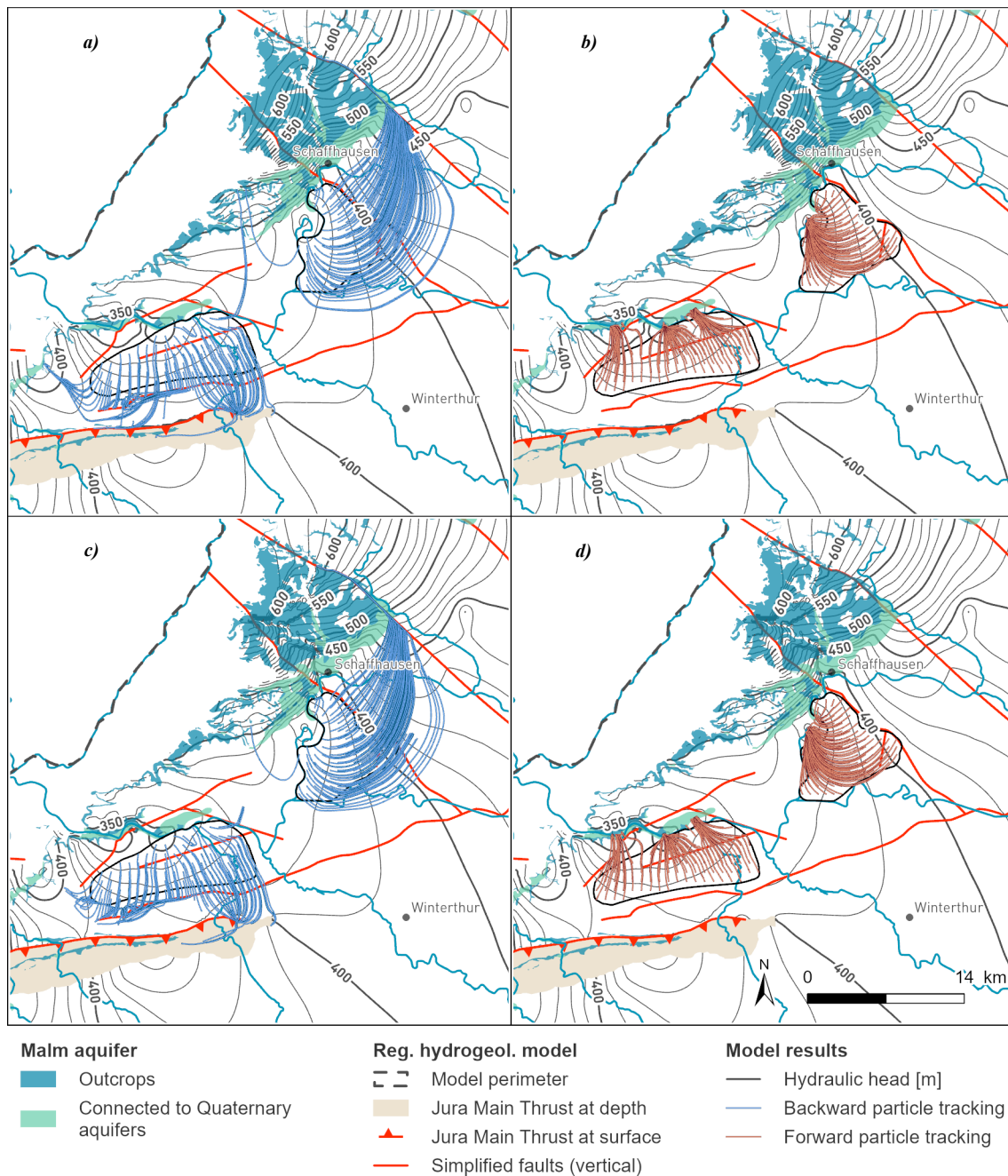


Fig. 8-8: Simulated hydraulic heads and the particle paths identifying recharge and discharge areas of the Malm aquifer

Hydraulic head situation at the top of the «Felsenkalke» and «Massenkalk» in the hydrogeological model. The map also shows Malm outcrops and the simplified regional fault pattern used in the model. The displayed particle paths are a 2D projection of the 3D particle traces. Note the site-specific groundwater flow systems and the strong resemblance to Fig. 7-22.

8.4.4 Summary

While in the base case, the model horizons from the top of «Felsenkalke» and «Massenkalk» to the bottom of the Villigen Formation have been assigned to be transmissive and hence act as an aquifer, the additional case Malm honours the fact that hydraulic tests during Nagra's recent drilling campaign indicated that mainly the top part of the Malm aquifer (i.e. the «Felsenkalke» and «Massenkalk») was found to include the transmissive zones. Adjusting the parametrisation of the base case to this showed almost no effect on head distributions or discharge/recharge areas. In comparison to the base case, the location of the recharge areas however moved slightly to the south from the outcrops of the Villigen Formation to the outcrops of the «Felsenkalke» and «Massenkalk». The increase of the hydraulic conductivity in the latter formation leads to higher Darcy Fluxes in comparison to the base case. The increased distance between the aquifers below and above the Opalinus Clay in comparison to the base case has only a limited impact on the vertical hydraulic gradients across the host rock.

9 Summary and conclusions

A regional steady-state hydrodynamic model has been developed to explore the regional ground-water flow system of Northern Switzerland. The model focuses on the aquifers above and below the Opalinus Clay and confining units, which effectively separate the upper and lower hydro-geological systems.

The meshed geometry of the model is based on several geological models and includes regional-scale faults important for the understanding of their effect on the hydrodynamic situation. Most of the regional-scale faults were implemented as vertical fault zones. They honour the lateral extent of the faults mapped in surface outcrops and on subsurface data in a simplified way and are represented as a row of three elements in the model with a constant total width of 150 m. The area of the Jura Main Thrust was extensively modelled in more detail because there, hydro-geologically important formations crop out and play an important role for the local and regional hydrodynamics as discharge and recharge areas or aquitards.

Model boundaries were placed either along well-defined hydraulic boundaries known from previous studies or based on conceptual considerations. While model parametrisation is based on observed data (e.g. hydraulic tests from boreholes) and on conceptual considerations, lateral boundary conditions are less well constrained by observations. Hence, to test the consistency and performance of the different boundary conditions, a preliminary sensitivity study has been performed. Based on different metrics (mean absolute error, correlation coefficients between simulated and observed data and sum of squared errors), the best fit model has been chosen for further calibration as a base case. The base case in turn has further been used for the analyses of additional cases.

Forward and backward particle tracking was performed to identify the recharge and discharge areas of the aquifers in northern Switzerland. The calculations were done using the groundwater velocity field and generic porosities. An arbitrary selected timeframe of 5 million years was considered for the particle tracking, which is well beyond the validity of the model.

In the base case, groundwater flow in the upper aquifers in the area of the siting regions (Malm and Hauptrogenstein aquifers) is clearly controlled by the topography, the surface waters and the location of outcrops. For the Malm aquifer in ZNO, recharge areas are mainly located along the topographically higher outcrops in the north-eastern part of the model and corresponding discharge is into the Rhine River (Rhine Falls area). In the area of the NL siting region, recharge mainly occurs through the thick Molasse units along the northern part of the Lägern Anticline and discharge via the Malm aquifer outcrops along the Rhine River in the area of Kaiserstuhl – Hohentengen. Low Darcy fluxes also prevail in the eastern part of the NL siting region as supported by hydrogeochemical data in the BUL1, STA2, and STA3 boreholes (Nagra 2024f). If only the Malm above the marly Schwarzbach Formation is considered in the model as an aquifer, results are virtually identical except that discharge and recharge areas appear to move very slightly southward. This slight movement is due to the outcrop situation where the upper part of the Malm simply crops out slightly more to the south.

The Hauptrogenstein aquifer is only present in the western part of the model because towards the east, a facies transition occurs to a more clay-rich lithology with lower hydraulic conductivity. Therefore, it is mainly relevant for the siting region Jura Ost. The local topography results in comparably small-scale flow systems with recharge in the topographically higher regions to the north (area south of the Mandach Thrust) and to the southwest (area north of the Jura Main Thrust) and discharge areas in the river valleys (Lower Aare Valley, Sissle Valley).

The Keuper aquifer is characterised by strong horizontal and vertical variations of lithology and also by strong variations of hydraulic conductivities. Several variants of parametrisation for the Keuper aquifer were tested to determine its significance. In the base case, different zones in the Keuper aquifer were considered in order to reflect the observed different lithofacies occurring in northern Switzerland (Nagra 2024f). Comparably low hydraulic conductivities and low hydraulic heads prevail in the NL siting region in agreement with the borehole data. Particle tracking in this area also highlights a limited groundwater flow and particles do not reach the surface during the timeframe considered for the particle tracking. Keuper groundwater in ZNO and JO is recharging at Keuper outcrops located along the Wutach Valley and to the north of the JO siting region. In both siting regions, forward particles do not reach any discharge areas during the timeframe considered for the particle tracking. Instead, they remain in the Keuper aquifer or are entrapped in the adjacent aquitards. More generally, the calibration of the base case led to a zone-specific parametrization with sharp changes of hydraulic conductivities between the zones. Overall, lower Darcy fluxes prevail in the Keuper aquifer in comparison to other aquifers.

Since gradual transition of hydraulic conductivities from one facies to another would generally be expected, an alternative homogeneous isotropic Keuper aquifer case was considered in which the considered aquifer is modelled with one single zone north of the Jura Main Thrust and the Baden – Irchel – Herdern Lineament. The alternative case led to a similar hydrogeological situation with respect to recharge and discharge areas as in the base case. The model calibration also led to a similar fit albeit less well than for of the base case. In particular, the model reproduces less well the low hydraulic heads observed in the NL siting region and the high values in the ZNO siting region. Despite higher hydraulic conductivities in the homogeneous case than in the base case, the particle tracking in the NL siting region shows the smallest travelling distance of all the siting regions. As for the base case, the forward particle tracking does not highlight any paths towards a discharge area: forward particles remain in the model during the considered time frame.

Two test cases were finally considered to study the large-scale potentiometry resulting from a regional channel system hosted in the Ergolz Member and identify the most likely associated recharge and discharge areas. The channel system was abstracted in the Keuper aquifer horizon using a large-scale anisotropy resulting from the preferential orientation of these fluvial deposits (i.e. with the highest hydraulic conductivity being parallel to the main channel orientation). Two possible orientations were tested, namely along a west-east and a north south axis. Both cases show lateral hydraulic gradients preferentially oriented in the direction of the lowest hydraulic conductivity. However, the W-E case led to a more consistent hydrogeological situation when compared with observations acquired in the NL siting region (i.e. low hydraulic head and direction of local lateral hydraulic gradients). While both models resulted in contrasting particle path lines, similar recharge areas were identified as in the base case and the alternative homogeneous isotropic case. Also, in a similar way, no paths towards any discharge zones could be identified using forward particle tracking as released particles remain in the Keuper horizons or are entrapped in the adjacent aquitards. Finally, the Muschelkalk aquifer represents the lowest, but generally most active aquifer implemented in the model. Similar to the Keuper aquifer, a piezometric depression is located in the area of confluence of the Aare River into the Rhine River, separating the hydraulic flow system into an eastern and western part. In the western part, recharge is mainly located in topographically higher outcrops while flow is towards topographically lower outcrops mainly in the Aare and Sissle Valleys. In the eastern part, recharge occurs in the outcrops along the Wutach Valley while discharge areas are located at the convergence of the Aare and Rhine Rivers. Darcy fluxes are generally higher compared to the Malm and Keuper aquifers.

Large-scale vertical hydraulic gradients were evaluated across the Opalinus Clay. Downward hydraulic gradients are generally observed in recharge areas from where they gradually change towards slightly upwards oriented gradients in the discharge areas. Downward hydraulic gradients thus dominate in the JO siting region as recharge of the aquifers occurs at nearby outcrops. Upward hydraulic gradients are found in the ZNO siting region due to low hydraulic heads in the

Malm (nearby discharge area) and comparatively high hydraulic heads in the Keuper. The NL siting region presents a mix situation. Indeed, downward hydraulic gradients are found in the northern part of the siting region as recharge of the Malm aquifer is occurring through the thick Molasse units. Upward hydraulic gradients are found further to the north as the Malm is discharging in the Rhine River.

The role of faults has been evaluated using a number of different simulations. Initially, the faults are transparent (faults inherit hydraulic conductivities from the surrounding hydrogeological units) and the effect of the fault is primarily the reduction of the flow-through cross-section. In the sensitivity analyses focusing on the impact of the regional-scale faults, the inherited hydraulic conductivity of each element was altered (increased or decreased) via a multiplicative factor based on the hypothesis that the fault conductivity is controlled by the orientation relative to the stress field. That is, faults oriented roughly E-W are changed to be less conductive (because they are oriented normal to the current stress field) while faults oriented roughly N-S are changed to be more conductive (because they are oriented roughly parallel to the stress field). For most cases, the simulations resulted in very similar flow fields and the actual absolute value of the multiplicative factor only had minor effects. The simulations showed that the model is most sensitive to the parametrisation of the Randen Fault and the Baden – Irchel – Herdern Lineament. The Baden – Irchel – Herdern Lineament (and the anhydrite in the Jura Main Thrust), which is oriented roughly E-W and hence is assumed to have low conductivities, reduces flow from the recharge areas in the North towards the South of the model. The Randen Fault (which is oriented roughly NS and hence is assumed to have an increased conductivity) enhances flow from outcrops in the Wutach Valley towards the south.

In general, the hydraulic situation in the modelled area is very robust in the sense that implemented changes of the hydraulic situation based on conceptual models or observed variabilities of lithologies only have a small impact on the regional flow fields and observed changes usually are very local. This already became clear during the initial sensitivity analysis. Though 76 simulations with different boundary conditions and initial parametrisations have been performed to determine the initial best-fit model, the calculated metrics (MAE, R and SSE) for all models are close. On average, correlation coefficients (R) between simulated and observed heads are, for most cases and units, between 0.8 and 0.85, head differences between the simulations are, again on average, less than 20 m. This is explained by the control of the altitudes of the recharge and discharge areas that are typically not far away. The probably largest uncertainties of the models are related to the parametrisation of the hydrogeologic units or the hydraulic properties of faults and much less to the different boundary conditions.

For the southern part of the model (south of the Jura Main Thrust and Baden – Irchel – Herdern Lineament) only very few observation points exist. However, the lack of observations here does not have a greater impact on the model results in the northern part because the southern boundary is (very) far from the areas of interest (which are situated close to the natural recharge and discharge areas in the north) and because the Jura Main Thrust partly breaks continuity of the units towards the northern part (and creates important discharge zones for the southern part). In addition, the roughly E-W-oriented Baden – Irchel – Herdern Lineament reduce N-S- (or vice versa) directed flow.

10 References

- Allenbach, R., Baumberger, R., Kurmann, E., Michael, C.S. & Reynolds, L. (2017): GeoMol: Geologisches 3D-Modell des Schweizer Molassebeckens – Schlussbericht. (Berichte der Landesgeologie, 10). Bundesamt für Landestopographie swisstopo, Wabern.
- Barton, C.A., Zoback, M.D. & Moos, D. (1995): Fluid flow along potentially active faults in crystalline rock. *Geology* 23/8, 683-686. DOI: 10.1130/0091-7613(1995)023<0683:FFAPAF>2.3.CO;2.
- Bense, V.F., Gleeson, T., Loveless, S.E., Bour, O. & Scibek, J. (2013): Fault zone hydrogeology. *Earth-Science Reviews* 127, 171-192. DOI: 10.1016/j.earscirev.2013.09.008.
- Bock, H., Dehandschutter, B., Martin, C.D., Mazurek, M., de Haller, A., Skoczylas, F. & Davy, C. (2010): Self-sealing of fractures in argillaceous formations in the context of geological disposal of radioactive waste. Review and synthesis. OECD/NEA, Paris.
- Brauchler, R. & Schulte, P. (2019): Borehole Benken: Analysis of long-term monitoring data. Nagra Arbeitsbericht NAB 18-01.
- Bussard, T., Tacher, L., Parriaux, A., Bayard, D. & Maö Tre, V. (2004): Dimensionnement des aires d'alimentation Zu. Document de base, available online at <https://infoscience.epfl.ch/handle/20.500.14299/18139>, status as of November 8, 2024.
- Doherty, J. (2004): PEST Model-Independent Parameter Estimation. User Manual. 5th ed. Watermark Numerical Computing, Brisbane, Australia.
- Fisher, Q., Kets, F. & Crook, A. (2013): Self-sealing of faults and fractures in argillaceous formations: Evidence from the petroleum industry. Nagra Arbeitsbericht NAB 13-06.
- Flechtner, F. & Scholz, H. (2012): Untersuchungen zur Verkarstungsfähigkeit von Molasse-konglomeraten des Hochgrat-Adelegg-Fächers im Südwesten Bayerns (Allgäu). *Grundwasser* 17/2, 69-78. DOI: 10.1007/s00767-012-0193-1.
- Funk, C., Peterson, P., Landsfeld, M., Pedreros, D., Verdin, J., Shukla, S., Husak, G., Rowland, J., Harrison, L., Hoell, A. & Michaelsen, J. (2015): The climate hazards infrared precipitation with stations – a new environmental record for monitoring extremes. *Scientific data* 2, 150066. DOI: 10.1038/sdata.2015.66.
- Gmünder, C., Jordan, P. & Becker, J. (2013): Documentation of the Nagra 3D geological model 2012.1. Nagra Arbeitsbericht NAB 13-28.
- Gmünder, C., Malaguerra, F., Nusch, S. & Traber, D. (2014): Regional Hydrogeological Model of Northern Switzerland. Nagra Arbeitsbericht NAB 13-23.
- Ishii, E. (2015): Predictions of the highest potential transmissivity of fractures in fault zones from rock rheology: Preliminary results. *Journal of Geophysical Research: Solid Earth* 120/4, 2220-2241. DOI: 10.1002/2014JB011756.
- Knott, S.D. (1993): Fault seal analysis in the North Sea. *AAPG Bulletin* 77/5, 778-792. DOI: 10.1306/BDF8D58-1718-11D7-8645000102C1865D.

- Nagra (2002): Projekt Opalinuston: Synthese der geowissenschaftlichen Untersuchungsergebnisse - Entsorgungsnachweis für abgebrannte Brennelemente, verglaste hochaktive sowie langlebige mittelaktive Abfälle. Nagra Technischer Bericht NTB 02-03.
- Nagra (2008): Vorschlag geologischer Standortgebiete für ein SMA- und ein HAA-Lager: Geologische Grundlagen (Bericht zur Geologie). Text. Nagra Technischer Bericht NTB 08-04.
- Nagra (2014): SGT Etappe 2: Vorschlag weiter zu untersuchender geologischer Standortgebiete mit zugehörigen Standortarealen für die Oberflächenanlage: Geologische Grundlagen Dossier II Sedimentologische und tektonische Verhältnisse. Nagra Technischer Bericht NTB 14-02 Dossier II.
- Nagra (2024a): 3D Seismic Interpretation of Stratigraphic Horizons and Structures in Time Domain Jura Ost. Nagra Arbeitsbericht NAB 23-17.
- Nagra (2024b): 3D Seismic Interpretation of Stratigraphic Horizons and Structures in Time Domain Nördlich Lägern. Nagra Arbeitsbericht NAB 23-18.
- Nagra (2024c): 3D Seismic Interpretation of Stratigraphic Horizons and Structures in Time Domain Zürich Nordost. Nagra Arbeitsbericht NAB 23-19.
- Nagra (2024d): Geological long-term evolution: Erosion. Nagra Arbeitsbericht NAB 24-15.
- Nagra (2024e): Geological Properties of the Jura Ost, Nördlich Lägern and Zürich Nordost Siting Regions for Safety Assessment. Nagra Arbeitsbericht NAB 24-10.
- Nagra (2024f): Geosynthesis of Northern Switzerland. Nagra Technischer Bericht NTB 24-17.
- Nagra (2024g): In-Situ Stress Field in the Siting Regions Jura Ost, Nördlich Lägern and Zürich Nordost. Nagra Arbeitsbericht NAB 24-19.
- Nagra (2024h): Post-Closure Safety Report. Nagra Technical Report NTB 24-10.
- Nusch, S., Gmünder, C. & Traber, D. (2013): Hydrogeologische Daten der Tiefenaquifere als Grundlage für die hydrogeologischen Modelle SGT Etappe 2. Nagra Arbeitsbericht NAB 13-43.
- Pochon, A. & Zwahlen, F. (2003): Ausscheidung von Grundwasserschutzzonen bei Kluft-Grundwasserleitern – Praxishilfe. Vollzug Umwelt. Bundesamt für Umwelt, Wald und Landschaft, Bundesamt für Wasser und Geologie, Bern.
- Preisig, G. (2013): Regional simulation of coupled hydromechanical processes in fractured and granular porous aquifer using effective stress-dependent parameters. Ph.D. thesis. Center for Hydrogeology and Geothermics, University of Neuchâtel.
- Voborny, O., Resele, G., Hürlimann, W., Lanyon, G.W., Vomvoris, S. & Wilson, W. (1994): Hydrodynamic synthesis and modeling of groundwater flow in crystalline rocks of Northern Switzerland. Nagra Technical Report NTB 92-04.
- Wessels, M., Anselmetti, F., Artuso, R., Baran, R., Daut, G., Geiger, A., Gessler, S., Hilbe, M., Möst, K., Klauser, B., Niemann, S., Roschlaub, R., Steinbacher, F., Wintersteller, P. & Zahn, E. (2015): Bathymetry of Lake Constance. State-of-the-art in surveying a large lake. Hydrographische Nachrichten 100, 6-11. DOI: 10.23784/HN100-01.