EDZ effects on rock chemistry and transport parameters

Chair: Philippe Lalieux - Peter Blümling
MODELLING OXIDISING PERTURBATIONS IN ARGILLACEOUS MATERIAL

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This paper presents the results of a numerical investigation of transient redox conditions in argillaceous material in the context of HLW deep geological disposal. The redox state is a crucial parameter not only for the lifetime of the canisters but also for the migration of radionuclides after canister failure. Since reducing redox conditions prevail in deep underground porous media, the digging of excavations to build the repository will induce an oxidising perturbation in the vicinity of the galleries and tunnels. After emplacement of waste packages and closure of galleries, other processes will control the evolution of the redox conditions such as the corrosion of steel canisters and structures, or the radiolysis of water close to the waste packages. Since reducing conditions are considered favourable for the confining function of the repository, the purpose of this study is to quantify the persistence in time and space of the initial oxidising atmospheric perturbation.

The system to be modelled is quite complex, both in physical and chemical terms. It consists in a argillaceous engineered barrier (EBS) and the zone in the argillaceous host-rock which was mechanically damaged during the excavation work (EDZ). One has ideally to take into account both thermal and hydric transient conditions, because of the significant heat release from waste packages and the initial unsaturated state of the EBS (and, to some extent, of the EDZ). In this study, we nevertheless considered that the system has reached a steady temperature gradient (105°C close to the canister to 65°C at the interface between the EDZ and the unperturbed host-rock) which lasts for the duration of the simulations (~ 100 years). We also considered that the saturation front is stationary during this period and that the porous media is reactive only when it is saturated (saturation > 90%).

The clayey material used in the EBS is the MX80 bentonite, which is essentially composed of Na-montmorillonite, but also contains secondary minerals including pyrite in small amounts. The EDZ composition and properties are based on those of the host-rock in the argillaceous series of the Callovo-Oxfordian at Bure (East of France). The initial water composition in the EBS and EDZ were calculated so that they satisfy equilibrium with respect to the mineral compositions.

In the simulations, the transport of aqueous species occurs only through diffusion and the exchange of matter with the unperturbed site water are allowed. The chemical reactions accounted for include kinetic dissolution and precipitation for minerals and multi-site ion exchange on clay surface for aqueous species.
The results of the simulations show that the key to the reactivity of the system is the dissolution rate of pyrite. In a system of metric size and in the presence of pyrite in the EBS (the only reducing mineral in MX80 bentonite), the oxidising perturbation lasts only for a hundred of years. The persistence of the oxidising perturbation may only be increased if the reactivity of pyrite is somehow inhibited (ca. 200 years at a maximum, due to the diffusion of oxygen into the EDZ). These results are consistent with other studies found in the literature. This means that the corrosion of canisters would essentially take place in reducing conditions. Different formalisms were tested for the pyrite kinetic law, with and without dependence on dissolved oxygen and pH, but the results are not significantly modified. Note also that the simulations were carried out using conservative hypotheses, i.e. that tend to increase the persistence of the perturbation: no steel structures at the interface between the EBS and the EDZ, no reducing bacterial activity, average (low) temperature, … No other parameter was identified that could possibly prevent the oxygen from being rapidly consumed in the system. The only major uncertainty lies in the chemical reactivity of the porous media, and the mineral clay in particular, when complete saturation with water is not reached.
MODELLING OF POREWATER FLOW IN THE VICINITY OF A DEEP GEOLOGICAL REPOSITORY IN OPALINUS CLAY

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INTRODUCTION
Nagra’s recent work for the Swiss high-level radioactive waste disposal programme has concentrated on the assessment of the Opalinus Clay formation located in the Zürcher Weinland of northern Switzerland (Nagra 2002a,b,c). The safety concept relies strongly on the Opalinus Clay as a geological barrier, which, together with the engineered barrier system, ensures that the release of radionuclides into the regional aquifers is low at all times such that resulting doses are well below the applicable regulatory guideline. As part of the geoscientific site characterisation process the emphasis of hydrodynamic modelling has been on the understanding of both the natural, undisturbed groundwater flow in the investigation area and the effects of repository-induced perturbations. The present paper is devoted to the repository-scale modelling, aimed at examining the following aspects:

• Darcy flux through the host rock formation
• changes in the natural flow field by the impact of the excavation disturbed / damaged zone (EDZ) around the backfilled tunnels
• effects of properties of the engineered barriers (backfilled tunnels, tunnel seals, shaft seals)

The impact of both the EDZ and the backfilled shafts and tunnels on porewater flow around the repository was assessed by systematic case studies (conceptual uncertainties) and sensitivity analyses (parameter sensitivity).

MODEL SET-UP AND MODELLING RUNS
The repository-induced perturbations were assessed with a 3-D repository model embedded in a local-scale groundwater model (Nagra 2002a). The lateral extension of the repository model is 3.8 × 2.2 km², in vertical direction it comprises the host rock formation and the adjacent hydrogeological units. All tunnels and caverns of the repository, including sealing structures were explicitly modelled in great detail. The EDZ was represented as a composite structure consisting of two concentric shells. The thickness of the shells depends on the tunnel radius and on the orientation of the tunnel axis relative to the principle directions of rock stress.

A reference case was defined, representing the most plausible model configuration with respect to geometry, parameters, boundary and initial conditions. More than 20 variations of the reference case were assessed, aimed at quantifying the model sensitivity with respect to individual component properties. In the reference case, values of $1 \times 10^{-13}$ and $2 \times 10^{-14}$ m/s were assigned to the horizontal and vertical hydraulic conductivity of the Opalinus Clay, respectively. An enhanced axial conductivity of the inner and outer zone of the EDZ was assumed with K-values of $1 \times 10^{-12}$ and $5 \times 10^{-13}$ m/s, respectively. According to the EBS design specifications the backfill of the access and construction tunnels exhibits a conductivity of $5 \times 10^{-11}$ m/s. A K-value of $1 \times 10^{-13}$ m/s was assigned to the seal sections and the bentonite backfill of the disposal tunnels. The demand for robust assessment of the safety functions of the multi-barrier system necessitated the use of conservative parameters in the sensitivity runs. For this reason, the conductivity of the EDZ was varied in a range of six orders of magnitude and, in some cases, the barrier function of
the seal sections was completely disabled. Further sensitivity runs evaluated the impact of porewater overpressures in the host rock formation on the flow conditions around the backfilled tunnels.

RESULTS AND CONCLUSIONS
Simulations of the undisturbed hydrogeological system (i.e. without repository) indicate a vertical (Darcy) flux of $2 \times 10^{-14}$ m/s upwards through the host rock into the adjacent Wedelsandstein. This corresponds to a total volumetric flow through the footprint of the repository in the order of 1 m$^3$/a. Consideration of the backfilled underground excavations does not significantly change the flow conditions, when the reference case is considered. The magnitude of flux into the Wedelsandstein is indistinguishable with respect to the undisturbed system, except for the immediate vicinity of the access ramp, where the Darcy flux is slightly enhanced by a factor of three. Further cases were investigated assuming higher conductivity of the seals ($5 \times 10^{-12}$ m/s); even a complete loss of barrier function of the main seal was examined. Notably, in none of the cases the local values of Darcy flux into the Wedelsandstein exceeded $2 \times 10^{-12}$ m/s.

An increase of the EDZ conductivity gives rise to marked changes of the porewater flow field around the backfilled excavations, because the EDZ starts draining the host rock formation. When the K-value of the EDZ exceeds $10^{-10}$ m/s the hydraulic conditions on the repository level are no more characterised by predominantly upwards directed flow, but the flow trajectories are concentrating along the backfilled tunnels. The length of the flow paths from the emplacement tunnels through the host rock into the Wedelsandstein increases substantially. The alignment of the flow field along the excavations stabilises, when the EDZ conductivity exceeds a value of $10^{-9}$ m/s. Even for the extreme case with $K_{EDZ} = 1 \times 10^{-6}$ m/s the total volumetric flow exfiltrating into the Wedelsandstein is less than 2 m$^3$/a.

Conclusions from repository-scale modelling are summarised as follows:
• the overall barrier function of the disposal system is guaranteed by the low permeability of the intact host rock, preventing any marked vertical porewater exchange between the local / regional aquifer systems. The estimated total volumetric flow exfiltrating into the Wedelsandstein is in the order of 1 - 2 m$^3$/a, irrespective of the hydraulic properties of the EDZ and the performance of the engineered barriers.
• On the repository level, the EDZ around the backfilled tunnels may substantially change the flow field. Enhanced EDZ conductivities give rise to marked prolongation of the exfiltration paths from the emplacement tunnels into the Wedelsandstein.

References:


MODELLING OF GROUNDWATER FLOW ALONG THE EXCAVATION DAMAGE ZONE OF A TUNNEL IN THE OPALINUS CLAY

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INTRODUCTION

In low permeability rocks, such as the Opalinus Clay (NAGRA 2002) of Northern Switzerland, fractures in the Excavation Damage Zone (EDZ) around emplacement tunnels may create a network of discrete pathways for fluid migration. This abstract describes work to develop groundwater flow models of the EDZ around tunnels in an underground research laboratory which account in a realistic way for the observed hydraulic, geological and geomechanical characteristics of the EDZ.

EDZ AT MONT TERRI ROCK LABORATORY

Observations from boreholes and tunnels at the Mont Terri Rock Laboratory (Martin & Lanyon 2003) have identified four failure modes:

• Stress-induced breakouts;
• Extensile fracturing;
• Bedding plane slip;
• Swelling and softening.

Breakouts and extensile fracturing occur as the excavation (or borehole) is made, whereas slip and swelling both show time and moisture dependent behaviour. The onset of swelling and slip can be limited by controlling humidity and excluding water from the excavation. Martin and Lanyon (2003) suggest a model for the EDZ at Mont Terri as shown in Figure 1 with zones of extensile fracturing (identified by a deviatoric stress criterion) and zones of potential bedding parallel slip. Brittle extensile fracturing is commonly seen in excavations around hard rocks (e.g. Martin et al 1997), while the bedding slip zone is similar in structure to that described by Økland & Cook (1988) based on laboratory tests simulating deformation behaviour of high angle boreholes in bedded shales.

\textbf{Figure 1}: Concept for the EDZ around the New Gallery at Mont Terri with stress induced fracturing in tunnel side walls and slip zone above and below the tunnel. Vertical cross-sections normal and parallel to the tunnel axis.
The results from Mont Terri have been extended to the situation expected at a hypothetical repository at 500m depth in the Zürcher Weinland where the stress field and orientation of bedding planes will differ from those at Mont Terri (NAGRA 2002).

MODELLING OF GROUNDWATER FLOW IN THE DISCRETE FRACTURE NETWORK OF THE EDZ

A structural model of the EDZ around an emplacement tunnel was developed on the basis of field observations and the results of coupled hydromechanical models. The structural model contained four classes of features:

- Extensile fractures in the tunnel sidewalls (see Figure 1)
- Disturbed bedding planes within the bedding slip zone (Figure 1)
- Highly disturbed bedding planes, associated with deformation zones predicted by the geomechanics modelling and observed in the work by Økland & Cook (1988);
- Bounding and inner shear fractures associated with the bedding slip zone.

The different classes were implemented within CONNECTFLOW, a hybrid discrete fracture network / continuous porous medium (DFN/CPM) groundwater flow code. A DFN representation of the EDZ is shown in Figure 2. EDZ effective conductivity and flow path geometry have been studied within the model by applying pressure gradients parallel to the tunnel axis. Sensitivity studies demonstrate that the effective conductivity along the EDZ is largely determined by the transmissivity of the bedding fractures, while locally transmissive sidewall fractures have a relatively minor effect.

Figure 2: CONNECTFLOW EDZ 20m tunnel section model: a) Fracture elements coloured by log-transmissivity b) Flow pathways (blue) and fracture traces coloured by flux (gradient parallel to tunnel).

RESULTS

The studies performed so far have used fracture properties as measured at Mont Terri. Recent model developments are focussing on the implementation of fracture closure mechanisms due to swelling of the buffer and self-sealing processes, which may result in significant changes in fracture properties. Mechanical and geochemical self-sealing processes have been observed in dedicated experiments at Mont Terri. The results from these experiments will be used to test the model developments.

References:


EFFECT OF EXCAVATION INDUCED FRACTURES ON RADIONUCLIDE MIGRATION THROUGH THE BOOM CLAY (BELGIUM)

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In Belgium, the Boom Clay at a depth of 200 m below surface is being evaluated as a potential host formation for the disposal of high-level nuclear waste. In order to investigate this option, an underground research facility composed of two access shafts and a 200 m long gallery was excavated in the Boom Clay for research purposes (HADES-URF). Around the gallery, excavation induced fractures are observed. The majority of these fractures are approximately parallel planes with an average spacing of around 70 cm, a strike approximately perpendicular to the tunnel axis and a dip between 30° and 70°. Fracturation and self-sealing processes in Boom (and Opalinus) Clay were studied in the EC SELFRAc project (EC contract FIKW-CT2001-00182). The research performed in the framework of this project shows that the excavation induced fractures around the connecting gallery are limited to a zone of 1 m. This gallery was excavated using an industrial technique and with minimal radial convergence. Moreover self-sealing processes, which will further limit the influence of these fractures, have clearly been demonstrated in laboratory and in-situ experiments.

The potential effect of these excavation induced fractures on the radionuclide migration through the clay is investigated in this study under the conservative assumption that no self-sealing occurs. A hydrogeological model of the clay is built with a radionuclide source in the middle of the clay surrounded by different fracture configurations. The radionuclide flux through the upper and lower boundaries of the clay into the surrounding aquifers is calculated and compared for different fracture configurations.

The hydrogeological model is a local 3D model of the 100 m thick Boom Clay. The vertical boundary conditions for groundwater flow are zero flux boundary conditions since the hydraulic gradient is vertical. The horizontal boundary conditions for groundwater flow are specified head conditions. The specified head at the upper boundary is 2 m higher than the specified head at the lower boundary since the downward vertical hydraulic gradient in the Boom Clay is approximately 0.02. The boundary conditions for transport at the upper and lower boundaries are zero concentration boundary conditions since the hydraulic conductivity contrast between the clay and the aquifers is so large that solutes reaching the aquifers are assumed to be flushed away by advection. The transport processes that were taken into account in the model are advection, dispersion, molecular diffusion, linear and reversible sorption and radioactive decay.

This local 3D hydrogeological model including different fracture configurations was run with FRAC3DVS, a simulator for three-dimensional groundwater flow and solute transport in porous, discretely-fractured porous or dual-porosity formations. The fractures were modeled as discrete planes with a saturated hydraulic conductivity proportional to the square aperture.
Two types of fracture configurations were inserted around the disposal galleries in the model. For the first type, the properties (extent, aperture, spacing, dip and strike) of the fractures are drawn stochastically from the probability distributions of the properties of the fractures observed around the previously excavated galleries, assuming that the fractures around the future disposal galleries in the Boom Clay will probably have similar properties. These fracture configurations are considered to be realistic although in this study it is conservatively assumed that no self-sealing occurs. The model was run for a large number of stochastically drawn fracture configurations and compared to a model without fractures. These calculations showed that the radionuclide fluxes through the clay are not significantly influenced by these fractures.

For the second type of fracture configurations, the fracture properties are varied over a much larger range. Fractures with much higher values of fracture extent, aperture, dip and frequency are modeled. With these fracture configurations, the critical values of the fracture parameters are determined. If the fracture extent, aperture, dip or frequency is larger than critical value, the fractures have a significant effect on the radionuclide fluxes through the clay. These critical values can be considered for the design of the waste disposal concept.