Elaboration of groundwater models for deep geological repository sites by using FEFLOW

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ABSTRACT

The Sectoral Plan Deep Geological Repositories ("Sachplan geologische Tiefenlager –SGT", developed by the Swiss Federal Office of Energy SFOE) is the Swiss road map to establish repositories for radioactive waste. SGT Stage 1 with focus on the selection of geologically suitable regions led to the proposal of the six geological siting regions for the L/ILW (low- and intermediate-level radioactive waste) repository (Südranden, Zürich Nordost, Nördlich Lägern, Jura Ost, Jura-Südfuss, Wellenberg) and the three geological siting regions for the HLW (high-level radioactive waste) repository (Zürich Nordost, Nördlich Lägern, Jura Ost). Four different host rock formations are assessed as part of the L/ILW program (Opalinus Clay, "Brauner Dogger", Effingen Member, Helvetic Marls). The Opalinus Clay is the proposed host rock formation for the SF/HLW/ILW program. SGT / Stage 2 requires the selection of at least two sites for each repository type (L/ILW and HLW). As a quantitative decision basis for the site selection process, provisional safety analyses studies are to be performed for all relevant repository configurations.

Comprehensive geoscientific data bases have to be prepared for the provisional safety analyses, the so-called geodata sets for safety assessment. In this context, conceptual and numerical models of the groundwater flow conditions are elaborated on different scales of interest, ranging from the regional scale to the immediate vicinity of the proposed repository. Accordingly, the proposed numerical analyses of groundwater flow are broken down in 2 work packages:

- WP 1 / Regional scale modelling, aimed at evaluating the recharge and discharge areas of the regional aquifer systems and at specifying the hydraulic boundary conditions for the local scale models
- WP 2 / Local scale modelling, aimed at evaluating the local groundwater flow conditions in the different siting regions at present and for relevant long-term evolution scenarios. Local scale modelling may also include the effect of the repository construction and operation on the use of groundwater (groundwater resources, mineral and thermal water exploitation)

In total WP2 includes setups of four local models based on the overall three dimensional (regional) hydrogeological GOCAD Model. As studies for the proposed siting region of the Wellenberg already exist, this region is not further considered here. The remaining four model-domains are named according to the geological sites Jura-Südfuss, Jura Ost, Nördlich Lägern and Zürich Nordost combined with Südranden. The size of the model areas varies from 214 km² to 427 km². The general objectives of the local scale models are aimed at evaluating the local groundwater flow conditions in the different candidate siting regions at present conditions and for relevant long-term evolution scenarios. The present paper focusses on different approaches of numerical model set up and discretisation based on the available geological models by using FEFLOW. In particular, the implementation of the complicated geology with regional faults and thrusts are presented and discussed. Examples of the elaborated local scale groundwater models (WP2) will be presented.

Key words: Groundwater modeling, repositories for radioactive waste, FEFLOW

INTRODUCTION

The Sectoral Plan Deep Geological Repositories ("Sachplan geologische Tiefenlager –SGT", developed by the Swiss Federal Office of Energy SFOE) is the Swiss road map to establish repositories for radioactive waste. SGT Stage 1 with focus on the selection of geologically suitable regions (NAGRA, 2008) led to the proposal of the six geological siting regions for the L/ILW (low- and intermediate-level radioactive waste) repository (Südranden, Zürich Nordost, Nördlich Lägern, Jura Ost, Jura-Südfuss, Wellenberg) and the three geological siting regions for the HLW (high-level radioactive waste) repository (Zürich Nord-Ost, Nördlich Lägern, Jura Ost). Four different host rock formations are assessed as part of the L/ILW program (Opalinus Clay, "Brauner Dogger", Effingen Member, Helvetic Marls). The Opalinus Clay is the proposed host rock formation for the SF/HLW/ILW program. SGT / Stage 2 requires the selection of at least two sites for each repository type (L/ILW and HLW).

As a quantitative decision basis for the site selection process, provisional safety analyses studies are to be performed for all relevant repository configurations, including conceptual and numerical groundwater flow models on different scales of interest, ranging from the regional scale (work package 1) to the immediate vicinity of the proposed repository (work package 2). Figure 1 gives an overview on the location of the regional and local models considered. WP 2 mainly aims at evaluating the local groundwater flow conditions in the different siting regions at present and for relevant long-term evolution scenarios.

In total WP2 includes setups of four local models based on the overall three dimensional (regional) hydrogeological GOCAD Model. These four models are named according the geological sites Jura-Südfuss (JS), Jura Ost (JO), Nördlich Lägern (NL), Zürich Nordost and Südranden (ZNO-SR), see Figure 1. The size of the model areas varies from 214 km² to 427 km². The general objectives of the local scale models are aimed at evaluating the local groundwater flow conditions in the different candidate siting regions at present conditions and for relevant long-term evolution scenarios. This paper focusses on different approaches of numerical model set up and discretisation based on the available geological models by using FEFLOW. In particular, the implementation of the complicated geology with regional faults and thrusts are presented and discussed.

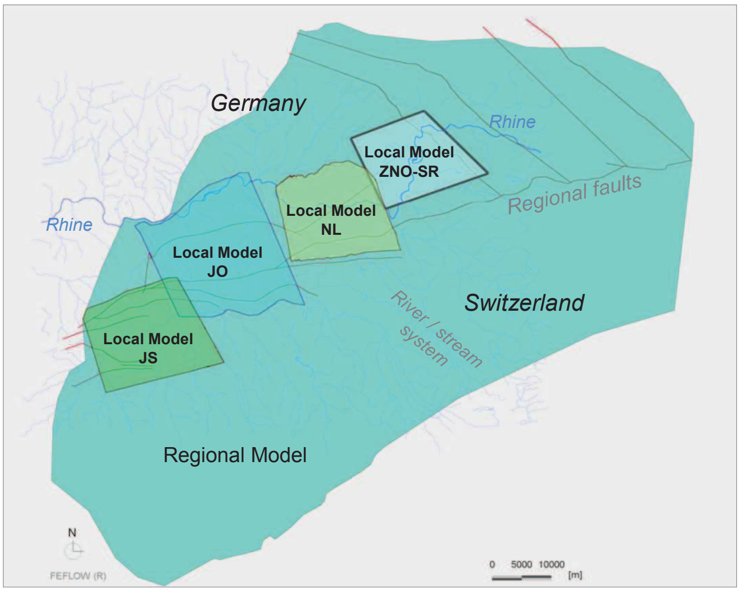


Figure 1. Location overview of the Regional Model and the Local Model areas

GENERAL APPROACHES OF MODEL SETUP

The model areas are located in Northern Switzerland. The model setup is based on the geological model data from the comprehensive geoscientific data bases available. The groundwater models considered 13 basic geological formations as shown in Table 1. Figure 2 and Figure 3 show different occurrences of the geological formations and complicated tectonic structures in the local model area.

Geological Era	Geological Formation	Layer / Unit	Slice / Layer surface	Lithology	Hydrogeologic function	Hydrogeologic model (Geol. GOCAD-Model)
			1			Top Quaternary = Land surface
Quaternary	Quartär	1	2	loose sediments	local shallow aquifer	Top OSM
Tertiary	Obere Süsswassermolasse (OSM)	2	3	claystone, siltstone, sandstone	aquitard	Top OMM
	Obere Meerwassermolasse (OMM)	3	4	sandstone, siltstone	porous / fractured aquifer	Top USM
	Untere Süsswassermolasse (USM)	4	5	claystone, siltstone, sandstone	aquitard	Top Oberer Malm
Malm (Upper Jurassic)	Villigen Formation	5	6	lime stone with lime amrl partition	fractured or karst aquifer	Top Effingen Member
	Effingen Member	6	7	marl, lime stone. Lime marl	aquitard	Top Oberer Dogger
Dogger (Middle Jurassic)	Oberer Dogger	7	8	lime stone, clay marl	aquitard	Top Hauptrogenstein / Klingnau-Formation
	Hauptrogenstein / Klingnau-Formation	8	9	oolitic lime stone and lime marl respectively	fractured or karst aquifer and aquiclude, respectively	Top Passwang
	Passwang Formation / Wedelsandstein	9	10	lime stone, clay marl with local aquifer	aquitard, local aquifer	Top Opalinuston
	Opalinuston	10	11	claystone	aquitard	Top Lias+Keuper
Lias (Lower Jurassic)	Toniger Lias			clay stone	aquitard	
	Arietenkalk			lime stone	local aquifer	
	Lias + Oberer Mittelkeuper	11		lime marl, clay marl, partly with sand and dolomite intercalation	aquitard	
Keuper (Triassic)	Gansinger Dol.			dolomite	local aquifer	
	Gipkeuper		12	dolomitic clay and anhydrite	aquitard	Top Oberer Muschelkalk
Muschelkalk (Triassic)	Muschelkalk Aquifer	12	13	lime stone, dolomite	fractured or karst aquifer	Top Mittlerer Muschelkalk
	Anhydrit-Gruppe	13	14	dolomitic clay, anhydrite and rock salt	aquitard	Top Kristallin

Table 1: Model structure with regional geological formations considered

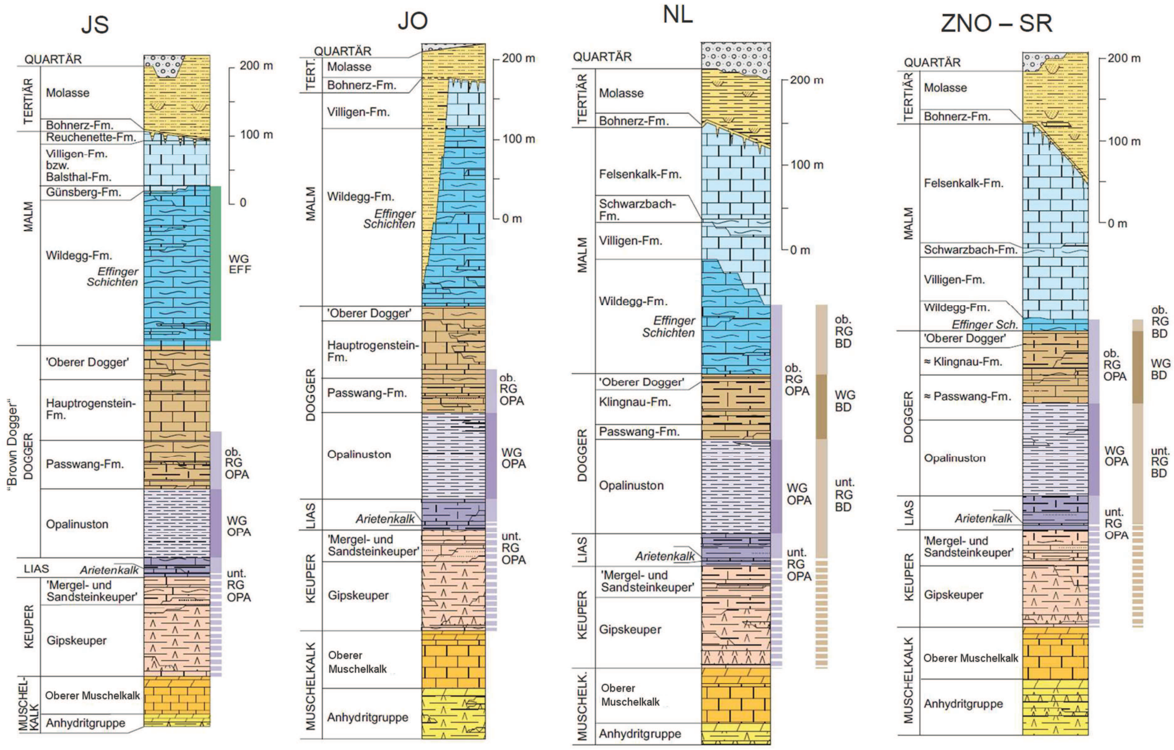


Figure 2. Geological profiles in the local model areas (after Nagra, 2008)

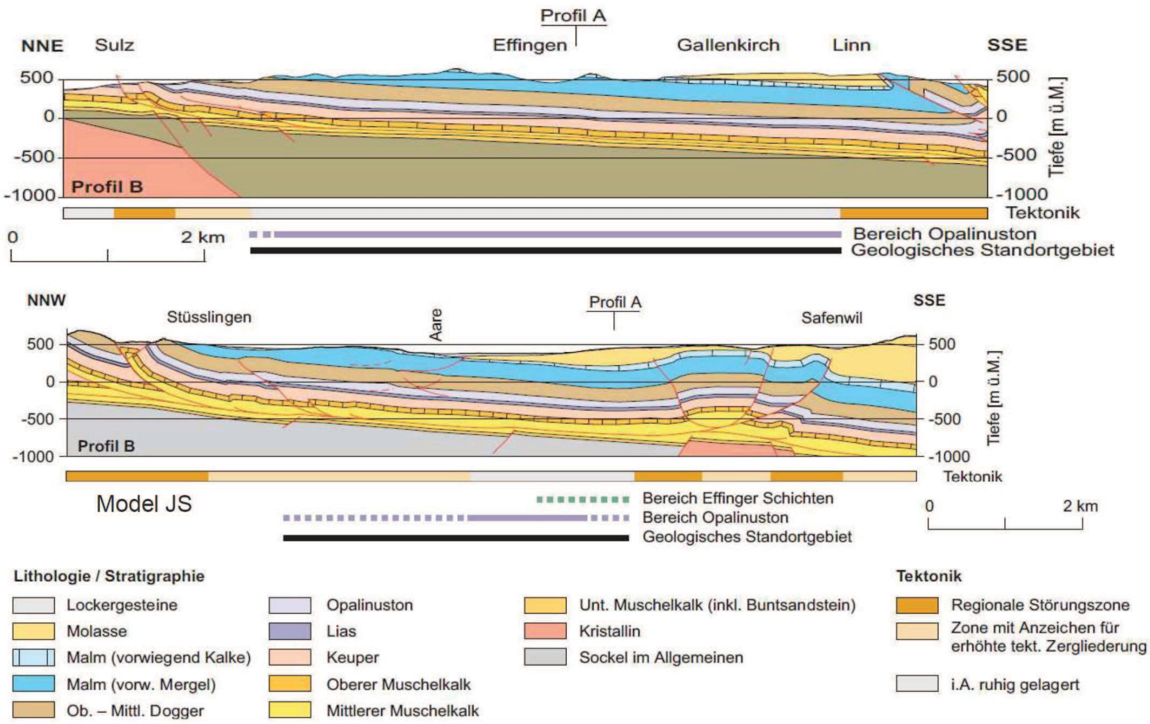


Figure 3. Geological sections in the local model areas JO and JS (after Nagra, 2008)

The model setup consists of two main stages:

- 3D model geometry constructing
- Parameter setting

Within the model geometry stage, the 3D model is built up first by a triangular mesh in the horizontal plane and then extended to the vertical direction forming 6-noded prismatic elements. Thereafter, the parameterization of the 3D model with material and/or hydraulic properties, boundary conditions and initial distributions of hydraulic heads was performed.

One important requirement for the model setup is an adequate implementation of relevant faults in the groundwater models. The relevant regional faults are implemented in the FEFLOW models according to their geological strike and dip or, if these data were not available, as vertical faults (see Figure 4).

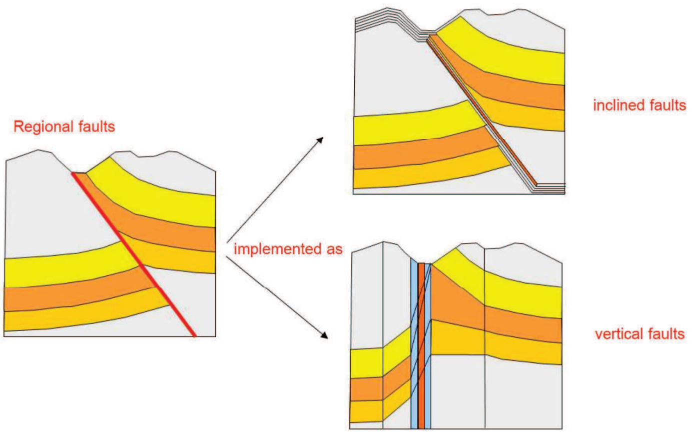


Figure 4. Illustration of fault implementation in FEFLOW-Model

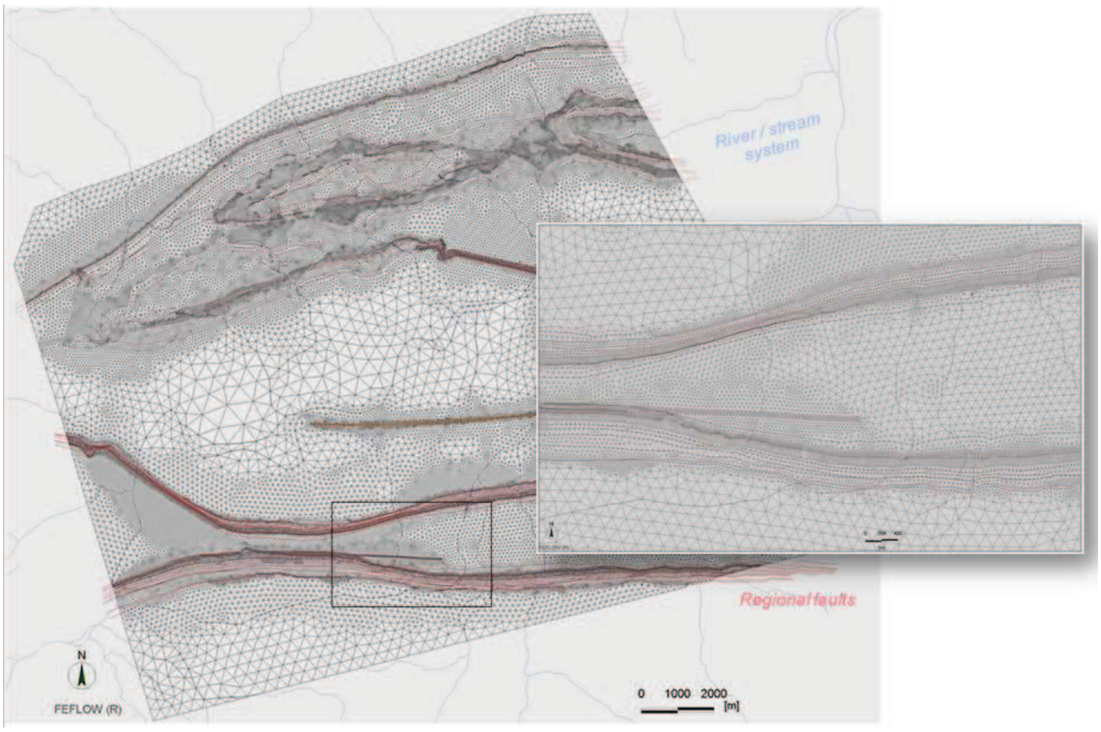
The horizontal discretisation of the model area is carried out first by designing a super element mesh considering the relevant geological features like faults and borders of geological formations at the different depths and river networks. Based on the generated super element mesh a finite-element mesh is then created. Figure 5 shows two examples of finite-element meshes for the local models ZNO-SR and JS

By vertical discretization, the generated 2D finite-element mesh is extended in the z-direction according to the elevation data of the GOCAD model, i.e. the regional geological model consisting of 13 basic geological formations from Mesozoic (Trias) to Cenozoic Era (Quaternary). In order to import the GOCAD geological layer-based data into a FEFLOW model, a FEFLOW plug-in (Ifm module) called "GOCAD2Elevation" was developed by DHI-WASY. The plug-in allows automated import and/or interpolation of elevation (and/or thickness) data of the geological layers according to the spatial distribution of the available data. In addition, the plug-in is capable to adapt hydraulic conductivities in the numerical model layers according to a user-defined minimal layer thickness or in combination with derived upper and lower angels of single finite elements. In this way, thin elements along a single fault can be assigned to adjacent geological layers if needed and a smooth transition of hydraulic conductivities along the faults can be guaranteed. To avoid that interpolation routines used for projecting GOCAD points to FEFLOW invoke misinterpretations of the geology, for example caused by an irregular distribution of GOCAD points, an additional step was needed. For this, a separate FEFLOW model was generated by SIMULTEC AG incorporating all GOCAD points in the horizontal mesh. The reason for setting up this model was that by importing the nodes from the local model mesh (for example Figure 5) as observation points, a correct interpolation of z-values could be achieved for all simulation nodes without depending on the original density of the GOCAD points. Furthermore, this model could be used to extract the outcrop borders and the interfaces between the geological units and the faults. These line elements could then be used to design the super mesh for the local simulation model. Although all this improved the representation of the geological layers around the faults significantly, an additional manual correction still had to be made to finalize the smoothing process along the fault faces. Figure 6 gives examples of cross sections for the present state of the Local Models built showing single characteristic elements. It can be seen that especially the local models JO and JS have complicated geological structures, which are represented by the mesh using the method described above.

The regional geological model includes only 13 basic (regionally distributed) geological formations. Some of these layers contain additional local distributed and, mostly, relatively thin geological layers (e.g. local aquifer layers), which have to be taken into account in the corresponding local models. The integration of these local geological layers required a division of the basic layers considered according to given thicknesses followed again, if needed, by a manual adaption of elevations and the geological unit assignment along the faults.

Figure 6 shows that the geological conditions in the local model ZNO-SR do not need complex geological modelling. As the regional faults in this local model shows dips of around 85°, the faults in this mod el has been implemented as vertical. The dense mesh in the eastern part of the ZNO-SR cross section represents an area in which a fault is located. The models NL and JO incorporate inclined faults only. In the model JS a combination of vertical and inclined faults has been applied. A challenge was the model JS in which local vertical faults are crossing inclined faults in some parts. For the models which are representing inclined faults it can be seen that the model is divided into several compartments. The local model JO, for example, is divided by four regional faults in five compartments. Each of the compartments includes a separate set of the 12 basic regional distributed geological units, some of which are again divided into sub layers required for representation of local geological units. These together made the number of model layers increase to a total of 85 (including separate layers for the faults themselves and the upper alluvial layer of Quaternary).

a) Finite-element mesh local model ZNO-SR with detailed view



b) Finite-element mesh local model JS with detailed view

Figure 5: Finite-element meshes of the local models ZNO-SR and JS

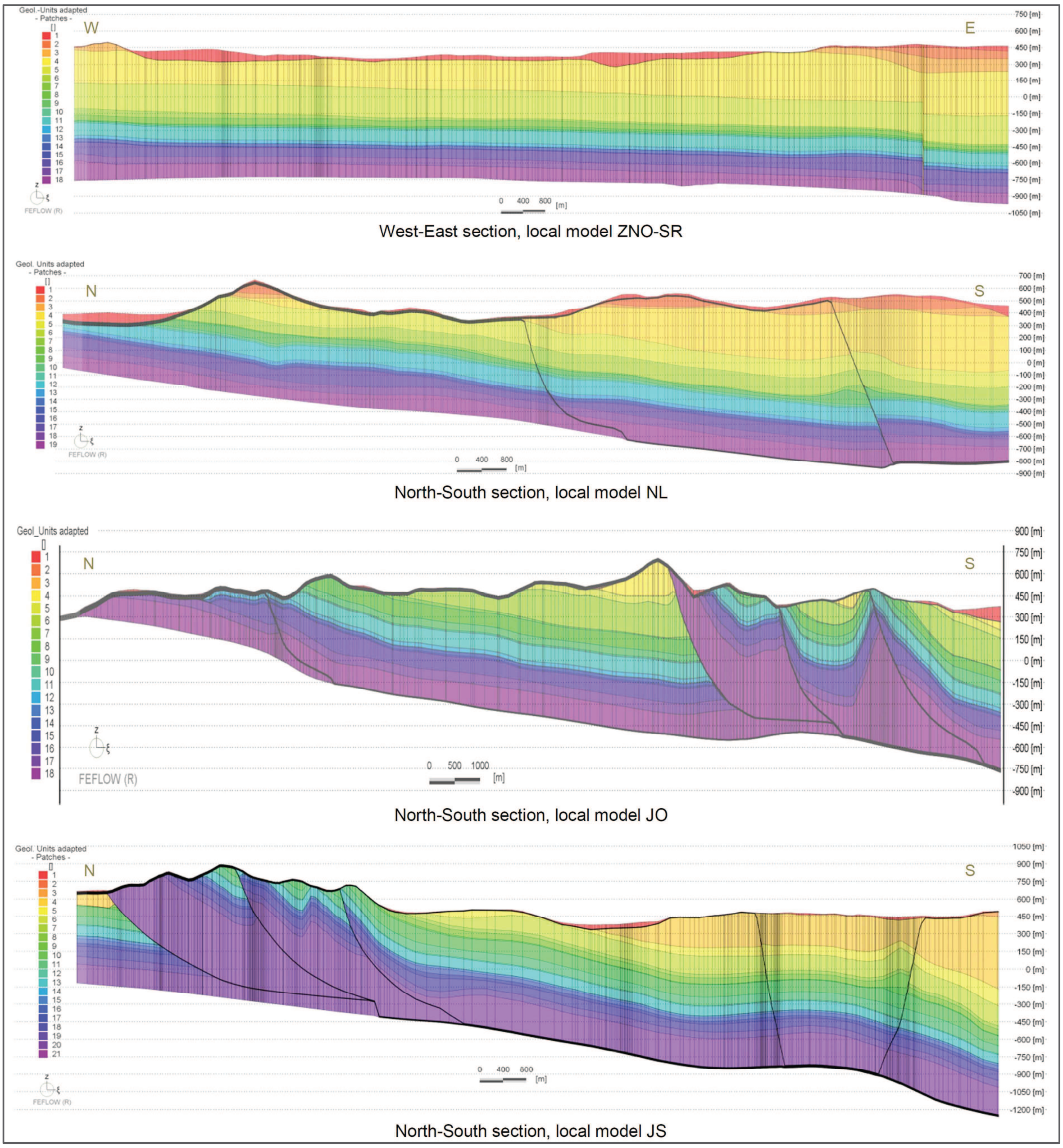


Figure 6: Exemplary cross sections of all local models

Parameter setting of the 3D FEFLOW models includes definitions of hydraulic parameters for the geological formations and of relevant regional faults considered, specification of necessary hydraulic boundary conditions as well as of initial hydraulic heads. In this regard, it's convenient first to define a reference data distribution for the geological formations or units considered ("geol. Units" for example). According to this reference data set, it's then straight forward to select, specify and modify hydraulic parameters using the selection tools now available in FEFLOW 6.1. In discussing the adaptation process with NAGRA, it was for example extremely helpful to define a reference data distribution called "Regional Faults" to verify the extent of the faults. Figure 7 exemplary shows the tectonic faults identified by this reference distribution implemented in the local model NL.

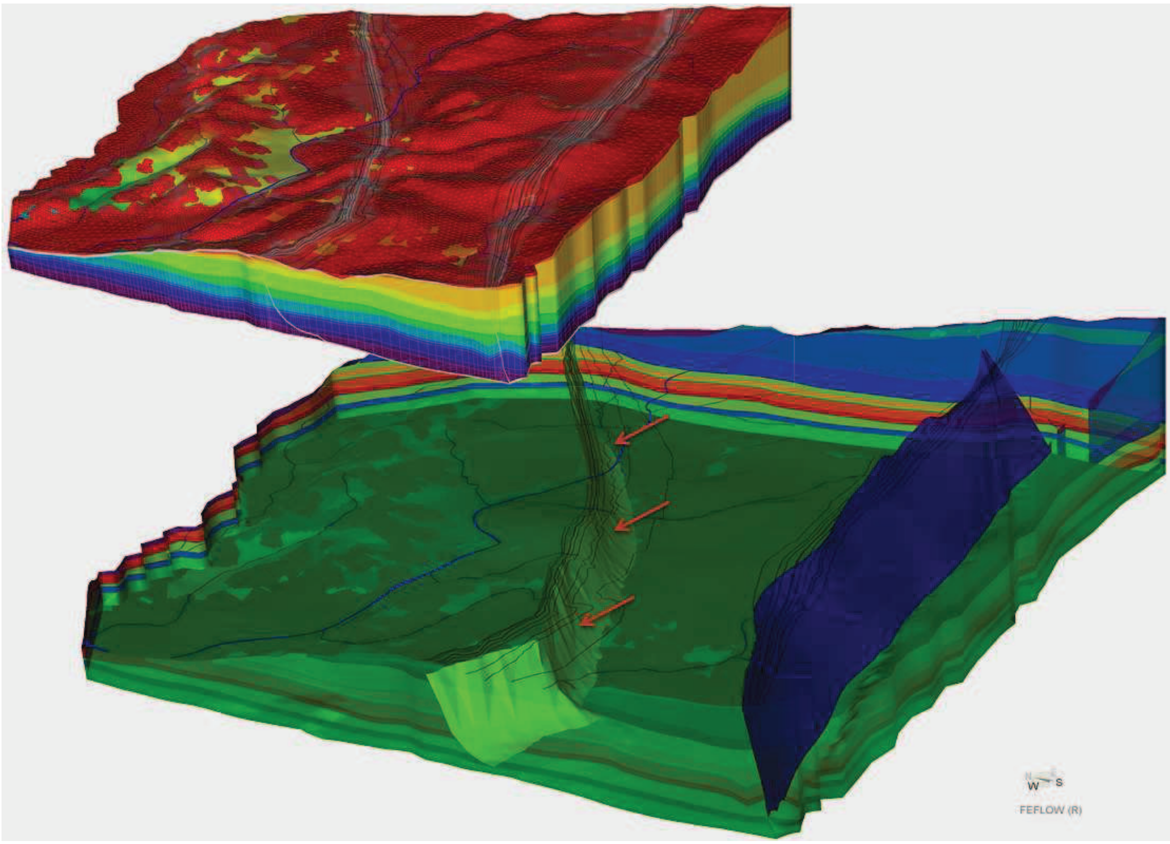


Figure 7. 3D representation of the implemented faults in the local model NL using reference data set selections.

STATUS AND OUTLOOK

The setups of the four local models according to the unique regional geological GOCAD-Model of 13 basic geological formations and with subsequent adaptions and implementations of locally distributed geologic sub layers have been finished. The corresponding reference data for the geologic formations or layer units and for the regional faults have also been specified as. A number of simulations with the local models ZNO-SR (with 18 numeric layers and about 1.2 Mio. elements), NL (with 56 numeric layers and 4.4 Mio. elements), JO (with 85 numeric layers and about 9.3 Mio. elements) and JS (with 92 numeric layers and about 25.5 Mio. elements) have successfully been carried out. These simulations also involved the definition of different characteristics of the faults and thrusts, in order to analyse their influence in detail.

Furthermore, the interaction between the local models and the regional groundwater model (elaborated by WP 1, SIMULTEC AG) has been implemented, which mainly involved the transfer of boundary conditions as well as recharge rates. A comparison between the models showed that the models provide essentially similar results. As the regional model was calibrated with available observation data, it can therefore be concluded that the local models are also capable to describe the relevant hydraulic processes. The next steps involve the simulation of further scenarios for sensitivity analyses and the long-term evaluation of groundwater flow processes with the local models. Until the final approval by the client, results of the simulations already performed have to be treated confidentially and therefore cannot be included in this paper. Nevertheless, the paper gives a good indication of the possibilities that the new FEFLOW 6.1 environment offers, in particular towards the representation of complicated multi-layered and fractured aquifer systems.

ACKNOWLEDGMENTS

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