Interreg
North-West Europe
DGE-ROLLOUT

HEATFLOW 3D-Modelling-application

Deliverable T2.1.12

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July 2023

Content

1 Introduction

Deliverable T2.1.12 is related to WP T2 “Decision and exploration support” and deals with the application of the HEATFLOW 3D-Modelling software. The target is the coupling of existing geological models with heat flow models and the improvement of the existing HEATFLOW 3D-modelling & simulation software (T2.1.11). In this regard, adaptation to the geological settings in NWE are performed. This will enable simulations of large, even transnational model spaces, the easy transfer of existing geological models into a HEATFLOW model space, the high accuracy modelling of fault systems, the coupling of deep geothermal reservoirs with underground heat storage and the simulation of chemical processes. In this deliverable two pilots are investigated:

- DMT simulates and assesses the possibility of storing geothermal energy in an old mine by modelling energy storage during summer and withdrawal in winter
- Application of the software to the planned deep geothermal energy (DGE) plant Weisweiler

1.1 Executive Summary

The aim of this study is to improve the existing HEATFLOW 3D-modelling & simulation software to be able to simulate large models with the coupling of deep geothermal reservoirs with underground heat storages and simulation of chemical processes.

Therefore, two different pilots are investigated in the following. The first pilot investigates the possibility of storing geothermal energy in an old mine. Based on different analytical and numerical calculations a preferred variant is developed with cyclic loading and different inlet temperatures in winter and summer, respectively.

The second pilot is the investigation of a planned DGE plant in Weisweiler. Here, the project partners GD NRW and RWE provided the geological subsurface model including available framework parameters. The initial process flow had to be changed during the project, such that in the end a new software package was developed, which transfers the geological model from GD NRW to the DMT software HEATFLOW. In this regard, it is possible to process complex geological conditions with a strong influence of faults. The heat flow including chemical reactions can be simulated. Different scenarios are investigated for the Weisweiler pilot, where the focus lies on the Kohlenkalk and Massenkalk formations, which comprise potential geothermal aquifers.

2 BoxModel – HEATFLOW

BoxModel represents a simulation software for 3D modelling of mine and groundwater flow, heat and (reactive) mass transport even in coupled systems \7\. It provides a toolbox for modelling of

- Mine water management (BOXMODEL)
- Groundwater flow including geochemical reactions (REACFLOW) and
- Deep geothermal reservoirs (HEATFLOW).

BoxModel contains the complete modelling workflow from geometry to postprocessing including conversion of several geological tools/software.

In the context of mine water management, BOXMODEL is used to calibrate historic flooding processes and forecast future developments, to optimize water management in operating mines, to simulate breakthrough scenarios or to predict mine water quality. In BOXMODEL, all relevant input

data can be considered, such as pump characteristics, complicated roadway networks, drifts and shafts, short cuts between mining fields, hydraulic connections and much more.

REACFLOW provides a flexible discretization similar to finite element models, which can optionally be transferred from e.g. SPRING (Delta H Software) or PETREL (Schlumberger) without loss of resolution. It allows the simulation of parallel multi-component transport, modified sorption potential per transport unit, geochemical reactions and microbiological degradation. Furthermore, REACFLOW offers a wide range of pre-installed transport units (MOH, PAH, VOC, SO4, CO3, Fe, pH-, Eh-calculation). The modification of the considered transport units and processes is freely extendable.

The focus of HEATFLOW is the direct transfer of structural geological models e.g. from PETREL for heat transport simulations including chemical processes. The improvement of the fault description contained therein ensures highly accurate modelling of flows in fault systems. Coupling of deep geothermal reservoirs with underground heat storage is possible.

2.1 Introduction to the software modules

The BoxModel simulation software is used to calculate the transient three-dimensional flow rate and the reactive mass transport. It consists of a freely structurally configurable model according to the volume balance method, which can consider defined irregular geometries (BOX) and a reactive mass transport model directly coupled to it. Both models are solved simultaneously.

The model part "BOX" serves in particular to consider various types of hydraulic elements such as groundwater conductors, aquifers, mining drifts, faults, drainage pipes etc. In accordance with the diversity of flow forms, laminar and turbulent flow as well as the temporal variability of hydraulic properties are treated equally.

In practice, conditions for the application of BOX3D are found, for example, when a mining tunnel connects mine fields that are more than a few kilometres apart and both areas are in hydraulic contact far below the groundwater surface. Here, the use of classic finite element or difference models is often inexpedient because of the complicated discretisation.

The data are processed with the integrated CAD program BOXCAD. The original model data from which the model is always generated, are CAD data. All changes - even if the user does not notice them directly via the special program interface - refer to the CAD data. The basic data format of BOXCAD is the internationally used SURPAC format.

The preparation of the data for the simulation is done with the pre-processor Praebox. Here, various settings can be made and geochemical mass properties can be adjusted. The generated data are primarily generic data files or text files in the form of character-separated values.

The simulation takes place in the Box3d or Box3d64 program module. Here, the calculation of the (in) stationary flow, the heat transport and the reactive mass transport takes place. The mass transport model has re-action terms that can take into account various sorption and desorption mechanisms as well as chemical reactions between and within phases.

Based on the calculated velocity field, the mass transport equation (convection equation) for the liquid phase is solved in parallel. Mineral phases were implemented for the solid phase. To describe the geochemical environment different species of a mineral phase are considered. Interactions can occur between migrants within the liquid phase, but also between liquid, gaseous and solid phase.

For example, dissolution and precipitation processes of mineral phases can take place, leading to a change in the concentration of the flowing components. These reactions are usually not in the chemical equilibrium but must be described by kinetic equations.

2.2 Flow Modelling

The flow of the total mass and of the momentum with the Darcy approximation in the flow in porous materials and the equations of state for the fluids and solids are called quantity flow. The BoxModel Box3D uses a three-dimensional structure. For this purpose, the flow equations are defined internally, discretised numerically and programmed. The flow equations of the quantity flow, the reactive mass transport and the heat transport are considered and formulated, for example, along a flow tube. The flow tube has the central streamline coordinate s and the variable cross-sectional area ΔA. Δs is the gradient distance related to the water level difference Δh between two element centres (box centre points).

Flow equations are formulated for a representative volume element RVE. An RVE is defined as constant. On the one hand, an RVE is sufficiently large and contains a sufficient number of microelements (pores, fissures, material components, fluid phases) to be able to form mean values over the RVE. On the other hand, the RVE is sufficiently small to be able to consider the location and time dependence of the mean values in the entire flow space. This definition helps to define the boxes in the model area.

The Finite Volume Method (FVM) is a numerical method for solving conservation equations (partial differential equations) based on a conservation law. In principle, the FVM is a generalisation of the finite difference method (FDM).

The flow equations differ between the confined and unconfined process. In unconfined flow, the transient of the flow process results mainly from the refillable porosity. This is the main variable affecting the water rise time. In confined flow, the transient behaviour is affected only by the compressibility of fluid and rock. This effect in terms of the duration of water rise is extremely small compared to that of refillable porosity.

2.2.1 Resting phase:

In mass transfer, a distinction is made between a flowing and a resting (active and passive) phase. Comparative calculations of real flooding examples have shown that a one-porosity-model is not able to realistically reproduce the data from practical examples. For this reason, in addition to the flowing or active phase (stretches), a second porosity was introduced, which assigns to the degradation areas (passive or quiescent or stagnant phase).

One of the main characteristics of this resting phase is that, although it is filled under saturated conditions, it flows extremely poorly thereafter. This is due to poor hydraulic contact with the flowing phase, which affects the releasable mass potential.

2.3 Mass-/heat transport model

When modelling the transport of mass dissolved in ground or mine water, the following transport mechanisms are represented:

- **advection** (transport of the mass with medium flow velocity)
- **molecular diffusion** (balancing of concentrations by Brownian molecular movement)
- **hydrodynamic dispersion** (compensation of concentrations due to different velocities in pore channels)
- geochemical **dissolution/precipitation processes** (phase change and chemical reactions)
- **adsorption / desorption**
- **microbial reduction**
- **time-dependent storage effects** in an aquifer.

The mathematical formulation of these individual processes is in the mass transport equation (convection-diffusion equation). Due to a similar mathematical description under certain assumptions of the diffusion and dispersion terms, they can be combined to one complex term.

In addition to the formulation of pure transport, the description of the pollutant release or retention (e.g. sorption, precipitation) during transport is of particular importance. This is considered in the source-sink term n_{vh}. The generic term for the exchange processes between phases and within a phase is "interaction".

The BOXMODEL is a multi-component mass transport model; therefore, the mass transport equation is solved in parallel for all transport units (note the previously mentioned solution of the mass balance equation for the resting and flowing phase). In the model, inorganic transport units (tenads: chemistry, trace metals), particle fractions, organic compounds and bacterial activity are considered as independent transport units.

The different particle fractions differ, among other things, in their sedimentation behaviour. In the BOXMODEL, the sedimentation is modelled by sedimentation kinetics. The sedimentation rate [mg/l/s] results from the particle concentration [mg/l] of a certain particle spectrum multiplied by the corresponding sedimentation rate constant [1/s]. These rate constants vary greatly for the grain spectra considered; as already mentioned, the fine spectrum is hardly sedimented. By delimiting the flow-dependent transport and deposition range, functions of the rate constants can be derived from the flow velocity.

For the extension of a mine water flow model to a mass transport model, further model input data are required. These will be described in the following section. A retardation coefficient is not used in the model, as sorption and desorption are always considered.

2.4 Initial and boundary conditions in multi-component mixtures - Source terms

For transient mass transport calculations, a start distribution of all chemical ingredients must be specified as the initial mass transfer condition. In addition, substance boundary conditions must be defined in the model. These determine the composition of the inflowing water (e.g. groundwater recharge, leachate from surface waters, boundary inflows).

The demand for a coherent ion balance between the chemical macro-components at any point in the model requires certain conditions. Therefore, the substance initial condition cannot be derived only from estimated concentration distributions (e.g. iso-concentration maps). In order to comply with this requirement, the approach described below is followed.

A specific composition is assigned to all water qualities relevant for the model area, which are to be differentiated spatially and qualitatively. This is defined and stored in the model as chemistry type (CT). Therefore, this includes groundwater, leachate and marginal inflows with the respective dissolved substances and their concentrations. The chemistry types are defined for each simulation or are adjusted during calibration. For the model, one type of chemistry represents a water quality balanced in the ion charges. Within the model, it can be used to define both the substance initial condition and the substance boundary conditions.

The data sets of the chemistry types are compiled from individual measurements and balanced geochemically. The balancing is continued until the measured pH- and EH- values correspond with the equilibrium model (PHREEQC or Reacflow). In case of an unbalanced ion balance, the dominating ions, mostly sodium or chloride/sulphate, are used for balancing.

2.5 Dissolution - precipitation reactions

Flowing water is nearly always in contact with a rock matrix. Due to this and mixing with other inflows, it is a subject to geochemical changes. Resulting thermodynamic imbalances between fluid and rock (under saturation/super saturation) lead to dissolution or precipitation reactions. The dissolution processes destabilize the matrix (increased permeability) whereas intensive precipitation can lead to collimation of the flow paths.

The requirement for the consideration of chemical reactions in models is the knowledge of the concentrations of substances (here especially ions/species), which participate in the chemical reaction. Therefore, these substances must be transported simultaneously in the numerical flow model. Thus, in each flow element at each time step the necessary ion concentrations, which are required for the reaction equations, are known. For many reaction equations, it is not enough to know the sum concentration, which is considered in the mass transfer equation, e.g., $\sum SO_4$ (= SO_4^{2-} + HSO_4^- + $CaSO_4$ + ...). Here, it is necessary to provide information on the specific ion or species distribution. For this reason, the geochemical system of all sum concentrations must be solved for the equilibrium state of the liquid species. Then it is examined whether the geochemical equilibrium system of the liquid phase is in balance with the solid phase. In the case of an imbalance, so-called kinetic interaction terms (reaction rates, phase exchange) are formulated, which shift the geochemical system towards equilibrium.

In the calculations of the dissolution and precipitation reactions, the redox conditions are always calculated and considered. Furthermore, the CO_2 partial pressure is also considered in the process of carbonate equilibrium. Carbonate dissolution and precipitation are a function of the CO_2 partial pressure, which in turn influences the pH value. The carbonate system and its temperature influence are integrated into the BoxModel. Therefore, the question must always be answered whether the considered reaction space is a closed system (no gas exchange with the atmosphere) or an open system (gas exchange with the atmosphere).

2.6 Mass input and release of macro-chemical components and trace metals

The input of substances into the model occurs by the inflow from the so-called inner boundary conditions. Each individual inflow within a box at a certain feed level must be evaluated regarding the installed transport units and allocated individually. For this purpose, the existing chemical analyses of partial water flows are evaluated.

On the flow path a leaching of already dissolved substances, e.g. from the resting phase, takes place. In order to model the underlying reactions in their entirety (including acid production and carbonate buffering) in a practicable way, a so-called initial water can be defined. When defining this as the resting phase of the model, it represents the net result of various mineral reactions. The total mass stored must be compared with the mass discharge already known from other sources. These values are refined during the calibration.

This stored mass is transferred kinetically inhibited from the resting phase to the flowing phase according to a diffusion law. The transfer for the individual transport units takes place according to a fixed stoichiometric ratio of the concentrations given in the initial water.

3 Application 1 – Energy Storage in an old mine

DMT simulates and evaluates the possibility of storing geothermal energy in an old mine, modelling summer energy storage and winter energy extraction.

The planned project describes the extraction of a sufficient amount of water from a shaft at a depth of about 20 m with subsequent use of a heat exchanger and a heat pump. After the heat has been extracted, the water should run back into the shaft. The feed into the shaft is at a depth of approximately 400 m via a pipeline. The water is circulated so that the shaft water level does not drop. Since the shaft water practically does not communicate with the groundwater, it is possible to feed in heat in summer (use of the shaft as heat store). A higher amount of heat that can be extracted is then to be expected. Therefore, two cases are investigated / calculated: one for pure heat extraction and one for the use as a heat storage tank with summer heat feed-in.

3.1 Site Characterization

The old coal mine under investigation is a c. 425 m deep shaft for the exploration of Carboniferous coal deposits (see Figure 1 and Figure 2). The diameter of the shaft is 6.2 m. Clinker masonry with rear stamped concrete was used to prevent strong water pathways. Mine adits were excavated in a depth of 407 m with a length of approximately 1,150 m to explore the hard coal deposits. The shaft was only in operation until 1958 and was flooded in 1959. In preparation for the flooding, the shaft was cleared and prepared in such a way that it was practically possible to put it back into operation.

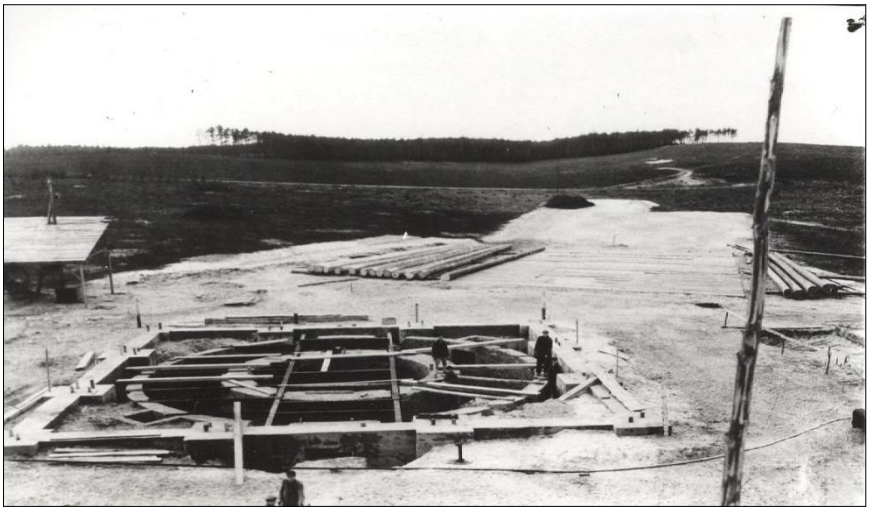

Figure 1: Shaft with foundation system. Freeze pipe cellar and winding tower foundation; Photo probably from the freezer house roof, viewing direction W.

Several exploration works were conducted. In 2008, depth-oriented water samples were collected with the aim of determining possible depth-dependent changes in water quality. The following parameters were determined:

- temperature
- conductivity
- pH value
- redox potential
- oxygen content

The temperature of the water sample in the upper part of the shaft was 17.5 °C. After that, a very small drop was registered (16.5 °C at 25.0 m, 16.1 °C at 75.0 m, 15.8 °C at 125.0 m, 15.7 °C at 225 m – 387 m) to 15.4 °C at 407 m depth. Conductivity also showed little variation over the entire depth interval, ranging from 200 to 225 µS/cm (based on above measured water temperature). The pH value ranged from 6.3 at the top of the shaft and increased with depth to 7.06 (at 407 m depth).

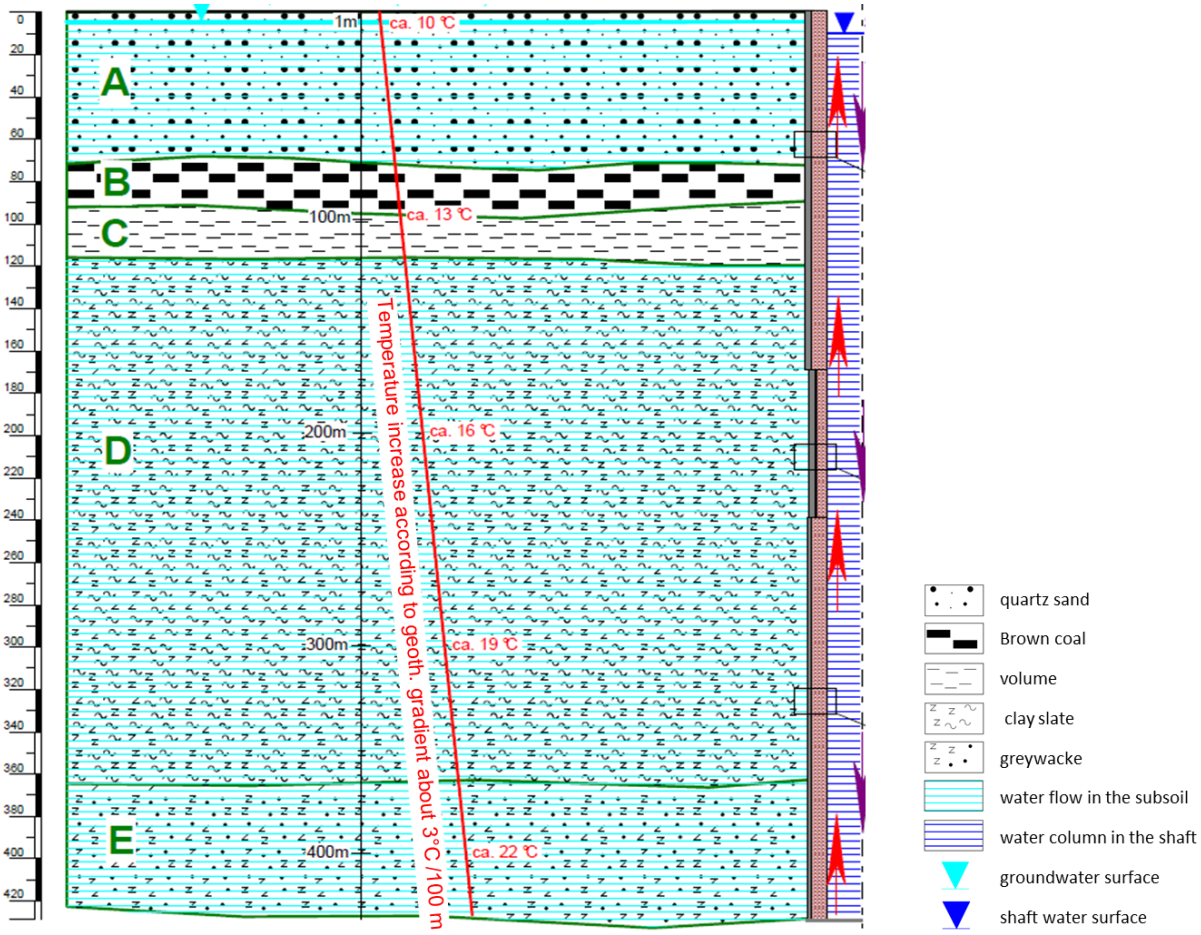

Figure 2: Cross section through the radially symmetrical shaft.

3.2 Calculation method

The DMT BoxModel tool HEATFLOW is used to calculate the heat transport in the shaft. In order to calculate the heat transport from the rock mass to the excavated shaft and water in it, the so-called cylindrical shell method with simple geometry can be used. I.e., the radially symmetric heat transport between rock mass and shaft is calculated with a numerical-discrete method based on the element balance shells constructed and solves the heat balance for each individual shell in each process time step (see Figure 3).

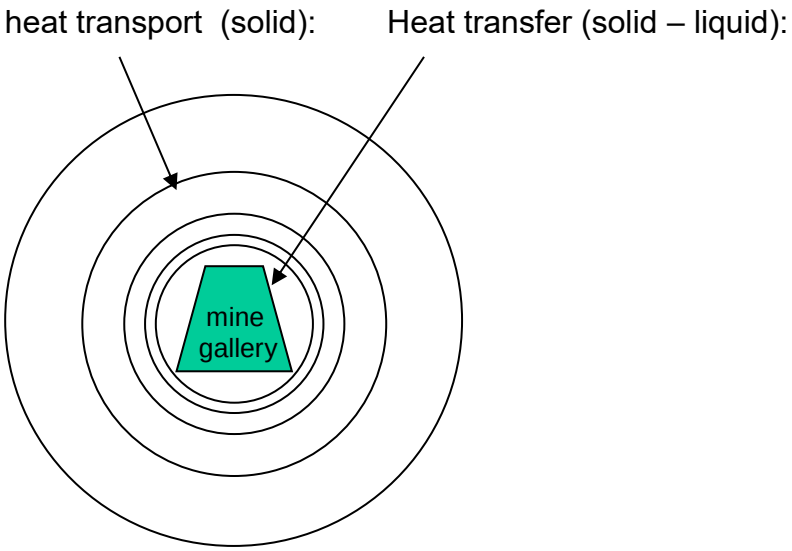

Figure 3: Cylindrical shell method. Radially symmetrical heat transport between rock and shaft.

3.3 Model setup

For the current example, 15 shells are selected, with the innermost shell having a thickness of 0.1 m. The thickness increases from shell to shell, so that a total depth of impact of 150 m (radially symmetric) in the rock mass is taken as a basis.

The shaft is vertically divided into 26 different slices, with the geometry of each slice shown in **Fehler! Verweisquelle konnte nicht gefunden werden.**. The properties of each model slides (thermal conductivity, storage coefficient etc.) are determined from the measurements.

Table 1: Relevant parameters of all slides, where kf: permeability, Poro: porosity, WLF: thermal conductivity, depth in [m].

Slice	kf [m/s]	Poro [1]	density [t/m³]	WLF [W/m * K]	heat capacity [MJ/(m³ * K]	Specific heat capacity [J/m³*K]	T [°C]	approx. depth
1	1.00E-04	1.00E-06	1.9	2.4	2.5	1315.8	15.50	108.8
2	1.00E-04	1.00E-06	1.9	2.4	2.5	1315.8	14.60	94.3
3	1.00E-04	1.00E-06	1.9	2.4	2.5	1315.8	14.60	79.8
4	1.00E-04	1.00E-06	1.9	2.4	2.5	1315.8	14.60	65.3
5	1.00E-04	1.00E-06	1.9	2.4	2.5	1315.8	14.60	50.8
6	1.00E-08	1.00E-06	1.0	0.4	2.0	2000.0	14.62	35.0
7	1.00E-09	1.00E-06	2.0	0.5	1.5	750.0	14.62	18.8
8	1.00E-09	1.00E-06	2.0	0.5	1.5	750.0	14.63	3.6
9	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.64	-12.7
10	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.64	-30.0
11	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.66	-47.4
12	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.67	-64.7
13	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.68	-82.1
14	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.69	-99.4
15	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.70	-116.8
16	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.70	-134.1
17	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.72	-151.5
18	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.74	-168.8
19	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.75	-186.2
20	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.76	-203.5
21	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.77	-220.9
22	1.00E-09	1.00E-06	2.5	2.1	2.5	1000.0	14.78	-238.3
23	1.00E-07	1.00E-06	2.5	2.3	2.2	880.0	14.79	-255.2
24	1.00E-07	1.00E-06	2.5	2.3	2.2	880.0	14.80	-271.7
25	1.00E-07	1.00E-06	2.5	2.3	2.2	880.0	14.88	-288.1
26	1.00E-07	1.00E-06	2.5	2.3	2.2	880.0	14.80	-304.6

3.4 Results shaft cooling

Example 1: Steady state solution

For the first example the following parameter are chosen:

- T_o rock and shaft = 14.7°C
- Geothermal gradient = 0K/100m -> T_{rock} = 10°C
- T inlet = 5°C

Therefore, the temperature in the mine gallery is constantly very low.
For comparison, the analytical solution for a radial symmetric heat transport in a cylinder is chosen which reads

$$\dot{Q} = 2\pi\lambda l / \ln(\frac{r_{shaft}}{r}) \cdot (T_{in} - T_{out}),$$

where

- $\dot{Q}$ [W] Heat flow
- λ [W/mK] Thermal conductivity
- l [m] Length of the cylinder (shaft)
- r_{shaft} [m] Radius of the shaft
- r [m] Radius
- T_{in} [°C] Temperature inside
- T_{out} [°C] Temperature outside

The parameter are as follows:

- q = 15 W/m
- λ = 2 W/mK
- r_{shaft} = 3.1 m

This input parameter results in a stationary temperature profile of the shaft as shown in Figure 4 for the analytical and numerical solution. The numerically derived temperature versus time is shown in Figure 5. It is plausible to see a moderate cooling of the shaft with time. Additionally, the analytical and numerical solution fit quiet well which validates the process.

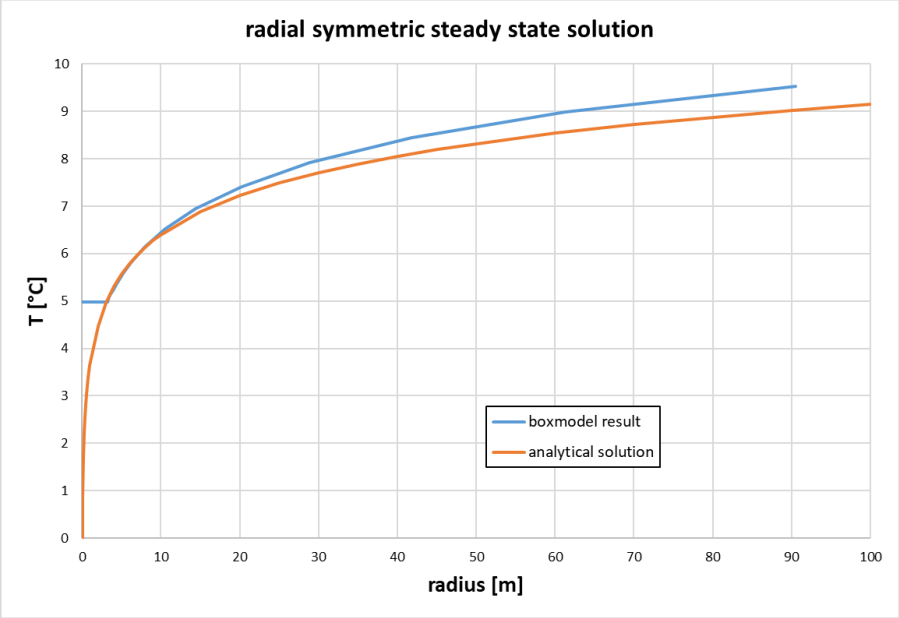

Figure 4: Steady state solution.

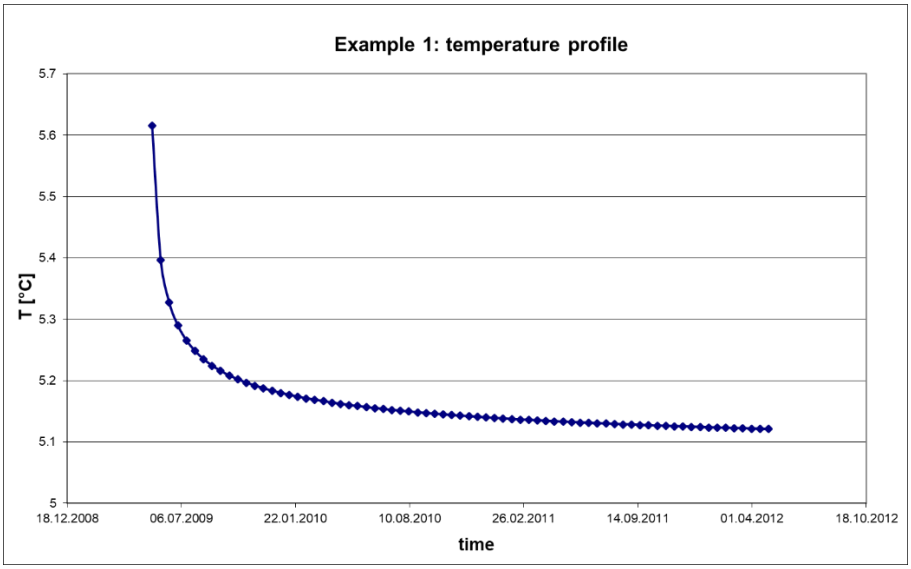

Figure 5: Temperature versus time for example 1.

Example 2: Transient solution

For the second example the following parameter are chosen:

- T_{shaft} = 14,7oC
- Geothermal gradient = 3 K/100m
- T_{inlet} = 10oC
- Q = 102 m3/h

Different tests are performed to find the optimal solution for heat storage, where the focus is set to the following setups:

a) Q = 10 and 100 m³/h
   - cyclic flow
   - permanent flow

b) Cyclic loading (10 m³/h)
   - flow from bottom to top
   - flow from top to bottom

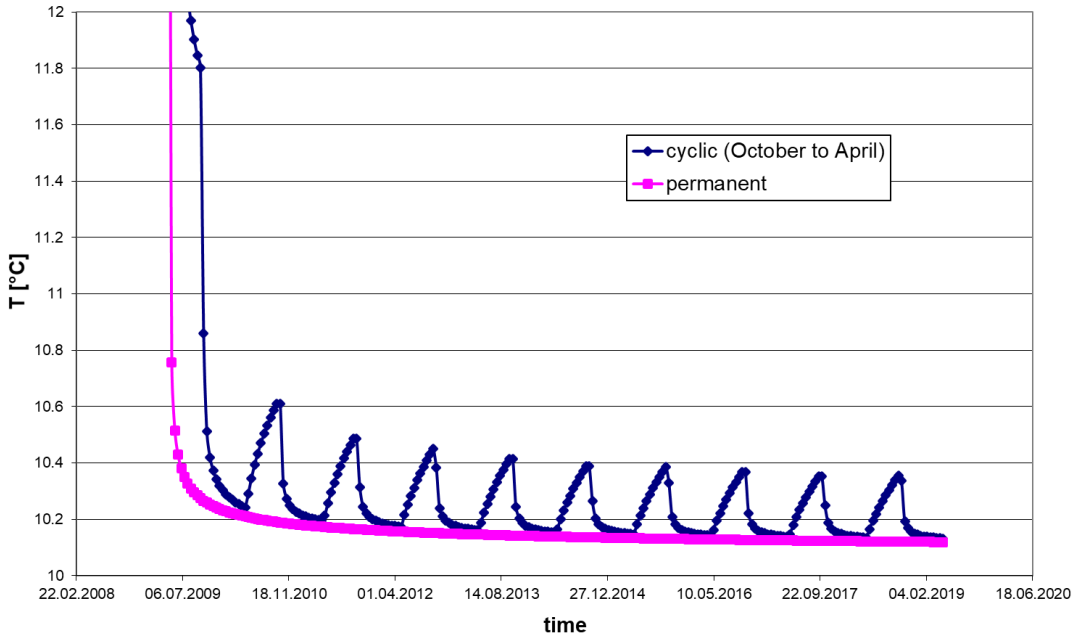

Figure 6: SetUp a): Comparison of permanent and cyclic operation with Q=100m³/h.

In the tests for a) a volumetric flow rate of 100m³/h is chosen. In Figure 6 the results are compared for a permanent inflow and for a cyclic flow, where between May and September the operation is stopped. In both cases a ΔT of approx. 0.15°C is usable after three years with a ΔT between cyclic and permanent flow of approx. 0.02°C.

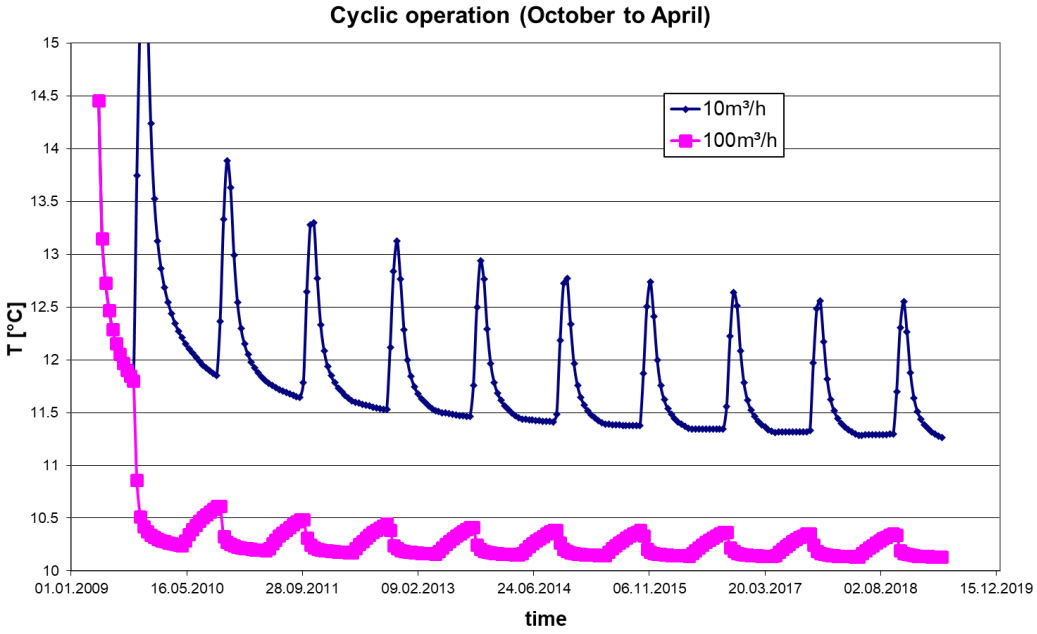

Figure 7: SetUp a): Comparison of cyclic operation with Q = 10 m³/h and 100 m³/h.

The results for a cyclic operation with a volumetric flow rate of 10m³/h is shown in Figure 7 in comparison to the results with a volumetric flow rate of 100m³/h. In this case a ΔT of approx. 1.35°C is usable after three years with a ΔT between the different flow rates of approx. 1.2°C.

For the setup b) the inlet temperature is reduced to 5 °C. The focus is now set on the flow direction. Considering a volumetric flow rate of 10 m³/h and a cyclic operation the fluid flow 'direction' is once set from bottom to top and once from top to bottom. The results are shown in Figure 8. The results show that about half a degree can be gained if the flow is from top to bottom (no cooling due to the geothermal gradient).

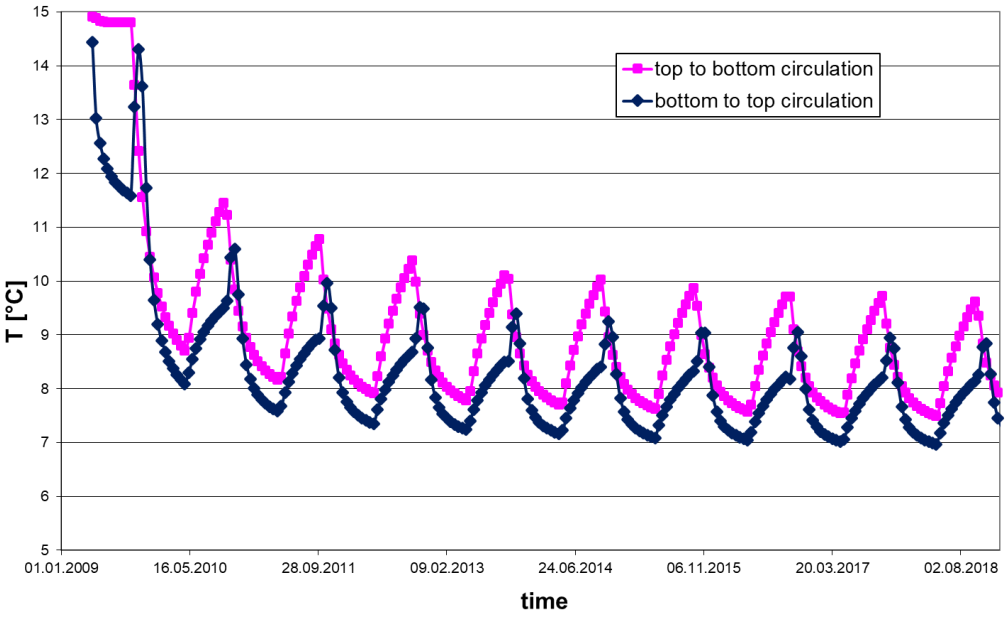

Figure 8: SetUp b): Different circulation techniques, T_{inlet} = 5°C, Q = 10 m³/h.

Based on the model tests and different setups, a preferred variant can be found which is shown in Figure 9. Here, the inlet temperature is set in summer to 20 °C and in winter to 5 °C.

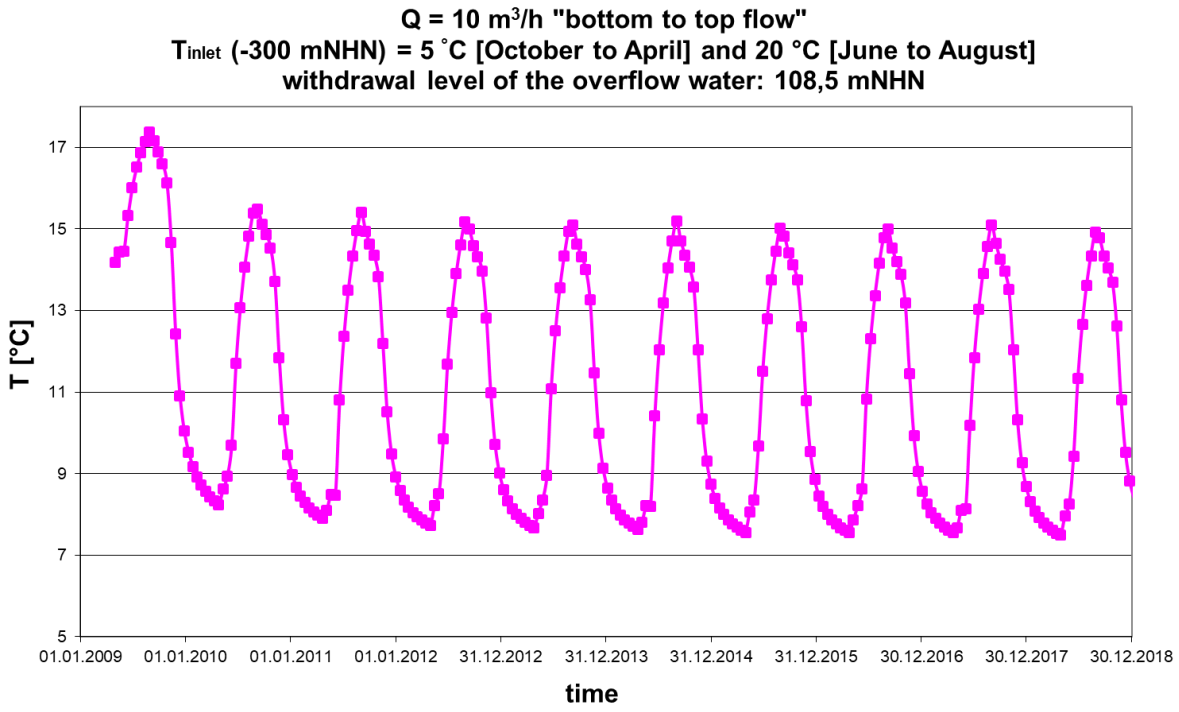

Figure 9: Preferred variant: Introduction in summer at 20 °C and in winter at 5 °C.

The heat storage in summer improves the situation significantly. The minimum at the end of winter is still ΔT = 2.5 °C but on average ΔT = 6 °C. Above all, no asymptote can be seen after ten years for this case.

4 Pilot 2 – Weisweiler Deep Geothermal Energy Site

4.1 Introduction

The Weisweiler project is connected to the oldest lignite power plant in western Germany. During the project it will be studied, exemplary for one large fossil fuel power plant, how a transition to renewable energy can be managed with DGE. In this regard, a process flow is developed to transfer and simulate heat flow in complex geological conditions with a strong influence of faults. The process includes the development of the DMT software module SpringToBox which can transfer SPRING to HEATFLOW models including all relevant parameters and connections. Additionally, the fault connections that cannot be processed with SPRING accurately, are included and created via the optimized DMT software. In the following sections first the model transfer software and process are explained. Afterwards the model set up is presented in detail. The section ends with different simulation scenarios in the Weisweiler model.

4.2 Model Transfer

Due to the available software tools, several model adjustments have been carried out that are explained in detail in the following sections.

4.2.1 HEATFLOW – Model Development

For the Weisweiler DGE site the modelling tool HEATFLOW was chosen to simulate the geothermal reservoir and underground heat storage. As the basic 3D subsurface model was delivered by project partner GD NRW in MOVE (Petroleum Experts Limited), the already existing interface to PETREL could not be used as originally intended. Also, the conversion of the MOVE model into a PETREL model for further processing with the PETREL interface in HEATFLOW would have required extensive additional work on the MOVE model or rework on the PETREL model and was found to be impractical. Therefore, a new procedure has been developed and integrated in the basic SpringToBox tool. The first step is to transfer the MOVE model to a SPRING model. This SPRING model can then be transferred by SpringToBox to a HEATFLOW model. Therefore, several software adaptions were carried out. The process is shown in Figure 10 and explained in detail in the following sections.

The HEATFLOW program developed by DMT is available for cases with more complex geology and a strong influence of geological disturbances on the underground flow, as well as for geochemical issues that require modelling of reactive mass transport (see chapter 2). To make complex geological models available for simulations with HEATFLOW, various methods are available that are continuously further developed, expanded, and optimized.

The focus of HEATFLOW is the transfer of structural geological models for heat transport simulations including chemical processes. The contained improvement of the fault description ensures a high accuracy modelling flow in fault systems. The coupling of deep geothermal reservoirs with underground heat storage is possible.

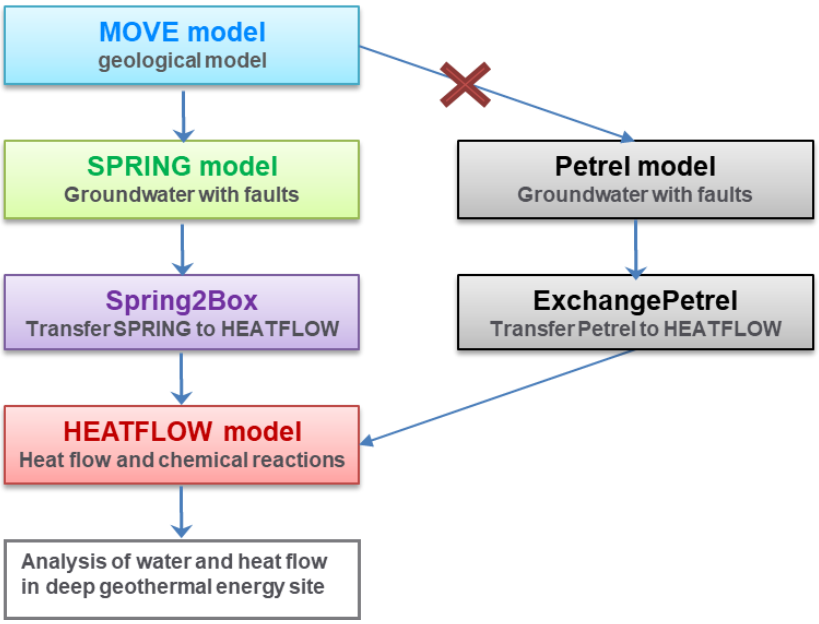

Figure 10: Flow chart for the model transfer

4.2.2 SPRING – Model adaptions

SPRING is an established and recognized software package for simulating flow in porous media, including heat and mass transfer. Less complex geology and simpler solute (non-reactive) transport issues can be handled effectively with these tools. Using this software as an intermediate step in the preparation of the HEATFLOW model offers three main advantages:

1. the model data of the SPRING models are available in a comprehensible ASCII format
2. the assignment of the parameters and boundary conditions relevant for the flow and transport modelling as well as suitable interpolation procedures are already implemented in the software
3. in suitable cases, flow and transport calculations, e.g. in the sense of comparative calculations, can be carried out with the software.

Within the project, a routine from the SPRING software to HEATFLOW has been developed. Models can be quickly transferred from one system to another. In particular, there is the possibility of transferring geological faults that cannot be solved within SPRING with high accuracy. The routine is described in the following.

To build the SPRING model, two data sets from the MOVE model were provided:

1. the elevations of the geological layer boundaries in a simple ASCII format (x, y, z).
2. the "cut-off-lines", i.e., the lines on the layer surfaces along which the faults intersect these layer surfaces in shape format, including heights along the lines.

The use of the simplest possible standard formats to transfer the model geometries of the MOVE model makes it possible to apply the procedure also to geological models that were created with other software packages.

For the construction of the SPRING model, a horizontal finite element mesh was first created within the boundaries of the MOVE model. In this mesh all cut-off lines, that remark the head and foot wall of a geological fault, are represented by element edges. Subsequently, the 3D layer structure was created by interpolating the provided point data and assigning the heights along the cut-off lines to individual node layers. Each node layer thus represents a geological layer surface.

In order to identify related cut-off lines, i.e. lines belonging to a specific fault, separated into foot wall and head wall, these lines have to be remarked with numbers following a special scheme. The first number marks the fault number, e.g. “Weisweiler Sprung” = 1, “Abbruch von Merode” = 2. An example of this assignment is shown in Figure 11, the individual faults are marked by different colours.

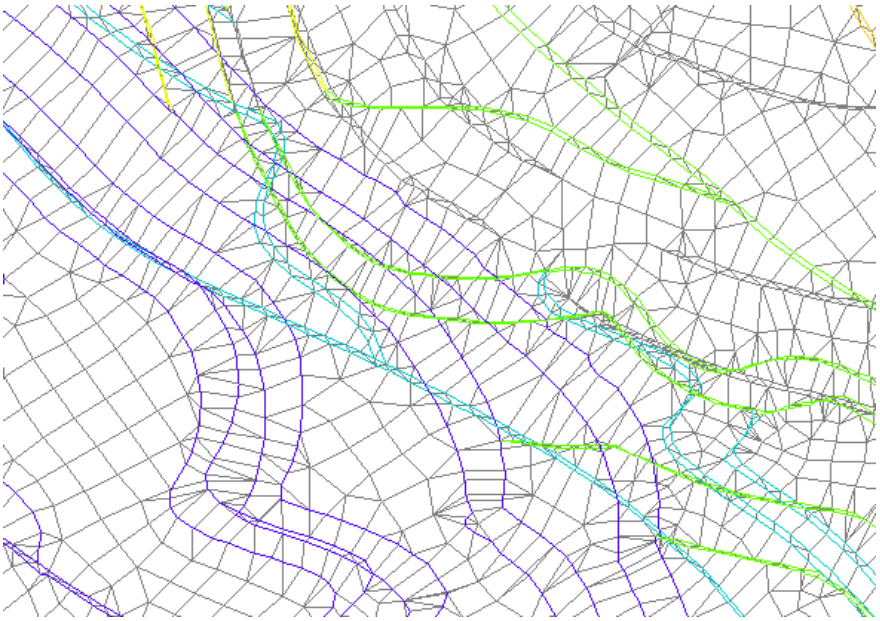

Figure 11: Detail of the Finite-Element-Mesh and assignment of the faults “cut-off lines” in the SPRING model. Faults coloured in blue, cyan, green and yellow.

These faults are later connected across the layers and several parameters are assigned which differ from one fault number to the other. These are the ‘height’ (thickness), the permeability and the porosity. The number after the comma is important for the transfer via the SpringToBox tool as it remarks different kinds of connections that are described in the following section. In general, the SPRING model needs to contain several parameters that are processed within the SpringToBox tool and transferred to the HEATFLOW model. These parameters are:

- KNOT – a defined volumetric flow rate (Neumann boundary condition, Type II BC)
- POTE – a fixed hydraulic head (Dirichlet boundary condition, Type I BC)
- KWER – the hydraulic conductivity kf
- KWEV – the vertical hydraulic conductivity
- SPEI – the effective porosity
- FLAE – the groundwater recharge
- GELA – ground surface elevation (top of the model)
- ZKOR – elevation of the individual geological layers
- STHW and STFW - the head and foot wall of the faults

4.2.3 SpringToBox – Software Adaptations

Based on the model preparation in SPRING, the BoxModel tool SpringToBox is used to transfer the SPRING model into a HEATFLOW model. With this model, a simulation applying the HEATFLOW tool is possible.

Software Adaptions in the SpringToBox tool were necessary. The interface of SpringToBox includes a checkbox for the faults and 'edit boxes' to present e.g. the fracture opening or the minimum thickness of the slices for the three-dimensional BoxModel. The code is written in the Object Pascal programming language Delphi and a program flow chart is given in Figure 13.

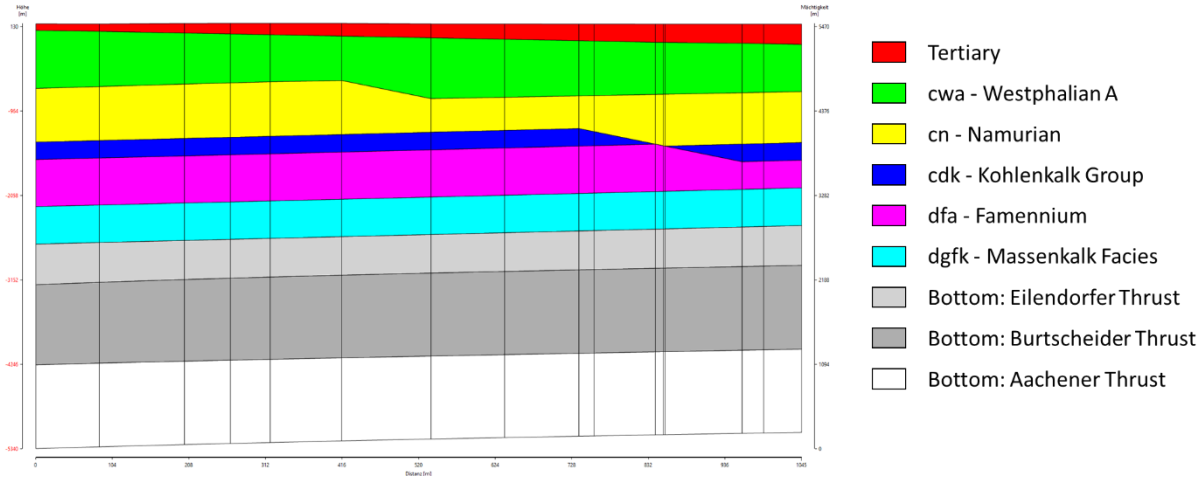

Figure 12: Cross section of SPRING model.

The faults are assigned in SPRING with numbers and separation in head wall (STHW) and foot wall (STFW). A cross section of the model in SPRING with the faults is shown in Figure 12. SpringToBox transfers the numbers of the SPRING model to fault boxes. This fault boxes are elements in HEATFLOW structure that are assigned with certain values such as the fracture opening or the hydraulic permeability. Due to the specific programming in HEATFLOW, this fault elements are located on the edge of the elements, right between two nodes with fault numbers assigned in SPRING. Additional information for the HEATFLOW model are the connections between the elements. We differentiate between geological connections and different types of fault connections. The geological connections are based on the equation:

$$K = k_f * \times \frac{l}{\Delta s}$$

For the hydraulic connection between boxes, which is based on purely geological causes, it must be expected that the water level will not reach the upper edge of the balance cell and that there will therefore be unconfined conditions. For this reason, the through-flow thickness M is constantly recalculated and multiplied during the model run.

The coefficient K has the unit [m/s]. Various options are available in the model for calculating the thickness of the flow. In addition to the variant preferred in MODFLOW (U.S. Geological Survey), of immediately including the thickness in the harmonic averaging of the k_f value and thus calculating the transmissivity straight away, there is the possibility of using the flow thickness from the upstream midpoint. This has proven to be the most stable procedure.

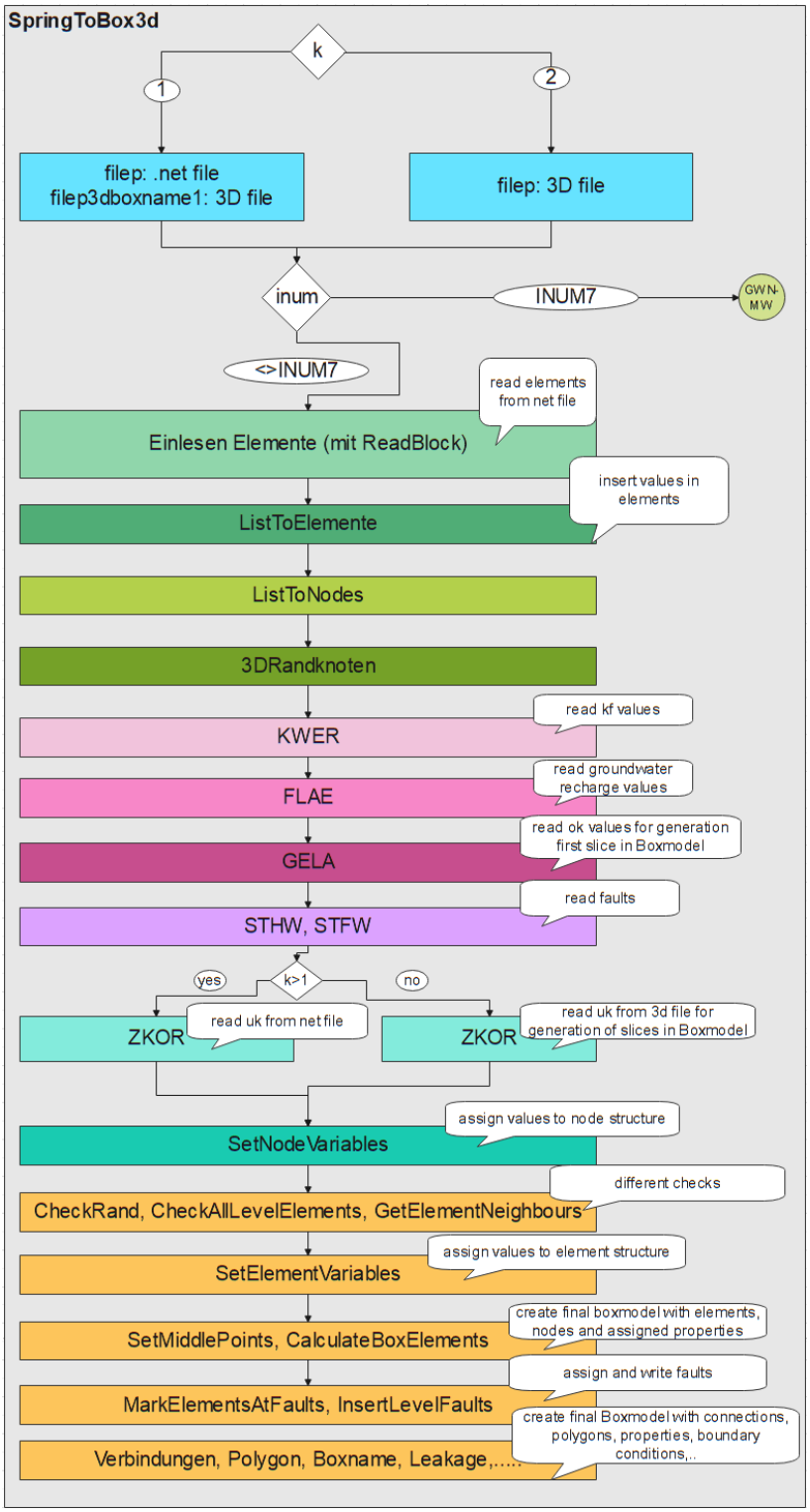

Figure 13: Program flow chart of SpringToBox3d.

In the model the coefficient K is multiplied by the corresponding thickness, which is not known from the outset in the case of unstressed conditions, and again leads to the conductance: L [m²].

The fault connections are simulated with a laminar cubic law and differentiated by overlapping of two layers, located in one layer or head wall to food wall connection as shown in Figure 14.

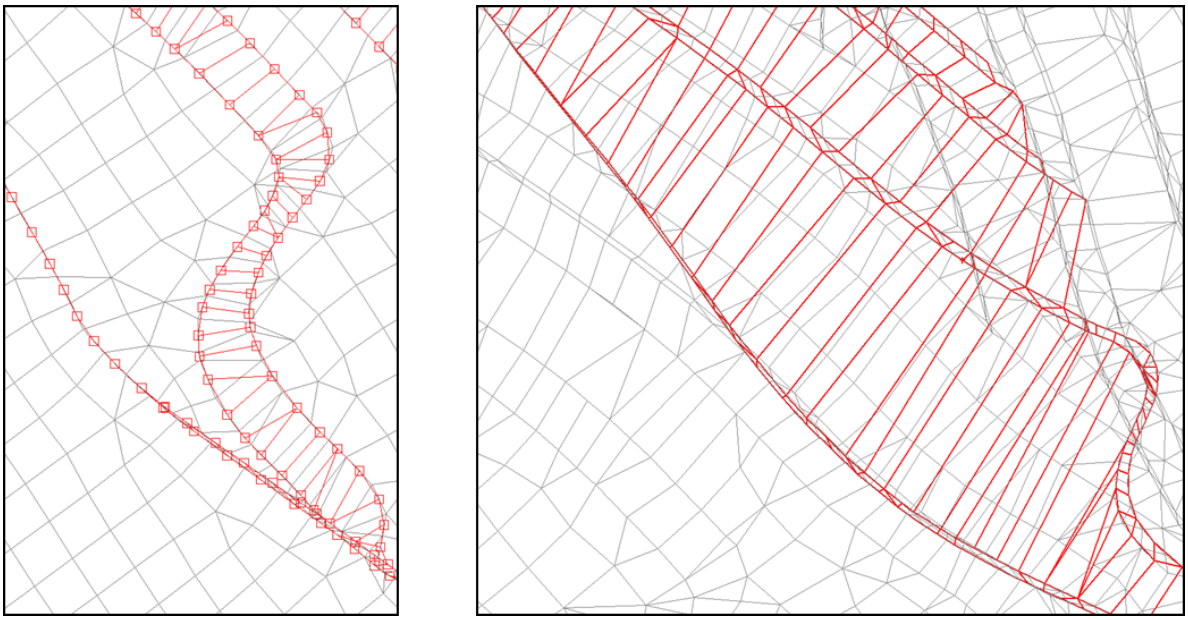

Figure 14: Left: Example of a head wall to foot wall fault connection. Right: Example of a fault connection overlapping layers.

In addition to the special type of connections, there is also an automatic linking of boxes lying one above the other according to the leakage concept.

In turn, the conductance is calculated from the leakage coefficient as follows:

$$L = Leak * \Delta Ag$$

$$Leak - Leakage - Koefficient\ [1/s]$$

$$Ag - horizontal\ area\ between\ superimposed\ boxes\ [m2]$$

4.3 Model set-up and Results

The Weisweiler model consists of ten layers and eight types of fracture zones have been adapted for the HEATFLOW simulation. In Figure 15 the geological sections are shown for the HEATFLOW model as well as the schematic geological model presented in Fritschle et al. 2021 \8\. The HEATFLOW model includes the Tertiary, Westphalian, Namurian, Kohlenkalk, Famennian as well as the Massenkalk horizons. The Eilendorfer, Burtscheider and Aachener thrusts are also included. A top view of the eight fracture zones is shown in Figure 16 and compared to the geological map given by the authors. The detailed information including all available fractures has been characterized by the eight fractures as well as by the thrust faults. The connection of the fractures is shown in Figure 17 in the full HEATFLOW model. Here, the center-cross-sections of the individual geological horizons are shown. The fractures are given with coloured connections. The chosen parameters for the numerical simulations are presented in chapter 6.

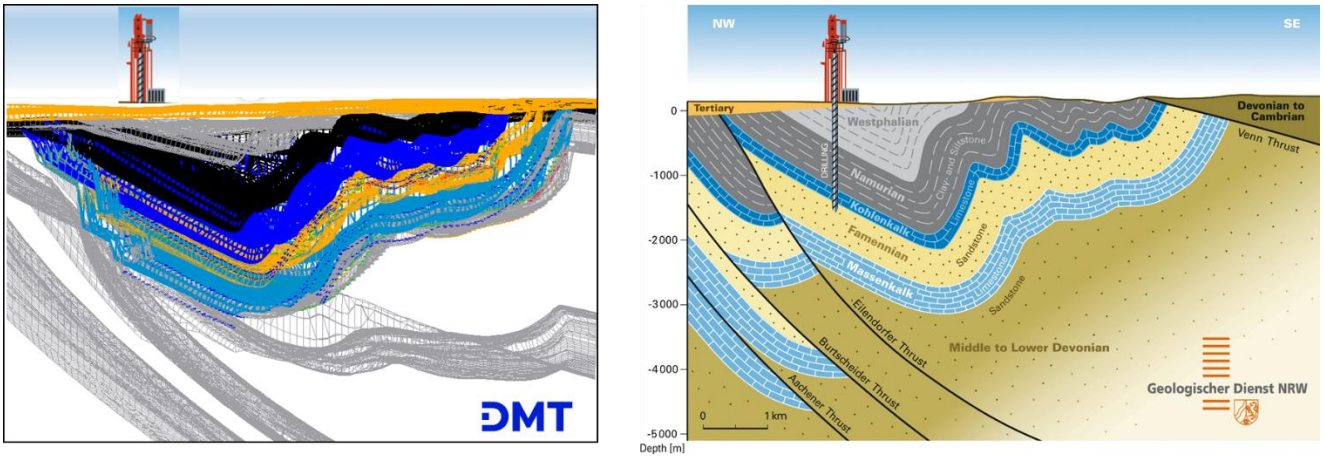

Figure 15: Left: Part of the geological section at the Weisweiler power plant, HeatFlow Model. The model shows a center-cross-section of each of the geological horizons. Right: Schematic geological cross section (Fritschle et al \8\).

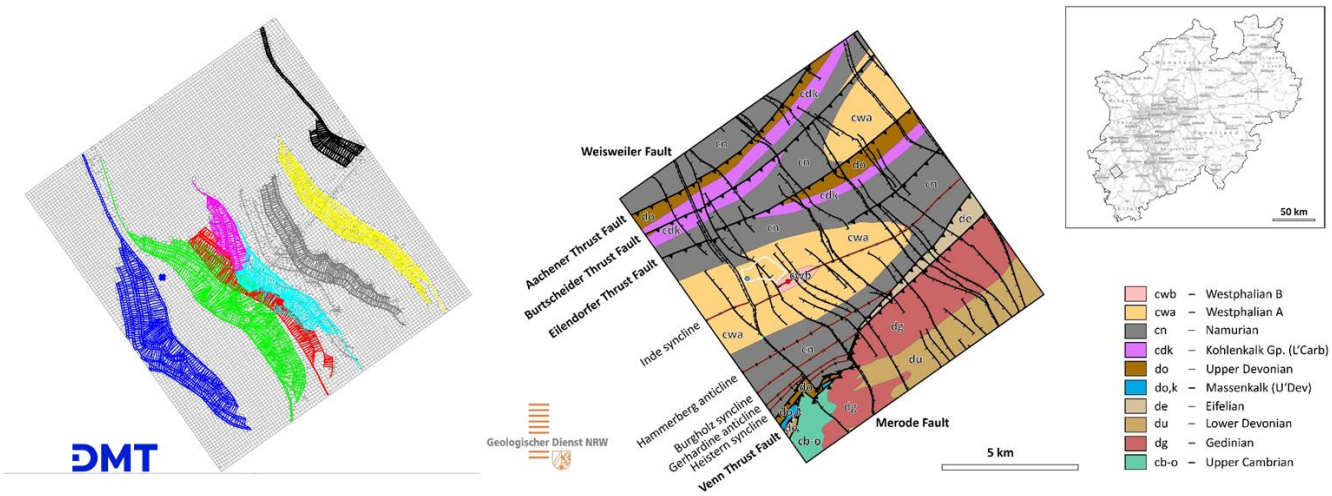

Figure 16: Left: Weisweiler model with fault elements and connections in HEATFLOW, top view. Right: Simplified geological map at the base of the Tertiary including the major structural features (Fritschle et al \8\) including the designated drilling spot for the exploration drilling on the premises of the Weisweiler power plant (blue spot).

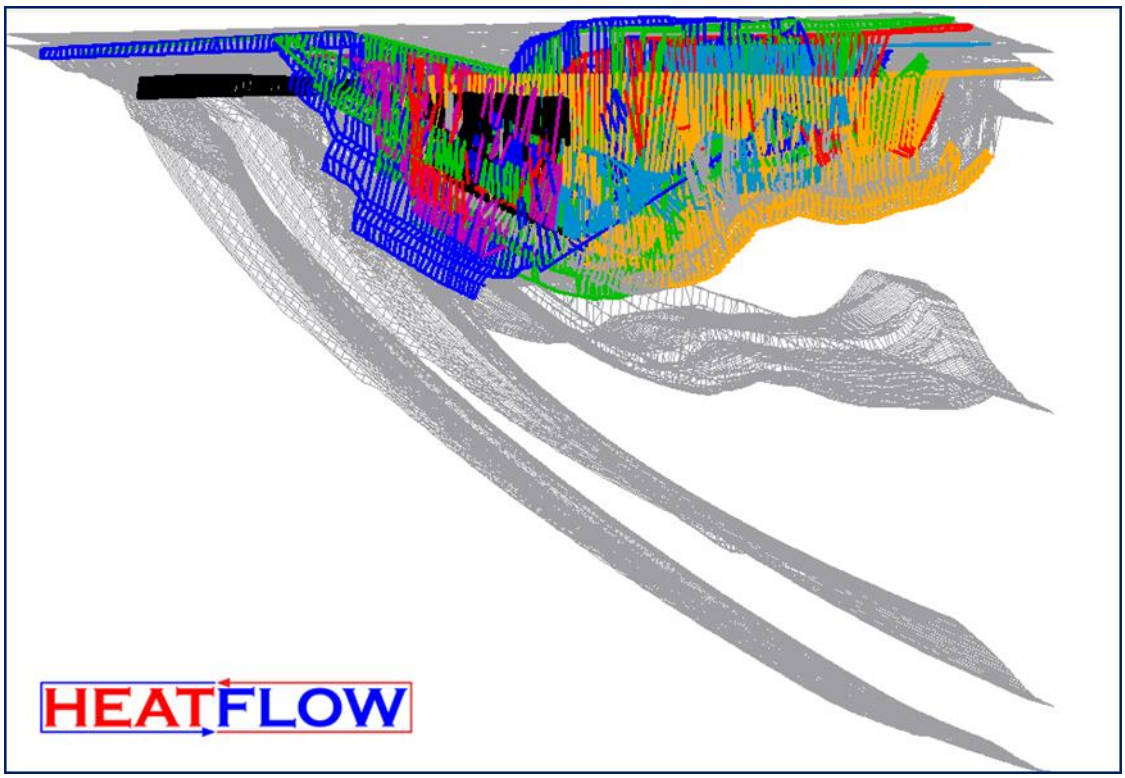

Figure 17: Weisweiler model with fault elements side view, coloured fault connections.

4.3.1 Example – Test phase

To test the general functionality of the simulation tool and the designated model the final input parameter for the scenarios have been modified in the way that the geothermal gradient is 2.45°C/100 m, the flow rate is 100 m³/min and the temperature of the induced fluid is 10°C. As tracer for the mass transport chloride is chosen with 1,800 mg/l for the induced fluid and 1,000 mg/l in the reservoir. Production I in Kohlenkalk level is chosen in the test example (compare Figure 29).

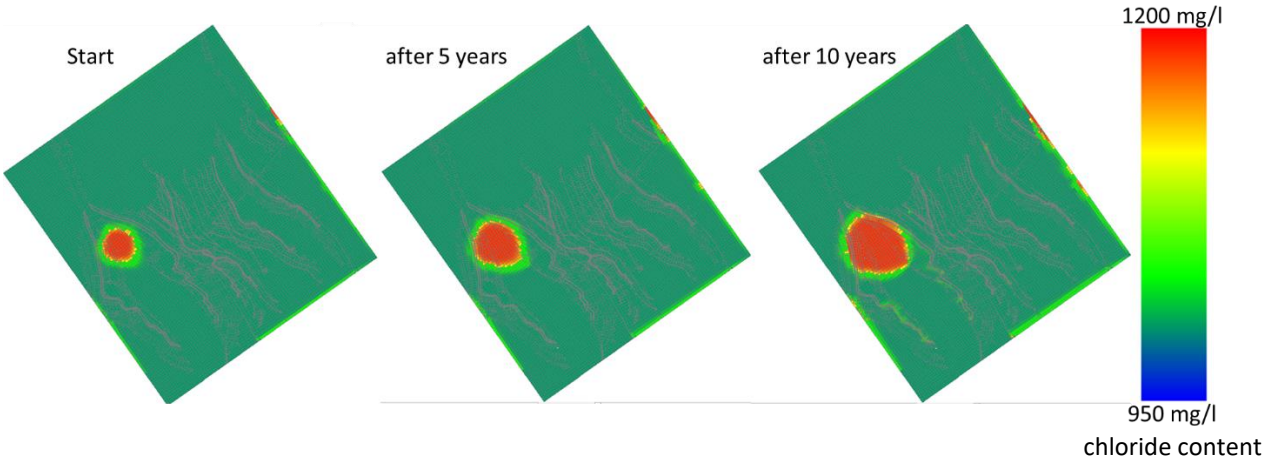

Figure 18: Test case ("Kohlenkalk"). Chloride concentration within ten years.

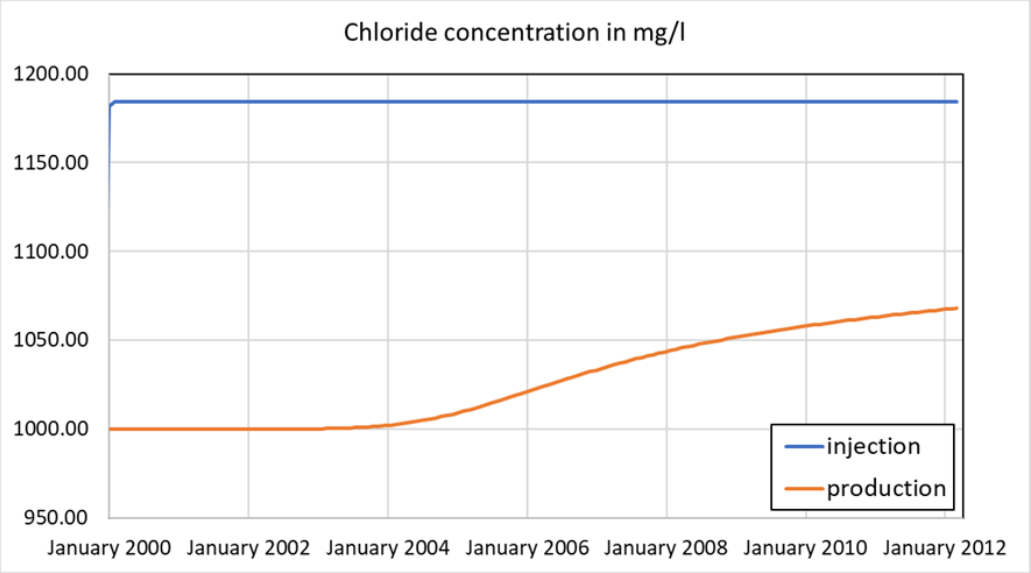

Figure 19: Test case ("Kohlenkalk"). Chloride concentration within twelve years.

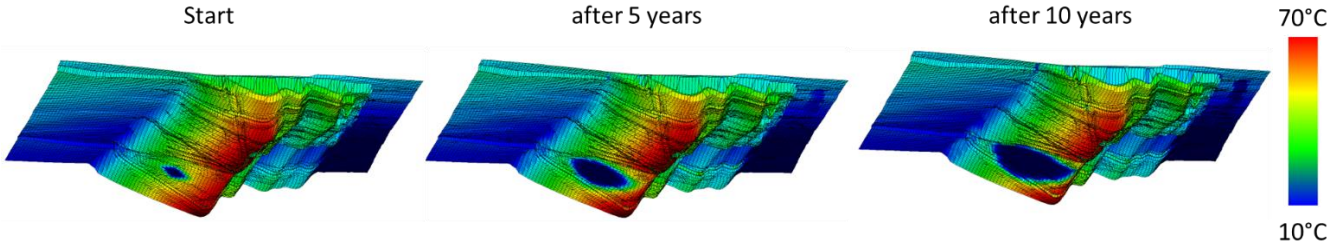

Figure 20: Test case ("Kohlenkalk"). Temperature in the Kohlenkalk after ten years.

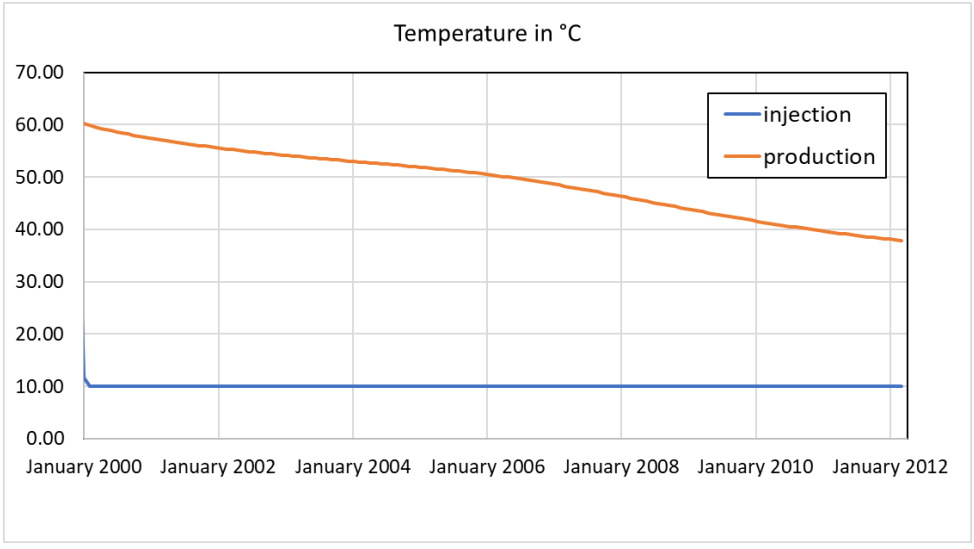

Figure 21: Test case ("Kohlenkalk"). Temperature in test example after twelve years.

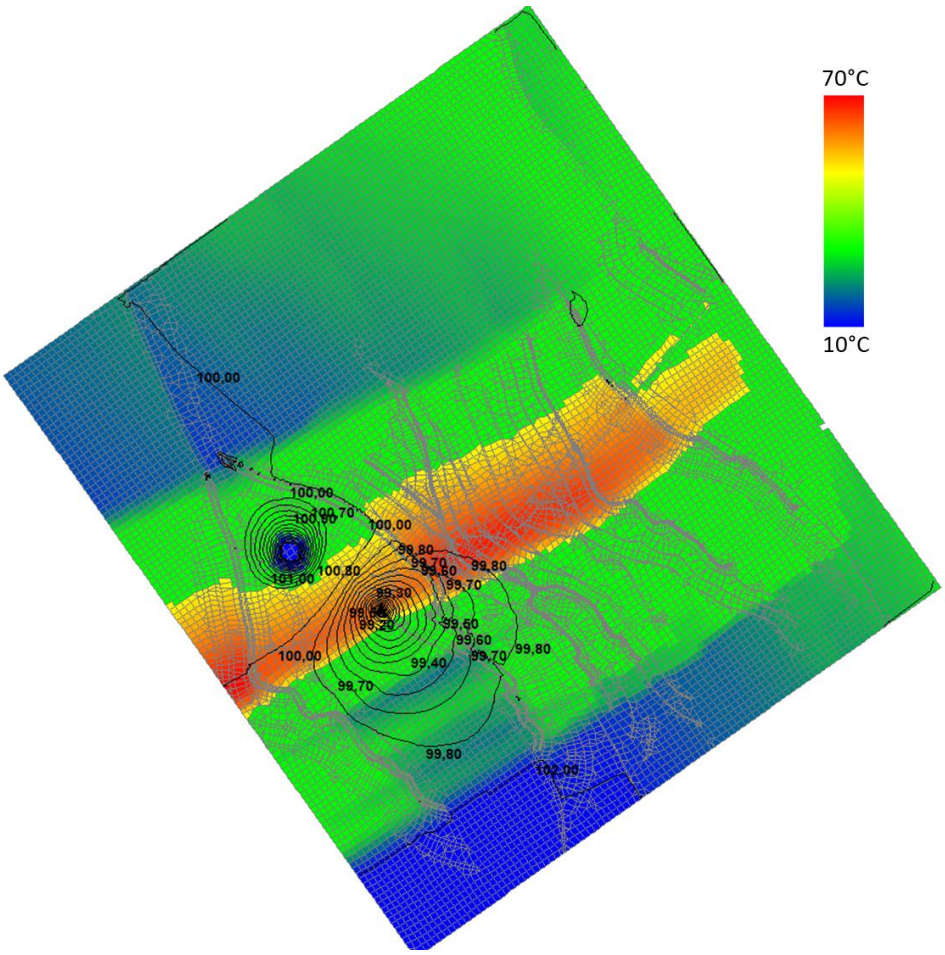

Figure 22: Test case ("Kohlenkalk"). Temperature with isolines after one year.

In Figure 22 the isolines are shown to visualize the area of influence of the injection and production wells. Here, a depression cone can be seen around the production point, with the area surrounding the injection point showing an increase in water level. The isolines and the temperature and chloride concentration pathways after twelve years show that the connection between the injection and production well is very active given such a high flow rate. The chloride concentration shown in Figure 19 starts to rise after four years in the production well. The temperature reacts faster (see Figure 21) as the production fluid temperature starts to decrease just in the beginning of the calculation. The temperature and chloride propagation in the carrier medium after ten years is shown in Figure 18 and Figure 20. A clear increase in the area of influence can be seen. It can also be concluded that the temperature change is concentrated on the Kohlenkalk level and only rarely active in the upper and lower levels. Adaptions of the input parameters are possible in a straightforward process. Hence, it can be inferred that the model simulation is feasible and operates in accordance with the expectations. Therefore, different scenarios have been simulated in the following chapters.

4.4 Scenarios

Two scenarios are chosen for the model simulations: Scenario 1: Kohlenkalk, Scenario 2: Massenkalk reservoir. The input parameters are taken from the comparable geothermal plant in Mol (Belgium) and from the investigations of the DGE-ROLLOUT partner RWE (\2\, \9\). Here, the geothermal gradient is 3°C/100 m, the flow rate is 140 m³/h and the temperature of the induced fluid is 35°C. Production I from Figure 29 is chosen. The scenarios have been investigated under the described assumptions for the input data and numerical model setup.

4.4.1 Scenario 1

In Scenario 1 the injection into the Kohlenkalk horizon is at -1,445.9 m depth and the production, which is approximately 1,500 m from the injection well, is at -1,839.15 m depth (see point I in Figure 29). The geofluid injection temperature is 35°C and the flow rate is 140m³/h. The isolines of the equilibrated fluid in the reservoir are shown in Figure 23.

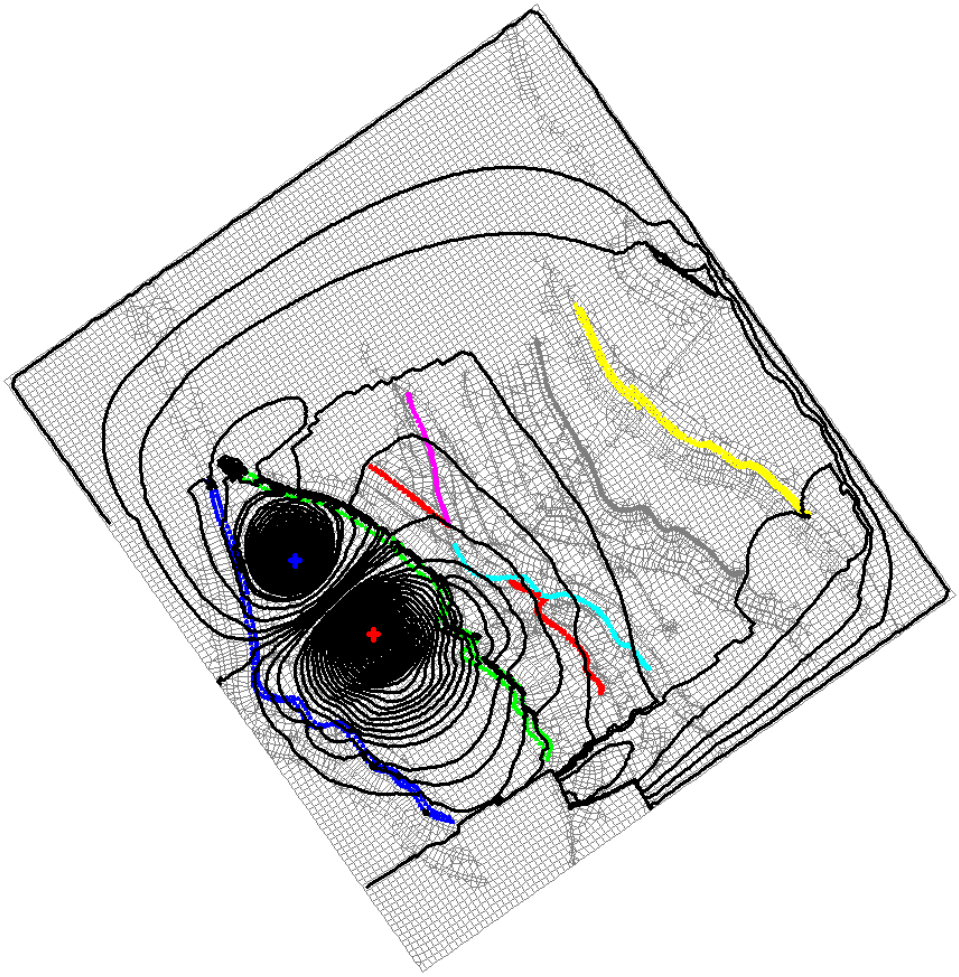

Figure 23: Isolines for Scenario 1 ("Kohlenkalk"). Blue: Injection well, red: Production well.

The resulting temperature profile for up to 100 years is shown in Figure 24. After 100 years, the temperature in a radius of about 500 m around the injection well has cooled down. The main part of the reservoir remains unchanged by the injected fluid even after 100 years of simulation time. Figure 25 shows the temperature change at the injection and production point in the model. The temperature at the production point cools down slightly from the initial temperature of 69.7°C to 63.8°C after 100 years calculation time. It is not expected that this moderate temperature change of about 0.06°C/year will have a large impact on the reservoir, however, the vicinity of the injection well shows a cooling of the reservoir within a radius of about 500 m. The injected fluid and the fluid in the reservoir have the same substance concentration and all modelled substances do not react to such moderate temperature changes. Therefore, chloride cannot be used as a tracer here as in the test example above.

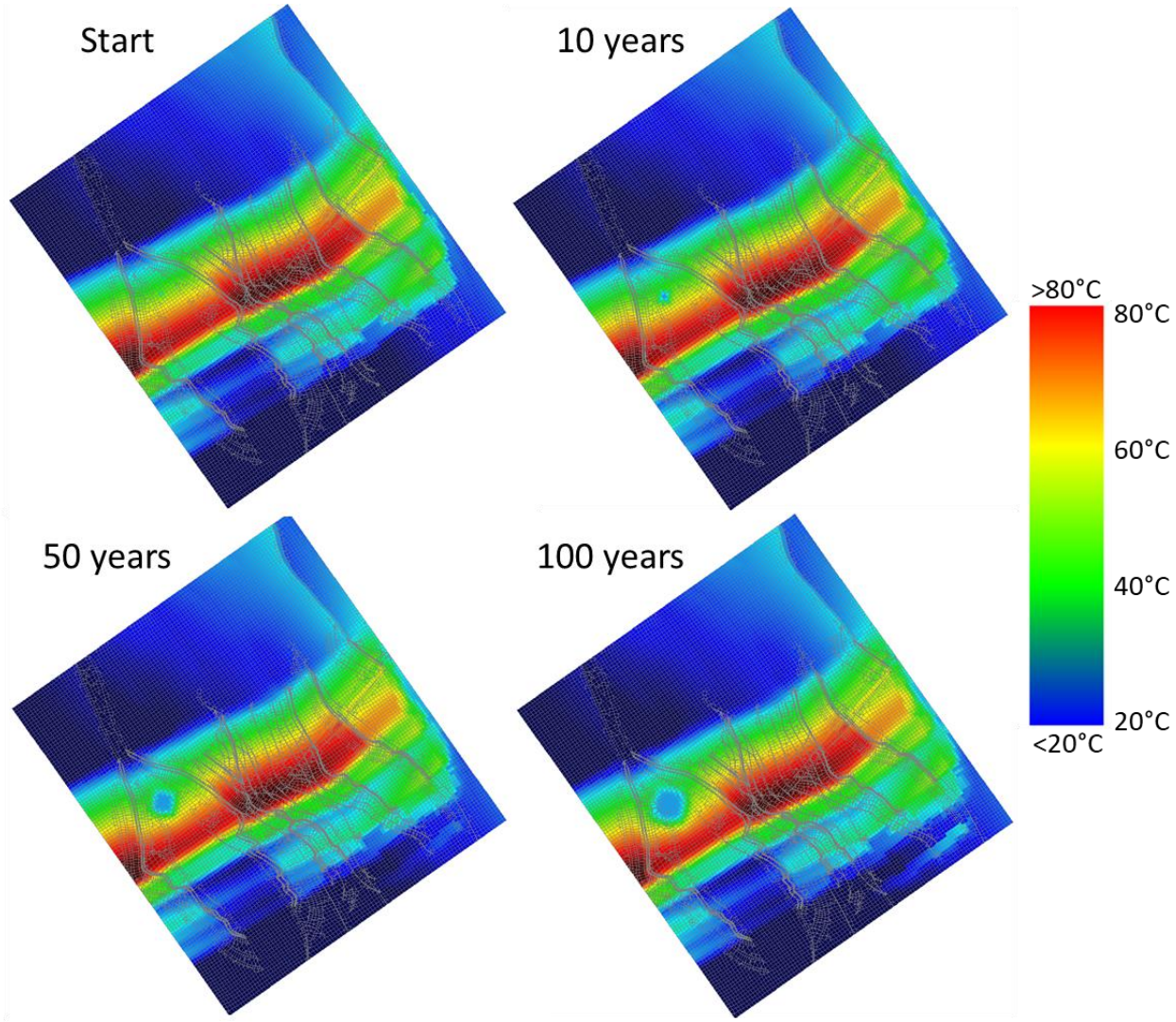

Figure 24: Temperature simulation in the "Kohlenkalk" after 100 years of production for scenario 1 with 35°C injection temperature.

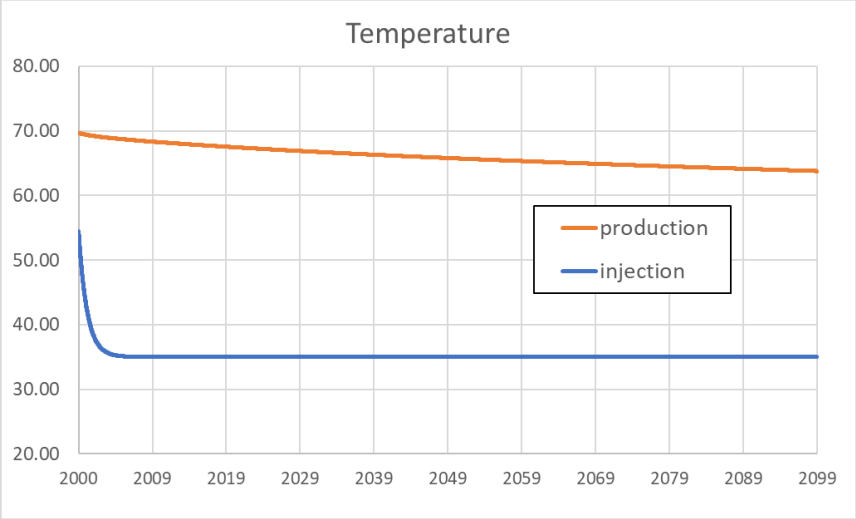

Figure 25: Temperature at injection and production wells in the "Kohlenkalk" formation for Scenario 1 with 35°C injection temperature.

4.4.2 Scenario 2

In Scenario 2, the injection into the Massenkalk layer is at -2,537.6 m depth and production, which is approximately 1,500 m from the injection well, is at -2,905.03m depth (see point I in Figure 29). The geofluid injection temperature is 35°C and the flow rate is 140m³/h. The isolines of the equilibrated fluid in the reservoir are shown in Figure 26.

The resulting temperature profile after 50 years is shown in Figure 27. Here, the rock temperature in a radius of about 300 m around the injection well has cooled down. The main part of the reservoir remains unchanged by the injected fluid even after 50 years of simulation time. Figure 28 shows the temperature change at the injection and production point in the model. After 50 years of calculation, the temperature at the production point cools slightly from an initial temperature of 101.7°C to 100.6°C. This moderate temperature change of about 0.02°C/year is not expected to have a major impact on the reservoir, however, the vicinity of the injection well shows a cooling of the reservoir within a radius of about 300 m. Again, the injected fluid and the fluid in the reservoir have the same substance concentration and all modelled chemical substances do not react on such moderate temperature changes.

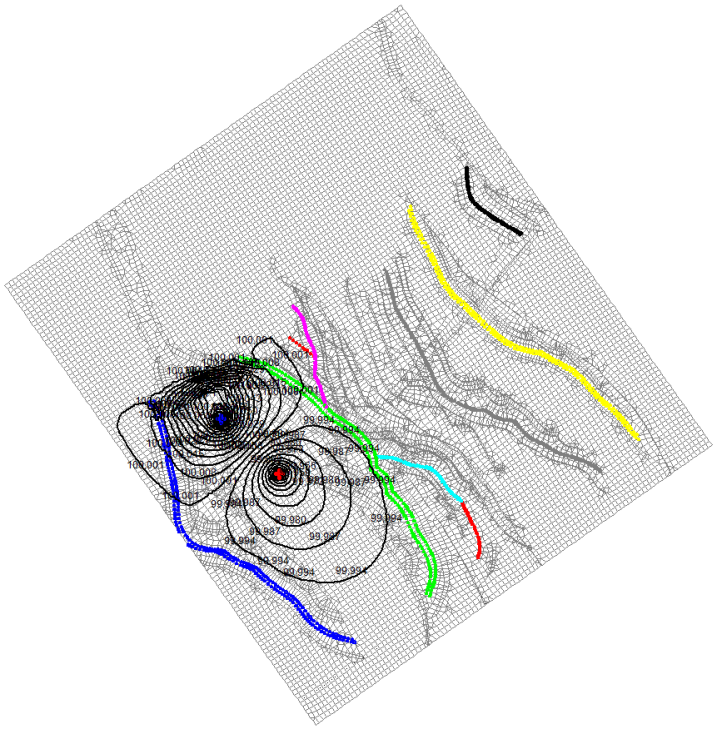

Figure 26: Isolines for scenario 2 ("Massenkalk"). Blue: Injection well, red: Production well

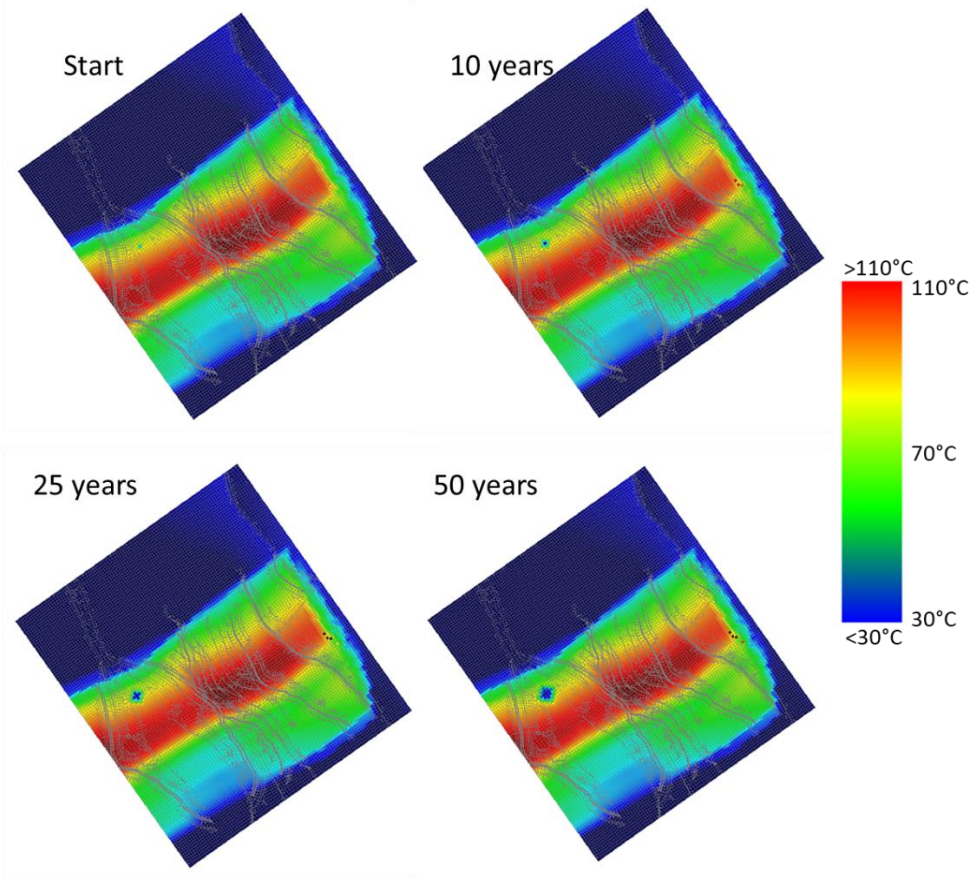

Figure 27: Temperature simulation into the "Massenkalk" after 50 years of production for Scenario 2 with 35°C injection temperature.

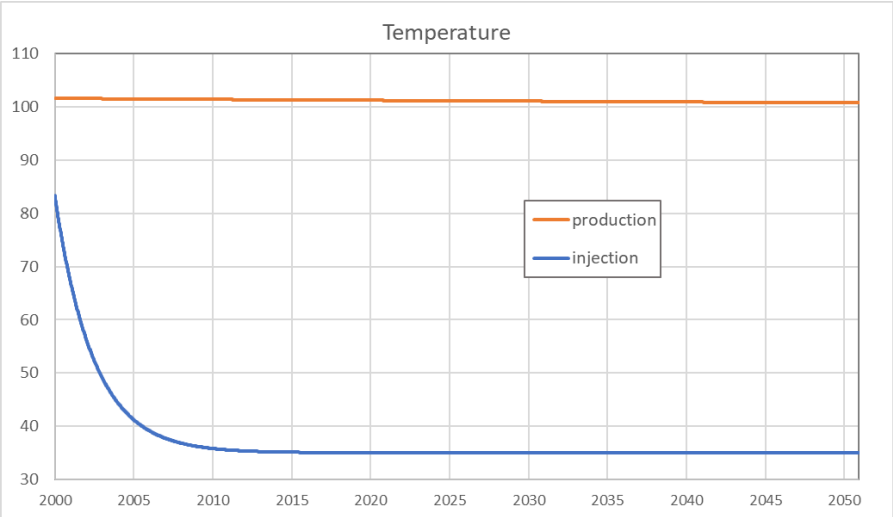

Figure 28: Temperature at injection and production well into the "Massenkalk" for Scenario 2 with 35°C injection temperature.

5 Summary & Recommendations

In the first part of the project DMT simulated and evaluated the possibility of storing geothermal energy in an old mine, modelling summer energy storage and winter energy extraction. Based on the model tests and different setups, a preferred variant can be found, in which the fluid storage temperature is set to 20°C in summer and in winter to 5°C.

In the second part of the project DMT simulated the geothermal characterization of the subsurface of the planned Weisweiler heat plant. Here, different scenarios for a possible reservoir in the Kohlenkalk or Massenkalk horizons were analyzed. The scenarios are based on the preliminary 3D geological subsurface model of the Weisweiler area and the geothermal reservoir characteristics of the deep geothermal power plant in Mol, Belgium.
Based on these available parameters, it can be assumed that the geothermal potential beneath the Weisweiler site is given with a flow rate of 140 m^3/h and a water temperature of 35°C. For Scenario 1 ("Kohlenkalk") the production temperature is around 70°C, whereas Scenario 2 ("Massenkalk") has a production temperature of 101°C. The rate of production temperature reduction is about 0.06°C/year in the "Kohlenkalk" and about 0.02°C/year in the "Massenkalk" scenario. The cooling around the injection well is limited to the near field in both scenarios.
Further investigations should be carried out in which alternative locations for the wells are examined. It is also recommended that the model should be updated once an exploration drilling has been completed on the prospective Kohlenkalk geothermal aquifer at depths less than 1,300 m. Nevertheless, the results indicate that the geothermal potential in the reservoir is given.

6 Attachment

6.1 Parameter

The input data are based on data from the comparable site in Mol with a flow rate of 140 m³/h and a temperature of 35°C. Two scenarios are selected for the model simulations: 1) “Kohlenkalk”, 2) “Massenkalk” reservoir. Following Deliverable T3.4.2 (RWE Power AG) the planned injection and production wells are separated 1,500 m from each other. Under this assumption, the possible locations shown in **Fehler! Verweisquelle konnte nicht gefunden werden.** and Figure 29 were determined. Production well site I is chosen for the model simulations. The hydrogeological parameter for the simulations (see **Fehler! Verweisquelle konnte nicht gefunden werden.**, **Fehler! Verweisquelle konnte nicht gefunden werden.**, **Fehler! Verweisquelle konnte nicht gefunden werden.**) are taken from different sources (\5\, \3\, \8\) and the hydrogeochemical parameters (see **Fehler! Verweisquelle konnte nicht gefunden werden.**) were taken from the comparable geothermal pilot site in Mol (\4\, \5\).

Table 2: Possible location of production wells.

Szenario 1	x	y	z Kohlenkalk (bottom)	z Massenkalk (bottom)	node no.
injection	310923.024	5634979.07	-1445.931	-2537.602	1861
production I	312172.385	5633781.67	-2028.198	-3126.473	1241
production II	312423.81	5634353.13	-2060.652	-3082.516	3354
production III	311933.923	5636322.65	-1255.425	-2193.316	6353
production IV	312656.152	5635446.21	-1875.075	-2710.314	18583
production V	311384.748	5633232.51	-1969.751	-3139.523	1080
production VI	309301.59	5634580.51	-1451.027	-2552.934	1303

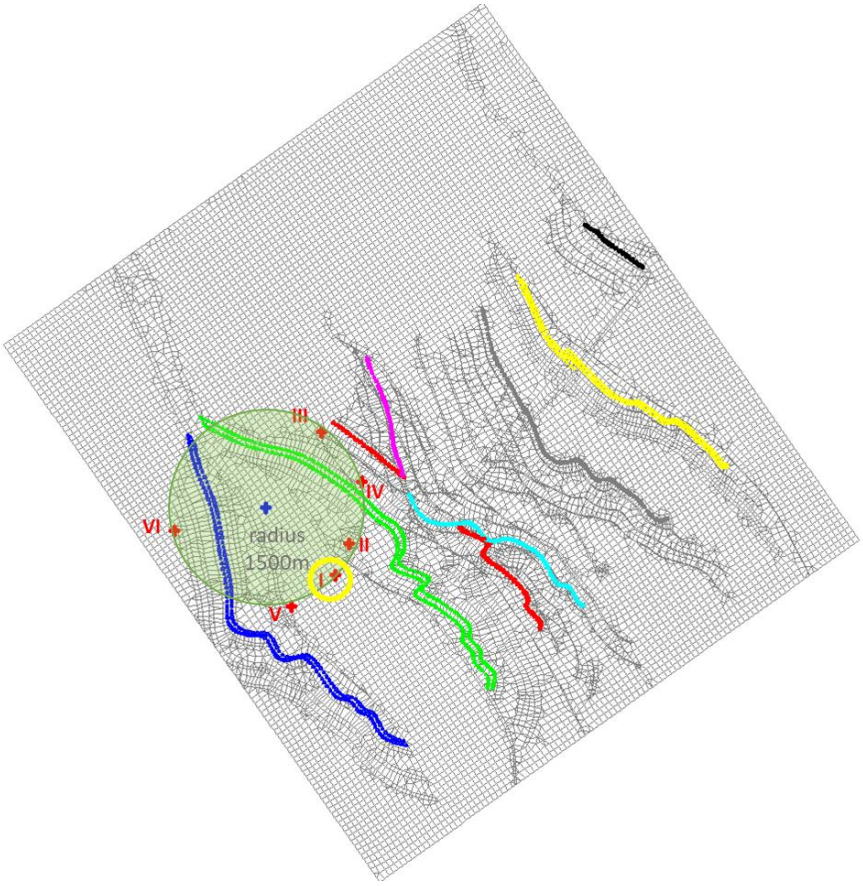

Figure 29: Possible production well locations, yellow: Chosen for model simulation.

Table 3: Parameter for HEATFLOW Simulation.

Parameter for HEATFLOW simulation	
3.0	T-Gradient (geothermal gradient 3°/100 m)
2.0	lambdaSolid [W/m/K = J/s/m/K] thermal conductivity rock
100	W_ue heat transfer coefficient [W/m2/K] (solid-fluid)
1000	cpSolid [J/kg/K] specific heat capacity rock
2000	rhoS [kg/m3] density
10	T [°C] temperature ground level
159	[W/m/K = J/s/m/K] thermal conductivity water
4184.18	[J/kg/K] specific heat capacity water

Table 4: Parameter from Stijn Bos and Ben Laenen \2\.

Parameter	Unit	MOL-GT01-3400m
Na+	mg/l	49800
K+	mg/l	2770
Ca2+	mg/l	9160
Mg2+	mg/l	557
Sr2+	mg/l	396
Ba2+	mg/l	16.8
Fe2+	mg/l	809
Mn2+	mg/l	13.6
NH4+	mg/l	267
Cl-	mg/l	98100
HCO3-	mg/l	1117
SO4 2-	mg/l	323
Br-	mg/l	153
F-	mg/l	<0.88
pH	5.47	5.44
EC	mV	184.8

Table 5: Hydrogeological parameter for the hydrostratigraphic units, source Burs et al \5\.

Hydrogeological parameter for the hydrostratigraphic units			
kf [m/s] - permeability coefficient	**Porosity (effective)**	**permeability**	**Geological unit**
1e-3 -> 1e-2	0.02 -> 0.46	strong permeable	quaternary
1e-5 -> 1e-4	0.01 -> 0.46	permeable	tertiary
6e-7 -> 3e-5	0.01 -> 0.41	low permeable to permeable	Walhorn formation
2e-6 -> 6.4e-4	0 -> 0.36	permeable to strong permeable	Kohlenkalk
1.4e-9 -> 1.4e-4	0.02 -> 0.4	very low permeable to strong permeable	sandstone
1e-5 -> 1e-4	0 -> 0.36	permeable	Massenkalk

Table 6: Parameter for the SPRING model setup.

slice in boxmodel	kwev [m/s]– vertical permeability coefficient	kwer [m/s]– horizontal permeability coefficient	spei – porosity [-]	GD data of Move
1	1.E-05	1.E-05	0.01	tertiary
2	1.E-06	1.E-06	0.15	cwa
3	6.E-07	6.E-07	0.01	cn
4	6.E-04	6.E-04	0.15	cdk
5	1.E-09	1.E-09	0.02	dfa
6	1.E-04	1.E-04	0.03	dgfk
7	1.E-10	1.E-10	0.10	Eilendorfer Thrust
8	1.E-10	1.E-10	0.10	Burtscheider Thrust
9	1.E-10	1.E-10	0.10	Aachener Thrust
10	1.E-12	1.E-12	0.00	
Faults	1e-3	1e-3	0.8	

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List of tables

List of figures

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