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THREE-DIMENSIONAL ANALYSES OF COMBINED GAS AND NUCLIDE TRANSPORT IN A REPOSITORY CONSIDERING COUPLED HYDRO-GEOMECHANICAL PROCESSES

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ABSTRACT

To study the coupled hydro-geomechanical processes and their influence on gas and nuclide transport in a two-phase flow configuration in a porous medium, a linear coupling of the hydrodynamic code TOUGH2 and the geomechanics code FLAC3D is described and applied to analyze three-dimensional isothermal gas and nuclide transport in a repository for nuclear waste in a deep geological rock formation like clay rock or rock salt. According to stress-dependent hydrological properties such as porosity, permeability and capillary pressure, the influence of coupled processes on two-phase flow can be relevant. The coupled analyses can be applied to quantify the safety margin related to hydro-fracturing due to fluid pressure build-up.

INTRODUCTION

To assess the long-term safety of a repository for nuclear waste in a deep geological rock formation, such as clay rock, fractured hard rock or rock salt, often a groundwater or brine flow into the repository is postulated. The water or brine can react with the radioactive waste or with its containers and can gradually disassemble them. The radioactive substances after being dissolved in the liquid phase can be transported out of the repository and subsequently can be released into the geosphere. The fluid flow and nuclide transport can be enhanced by gas generation, mainly hydrogen produced due to corrosion of metallic materials, at least within the repository building and possibly also in the host rock. The pressure build-up due to gas generation can also influence the geomechanical behavior of the filling and sealing materials and host rock. The transient stress situation, especially if the fluid pressure approaches the lithostatic pressure, can reactivate an unfavorably oriented fault or can lead to new fracturing. This can in turn affect the hydro-geological properties, chiefly porosity, permeability and capillary pressure of the host rock.

To study the coupled hydro-geomechanical processes and their influence on gas and nuclide transport in a two-phase flow configuration, TOUGH2 and FLAC3D are linearly coupled as a first order approximation to estimate the impacts of the coupled processes. This linear coupling is based on the detailed sequential coupling suggested in (Rutqvist et al. 2002). FLAC3D is developed for rock and soil mechanics and can also handle some features of the thermal-hydrologic-mechanical processes for single-phase flow but not for two-phase flow situation (Itasca 2002).

Within GRS, the TOUGH2 code has been modified to study gas, heat and nuclide transport under various conditions in one-, two- and three-dimensional configurations. For instance, in Javeri (2000), combined gas and nuclide transport in a two-dimensional repository in rock salt is analyzed with TOUGH2 including variable brine fraction and rock convergence and also considering porosity and permeability of crushed salt depending upon pressure and rock convergence without performing geo-mechanical analysis. In Javeri and Mielke (2001), mechanical stability and integrity of the rock salt following an excavation of disposal chambers are investigated using the mechanical code ADINA but neglecting hydrological processes. Hence, this paper extends the previous analyses of separate treatment of hydrological and mechanical processes. The main objective of the present scoping analysis is to develop a procedure that allows the study of coupled hydro-geomechanical processes at least in an elementary but reasonable manner.

HYDROLOGICAL ANALYSIS WITH TOUGH2

The computer code TOUGH2/EOS7 (Pruess 1991a; 1991b) is employed to analyze gas and nuclide transport in two-phase flow conditions in a three-dimensional porous medium. For numerical simulation, the region to be modeled is discretized into volume elements. The conservation equations are solved simultaneously with the integral finite difference method. The scalar quantities like pressure and temperature are determined at the center of the elements and the vector quantities such as velocities and mass fluxes are determined at the interfaces of the elements.

MECHANICAL ANALYSIS WITH FLAC3D

FLAC3D is a three-dimensional explicit finite difference code for engineering mechanics computation and can describe the behavior of structures built of soil, rock or materials that undergo plastic flow when their yield limits are reached. Materials are represented by polyhedral elements within a three-dimensional grid that is adjusted by the user to fit the shape of the object to be modeled. Each element behaves according to a prescribed linear or non-linear stress/strain law in response to applied forces or boundary constraints. To analyze coupled processes, fluid or pore pressure can be prescribed by invoking the fluid configuration and the mean effective normal stress can be calculated as:

$\sigma_{mean} = (1/3)(\sigma_1 + \sigma_2 + \sigma_3), \quad \sigma_{mean,eff} = \sigma_{mean} + p,$

For the analysis of coupled thermal-hydrologic-mechanical processes, it is to be noted that the displacements, total stresses, pore pressure and temperature are calculated at the grid points (corner nodes of a zone) and the principal stresses and the average pore pressure at the center of a zone.

COUPLING OF TOUGH2 AND FLAC3D

The essential assumption for the coupling of TOUGH2 and FLAC3D is that the two codes are executed on an identical numerical grid. The number of FLAC3D zones and the number of TOUGH2 elements must be equal (Fig. 1). In (Rutqvist et al 2002) a detailed procedure is described to couple TOUGH2 and FLAC3D sequentially to study two-phase flow behavior in a porous sedimentary rock and in a highly fractured hard rock including the impacts of stresses on the hydrological properties. In their procedure, which assumes that TOUGH2 and FLAC3D are executed in an environment of the same operating system, the key parameters and data such as pressure and temperature are transferred from TOUGH2 to FLAC3D and stresses are transferred from FLAC3D to TOUGH2 at every time step. This rather laborious procedure results in a tight sequential coupling, which can be relevant if the hydrological parameters depend strongly on mechanical behavior.

Here, to limit the computational efforts, a simpler procedure is suggested to couple TOUGH2 and FLAC3D. The following linear scheme, based on the sequential approach of (Rutqvist et al. 2002), does not presume that the two codes are running in an environment of the same operating system. This linear coupling consists of three steps (Fig. 2):

Step one: Hydrological analysis: As usual, a complete TOUGH2 run up to the end of the problem time is carried out with hydrological parameters which do not depend on stresses, and the distribution of pressure and temperature are saved for all TOUGH2 elements and time steps.

Step two: Mechanical analysis: In the beginning of the FLAC3D run, the complete pressure and temperature distributions computed by TOUGH2 are read for all elements and all time steps. Since the TOUGH2 mesh uses one center point within an element to determine pressure and temperature in an element, and FLAC3D grid points for temperature and pressure are located at the corners of the elements, data have to be interpolated from mid-element of TOUGH2 to corner grid points of FLAC3D. At each time step of TOUGH2, the volume-averaged pressure at all grid points n of FLAC3D is determined as:

$p_n = [\sum p_k V_k] / \sum V_k.$

where k are the centers of the zones around n. In the same manner, the temperature at the grid points of FLAC3D can also be calculated. This relation represents one possible scheme to compute the pressure at the grid points. Depending upon the problem, other interpolation schemes could also be considered. After prescribing the pressure at all grid points at each time step of TOUGH2, the stresses are computed with FLAC3D. At the end of the mechanical analysis for all time steps of TOUGH2, the distributions of input fluid pressure, principal stresses and the mean effective normal stress for all zones or elements and all time steps are saved and can be interpreted as tabular functional relationships between fluid pressure and stress:

$\sigma_{principal,j}(t,i) = f[p(t,i)], \quad \sigma_{mean,eff}(t,i) = f[p(t,i)].$

Step three: Hydrological analysis with variable properties: In the beginning of this modified TOUGH2 run using basically the same input data of step one, the complete distributions of the input pressure for step two, and corresponding output principal and effective stresses computed by FLAC3D are read. Since these quantities are determined at the center of the zone, they can directly be allocated to the corresponding elements of TOUGH2 without performing any spatial interpolation. Now, at each time step of TOUGH2 employing tabular functional relations between fluid pressure and stress for each element of step two, corresponding stresses for the new pressure are determined, if required, considering appropriate interpolation. Subsequently, porosity, permeability and capillary pressure for all elements are calculated as functions of mean effective stress at each time step. Usually, these coupling functions are highly non-linear empirical relations and should be determined considering site-specific data. Here, for instance, the following functions are introduced:

$\Delta\sigma_{mean,eff} = \sigma_{mean,eff}(t) - \sigma_{mean,eff}(t = 0),$

$\varphi_0 = \varphi(t = 0), \quad k_0 = k(t = 0),$

$\varphi = \varphi_0 \exp(a\, \Delta\sigma_{mean,eff}), \quad k = c\, \varphi^b,$

$p_{cap} = p_{Gas} - p_{Liquid} = p_{cap}(S_{Liquid})[(k_0\varphi)/(k\varphi_0)]^{1/2},$

where a, b, c are constant parameters.

To avoid a violation of mass conservation of the solute being the important liquid component due to porosity change at each time step, the mass fraction of solute in the liquid phase may be corrected:

$X_{s+1}(\text{solute}) = X_s(\text{solute})\ \varphi_s/\varphi_{s+1}$.

This linear coupling of TOUGH2 and FLAC3D, in which the codes are executed separately up to the end of the problem time, is rather simple. Hence, it is viewed as a first-order approximation of simulation of coupled hydrologic-mechanical processes. However, this linear coupling can deliver first estimation of the impacts of the coupled processes and can certainly be improved by introducing an iterative sequential coupling of two codes at each time step according to the approach of (Rutqvist et al 2002).

GAS AND NUCLIDE TRANSPORT IN CLAY

In (Javeri and Baltes 2001), a two-dimensional parametric investigation is performed to analyze the gas and solute transport in a simplified isothermal repository system for radioactive waste to define site-selection criteria. This model is now extended to study a three-dimensional situation and to demonstrate the linear coupling of TOUGH2 and FLAC3D (Fig. 3 and Table 1). The model with reasonable parameters consists of three material domains: the upper 400 m represents a barrier rock, the lower 200 m a clay-type host rock and a 10-m-high repository within the host rock at the bottom. Initially, the complete system is flooded with groundwater. To simplify the analysis, the radioactive substances in the repository are simulated by a single non-decaying solute. The homogeneous gas generation in the repository is represented by hydrogen formation rates in three time segments:

1. $0 \le t \le 1000$ years: linear increase from 0 to Q_{Gas},
2. $1000 \le t \le 5000$ years: $Q_{Gas} = 45$ kg/year,
3. $5000 \le t \le 6000$ years: linear decrease from Q_{Gas} to 0.

The fluid consists of three components: ground water, solute in liquid phase, and hydrogen. The solubility of hydrogen in the liquid phase is given by:

$X_{Gas\ in\ Liquid} = m_{Gas}/m_{Liquid} = (p/C_{Henry})(M_{Gas}/M_{Liquid})$.

To describe two-phase flow, the modified Brooks-Corey functions are used to calculate relative permeability and capillary pressure:

$S_{Liq,Eff} = (S_{Liquid} - S_{Liq,Res}) / (1 - S_{Liq,Res} - S_{Gas,Res})$,

$k_{Liq,Rel} = (S_{Liq,Eff})^4$, $\quad k_{Liq} = k k_{Liq,Rel}$,

$k_{Gas,Rel} = (1 - S_{Liq,Eff})^2\ (1 - S^2_{Liq,Eff})$, $\quad k_{Gas} = k k_{Gas,Rel}$,

$p_{cap} = p_b(1 - S_{Liqid})/S_{Gas,Res}$, if $(1 - S_{Gas,Res}) \le S_{Liqid} \le 1$,

$p_{cap} = p_b\ /(S_{Liq,Eff})^{1/2}$, if $S_{Liquid} \le (1 - S_{Gas,Res})$,

$p_b = 0.56\ k^{-0.346}$, $\quad$ k in m², $\quad$ p_b in Pa.

Case HC31: Hydrological analysis: Assuming hydrological properties independent of stress, TOUGH2/EOS7 is executed up to the problem time of 10^4 years in 494 time steps with a maximum time step of $4 \cdot 10^9$ s. The fluid pressure for all elements and time steps are saved.

Case MC31: Geomechanical analysis: To determine the spatial stress situation with FLAC3D, an isotropic elastic material model for the barrier rock and repository is postulated. Further, it is assumed that the host rock is a clay-type rock, which obeys the elastic plastic material model according to the Mohr-Coulomb formulation. Using the pressure distribution from case HC31 and prescribing the fluid pressure at all grid points and all time steps, FLAC3D is executed for the same number of time steps as in case HC31 and principal stresses and mean effective stresses for all zones and time steps are saved.

Case HMC31: Hydrological analysis with variable properties: Employing basically the same input data of case HC31 and allocating the stresses of case MC31 to corresponding TOUGH2 elements, TOUGH2 is executed up to the same problem time. However, employing tabular functional relations between stresses and pressure of case MC31, at each time step, the hydrological properties of host and barrier rock, porosity, permeability and capillary pressure, are determined as mentioned above:

$\varphi = 0.05 \exp[5 \cdot 10^{-8}\ (1/\text{Pa})\ \Delta\sigma_{mean,eff}]$,

$k = (1.6 \cdot 10^{-14}\ \text{m}^2)\ \varphi^4$.

Fig. 4 shows the pressure distributions of case HC31 in the boundary plane (y = 5 m) at t = 5000 years, around which maximum values occur. The gas generation influences the fluid pressure significantly within 1000 m in the x-direction away from the repository but not in y-direction, as the width in the y-direction is relatively small. Because of the relatively low permeability and high capillary pressure of the host rock, the gas saturation remains below 1 % beyond 100 m from the repository in the first 10^4 years (Fig. 5). Due to significant capillary pressure difference between host rock and repository and due to increasing gas solubility with increasing pressure, slightly more gas is released at the ends than at the center of the repository. The solute with initial mass fraction of 0.25 in the liquid phase in the repository does not migrate vertically beyond 100 m from the repository within 10^4 years (Fig. 6).

The mechanical calculation of case MC31 indicates a failure due to tensile stress in the host rock right above the repository and a failure due to shear stress a little away from the repository; around 45 % of the host rock is affected (Fig. 7). Assuming that the hydro-fracturing due to pressure build-up in the rock can occur, if the fluid pressure reaches the minimum compressive principal stress, the factor of safety related to hydro-fracturing can be defined as in Javeri and Mielke (2001):

$F_{Fracture}$ = |minimum compressive principal stress| / p,

$F_{Fracture} = 0$, if any principal stress > 0 or $\sigma_{mean} > 0$.

In Fig. 8, the factor of safety related to hydro-fracturing in the boundary plane (y = 5 m) at t = 5000 years for the case HMC31 is depicted. In the lower area of the host rock, the safety factor is a little higher than in the upper area, as the difference between the fluid pressure and the lithostatic pressure increases with depth. In the region right above the repository, the safety factor is little higher than at the horizontal ends of the repository in x-direction, as slightly more gas is released at the ends of the repository. Postulating that a risk of hydro-fracturing is given for a safety factor below 1.2, almost all of the region above the repository is affected.

In case HMC31, due to fluid pressure build-up and due to associated changes in mean stress, the porosity of the rock increases from 0.05 to 0.0615 and the permeability from 1E-19 to 2.29E-19 m². One can expect that theses maximum values could not be exceeded, even with a tighter coupling of codes at each time step according to (Rutqvist et al. 2002) is applied, as in that case the fluid pressure could be a little lower and thus porosity and permeability could also be little lower. Employing the maximum values of porosity and permeability for all elements of case HMC31, a bounding case for the hydrological analysis is defined:

Case HC32: same as case HC31, but porosity and permeability are prescribed as:

$\varphi_i = \varphi_{max,i}$(case HMC31), $k_i = k_{max,i}$(case HMC31).

Fig. 9 shows the pressure in the repository for the case HC31, HMC31, and HC32. As the maximum repository pressure lies between 12.9 and 15.6 MPa and is well above the lithostatic pressure of 12 MPa, a failure of mechanical stability of the host rock and also of the repository is to be expected. According to the postulated stress-porosity-permeability relationship, the impact of coupled processes is moderate in case HMC31, which can be bracketed reasonably by the limiting hydrological cases HC31 and HC32. In Fig. 10, the migration of the nuclide from the repository is presented. As expected, in all three cases the migration is nearly the same, around 55 % of initial solute mass of 10^7 kg within 10^4 years, as the driving pressure difference is not very different. However, the higher permeability in cases HMC31 and HC32 leads to a little higher release than in case HC31. In other situations with a more sensitive stress-porosity-permeability relationship, the impact of the coupled processes can be substantial.

GAS AND NUCLIDE TRANSPORT IN SALT

To study the gas and nuclide transport in rock salt, the same model (Fig. 3 and Table 1) is employed, however, the host rock is now rock salt. Accordingly, reasonable properties for rock salt are introduced and the following cases are defined.

Case HS31: Hydrological analysis: Case HS31 is the same as HC31, but for host rock:

$\varphi = 0.01$ and $k = 1\cdot10^{-19}$ m².

Case MS31: Geomechanical analysis: Case MS31 is the same as MC31, but the pressure distribution of HS31 is applied and the material behavior of rock salt is described by neglecting primary but considering secondary creep rate (Javeri and Mielke, 2001):

$(d\varepsilon/dt)_{secondary} = D \exp(-A/\theta) (\sigma^{dev} / \sigma_{ref})^5$,

$\sigma^{dev} = [(3/2)\, \sigma_{ij,dev}\, \sigma_{ij,dev}]^{1/2}$,

$\sigma_{ij,dev}$: deviatoric part of total stress σ_{ij},

D = 0.18 1/day, A = 6495 K, θ = 298 K, σ_{ref} = 1 MPa.

Case HMS31: Hydrological analysis with variable properties: Case HMS31 is as HMC31, but the pressure and stress distribution of case MS31 are invoked and the porosity and the permeability of the host are calculated as:

$\varphi = 0.01 \exp[5\cdot10^{-8}\ (1/\text{Pa})\ \Delta\sigma_{mean,eff}]$,

$k = (1.0\cdot10^{-11}\ \text{m}^2)\ \varphi^4$.

The pressure development in cases HC31 and HS31 is very similar, as other relevant parameters are same and the lower porosity 0.01 of host rock does not influence the flow situation significantly. To characterize the mechanical stability of rock salt, the factor of safety related to dilatancy (increase of volume due to opening or widening of cracks) can be defined by using dilatancy boundary conditions derived from experimental observations (Hunsche 1993):

$F_{dilatancy} = \tau_{dil} / \tau$,

$\tau = (1/3) [(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2]^{1/2}$,

$\tau_{dil} = 0.86|\sigma_{mean}| - 0.0168|\sigma_{mean}|^2$, ($\tau_{dil}$; σ_{mean} in MPa),

$F_{dilatancy} = 0$, if any principal stress > 0 or $\sigma_{mean} > 0$,

$F_{dilatancy} < 1$: Mechanical stability is affected.

Since in case MS31 the factor of safety related to dilatancy lies far beyond one (1), the mechanical stability of the entire rock salt mass based on above criterion is expected (Fig. 11). However in case HMS31, as in the case of clay rock, hydro-fracturing of nearly the entire region directly above the repository can be expected, since the stress situation in both cases is similar (Fig. 12). The criterion for hydro-fracturing is clearly stricter than the dilatancy criterion, since for the dilatncy criterion all principal stresses should only be negative,while for the hydro-fracturing criterion all principal stresses should be sufficiently negative.

In case HMS31, due to the fluid pressure build-up and due to associated changes in mean stress, the porosity of rock salt increases from 0.01 to 0.0122 and the permeability from 1E-19 to 2.22E-19 m². Using the maximum values of porosity and permeability for all elements of case HMS31, a bounding case for hydrological analysis is defined:

Case HS32: same as HS31, but porosity and permeability are prescribed as:

$\varphi_i = \varphi_{max,i}$(case HMS31), $k_i = k_{max,i}$(case HMS31).

As the maximum pressure in the repository exceeds the lithostatic pressure of 12 MPa, a failure of mechanical stability of the rock salt cannot be excluded (Fig. 13). Case HMS31 can be reasonably bracketed by the bounding hydrological cases HS31 and HS32. Nearly the same nuclide migration as in case of clay rock is observed, and hence, it is not depicted.

CONCLUSIONS

To study the coupled hydrologic-geomechanical processes and their influence on gas and nuclide transport in a two-phase flow configuration in a porous medium, a linear coupling of the hydrodynamic code TOUGH2 and the mechanics code FLAC3D is described and applied to analyze three dimensional gas and nuclide transport in an isothermal repository for radioactive waste in a deep geological formation like clay rock or rock salt. The scoping coupled hydro-geomechanical analyses show that the transport behavior of the contaminated two-phase fluid is noticeably influenced by the transient stress conditions. The coupled analyses can be applied to quantify the safety margin related to hydro-fracturing due to fluid pressure build-up if the hydrological properties, such as porosity, permeability, and capillary pressure depending upon mean effective normal stress are employed.

Summarizing, it is concluded that the current linear coupling, which is rather simple, is to be viewed as a first-order approximation of simulation of coupled hydrologic-mechanical processes. However, it can deliver a reasonable estimation of impacts of the coupled processes. In the future, the present linear coupling should be verified and improved by introducing iterative sequential coupling of two codes at each time step.

SYMBOLS

A: normalized activation energy [K]
k: permeability [m²]
M: molecular weight [g/mol]
m: mass [kg]
p: pressure [Pa]
p_b: bubble entry pressure [Pa]
Q: mass flow [kg/s]
S: phase saturation
t: time [s]
T: temperature [C]
V: volume [m³]
X: mass fraction
ε: strain
σ: stress [Pa] (tensile: > 0; compressive: < 0)
σ_j: principal stress (j: 1 to 3) [Pa]
φ: porosity
θ: temperature [K]
τ: octahedral shear stress [Pa]

SUBSCRIPTS

i: index of TOUGH2 element
k: index of a FLAC3D connected zone
n: index of a FLAC3D grid point
s: time step

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Table 1. Modeling parameters

Property	Value
Volume of repository	1E5 m³
Density of liquid phase	$\rho_{Water}(p,T)$
Dynamic viscosity of liquid phase	$\mu_{Water}(p,T)$
Dynamic viscosity of hydrogen	8.95 E-6 Pas
Gas constant of hydrogen	4124J/(kgK)
Molecular weight of liquid phase	18 g/mol
Molecular weight of hydrogen	2 g/mol
Henry constant for hydrogen, C_{Henry}	7.31E9 Pa
Mol. diffusion coefficient in liquid	5E-11 m²/s
Porosity of barrier and host rock	0.05
Permeability of barrier and host rock	1E-19 m²
Porosity of repository	0.4
Permeability of repository	1E-12 m²
Residual liquid saturation, $S_{Liq,Res}$	0.2
Residual gas saturation, $S_{Gas,Res}$	0.05
Mechanical properties	
Dry rock density	2000 kg/m³
Elastic bulk modulus of barrier rock	2E9 Pa
Elastic shear modulus of barrier rock	1.2E9 Pa
Elastic bulk modulus of repository	30E6 Pa
Elastic shear modulus of repository	2E6 Pa
Host rock (clay rock): Mohr-Coulomb-parameter	
Elastic bulk modulus	2E9 Pa
Elastic shear modulus	1.2E9 Pa
Cohesion	1E6 Pa
Dilatation angle	30 degree
Internal angle of friction	30 degree
Tension limit	1E6 Pa
Host rock (rock salt)	
Elastic bulk modulus of rock salt	18.12E9 Pa
Elastic shear modulus of rock salt	9.843E9 Pa

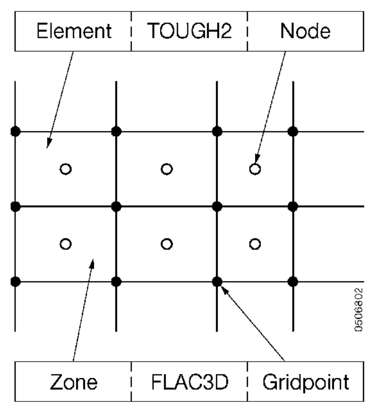

Figure 1. Identical mesh for TOUGH2 and FLAC3D

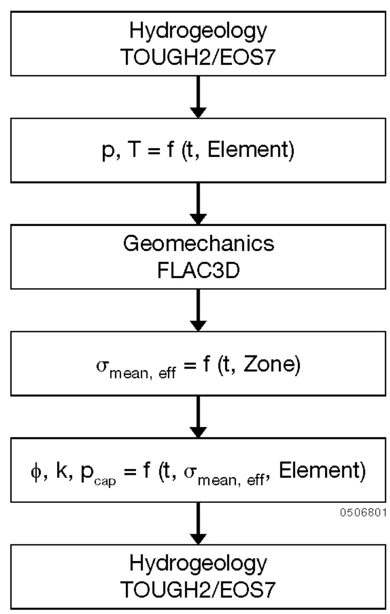

Figure 2. Linear coupling of TOUGH2 and FLAC3D

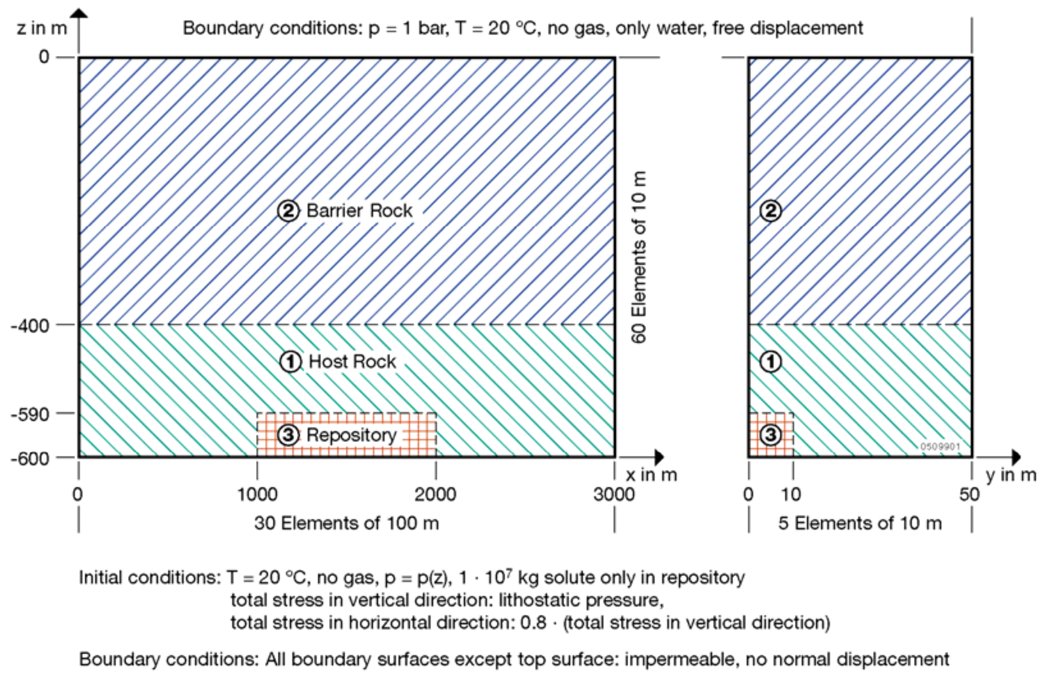

Figure 3. Three-dimensional model of a repository

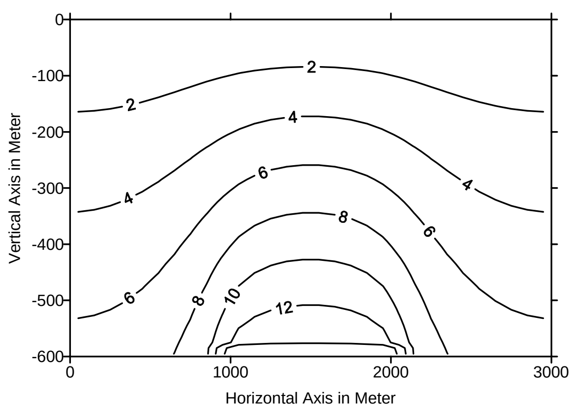

Figure 4. Pressure (MPa) at y= 5 m and t = 5000 years in case HC31

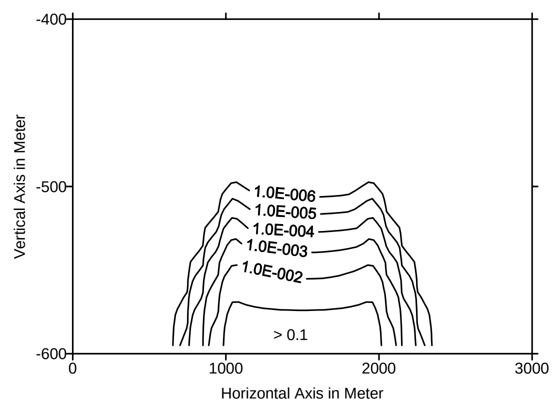

Figure 6. Solute mass fraction in liquid phase at y = 5 m and t = 10,000 years in case HC31

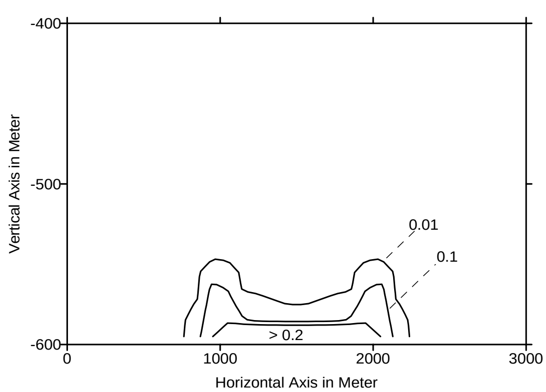

Figure 5. Gas saturation at y= 5 m and t = 10,000 years in case HC31

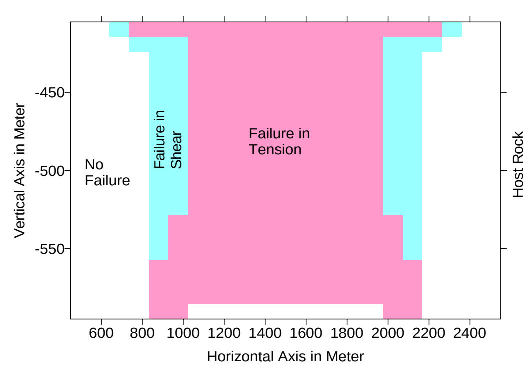

Figure 7. Failure state in case MC31

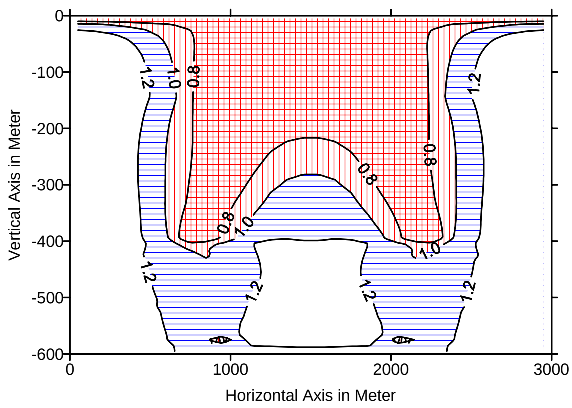

Figure 8. Factor of safety regarding hydro-fracturing at y = 5 m and t = 5000 years in case HMC31

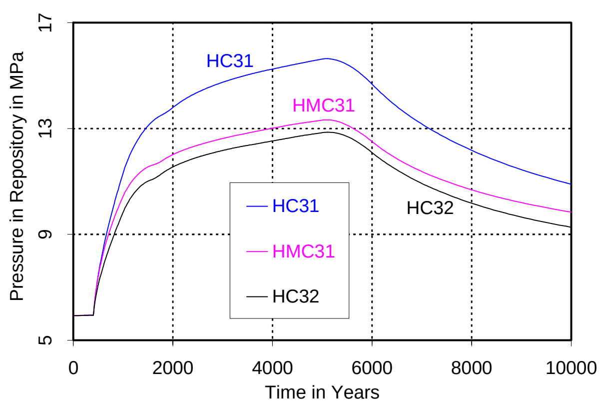

Figure 9. Pressure at the center of repository in clay

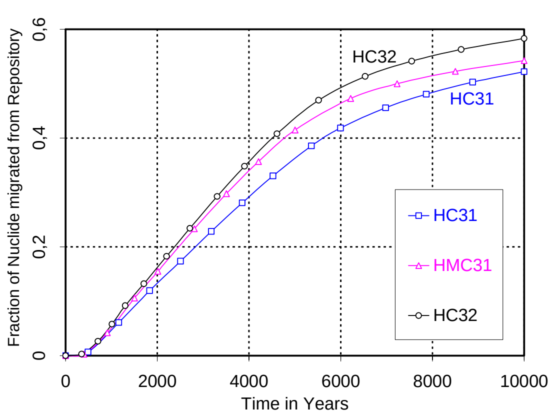

Figure 10 Fraction of nuclide migrated from repository in clay

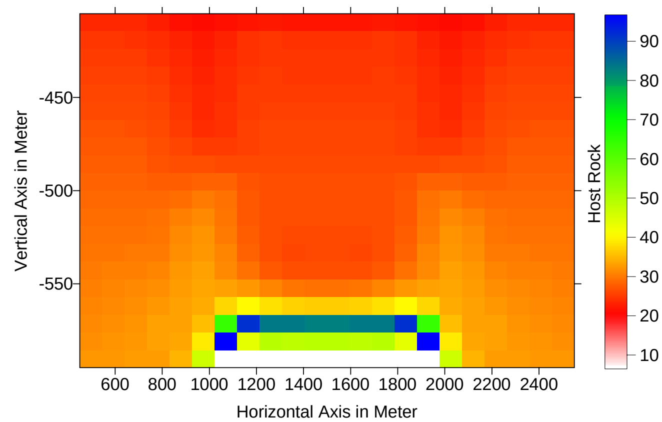

Figure 11. Factor of safety regarding dilatancy at y = 5 m and t = 10000 years in case MS31

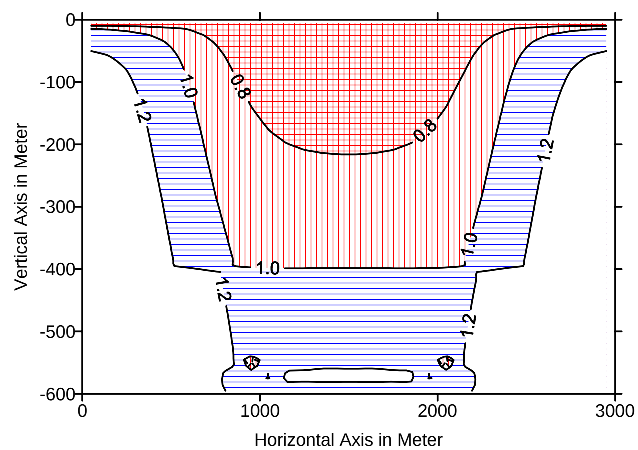

Figure 12. Factor of safety regarding hydro-fracturing at y = 5 m and t = 5000 years in case HMS31

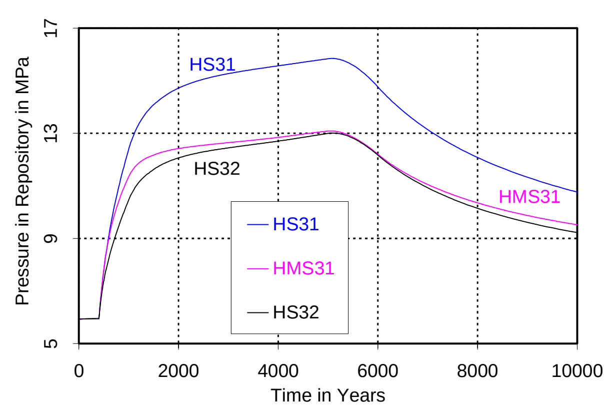

Figure 13. Pressure at the center of repository in salt