

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 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 mechanic 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 a 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 the 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 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 the gas generation, mainly hydrogen produced due to corrosion of metallic materials, at least within 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, specially, 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 hydrologic-mechanical processes and their influence on gas and nuclide transport in a two phase flow configuration, two 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 a single phase flow condition but not for two phase flow situation (Itasca 2002).

In GRS, 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 geomechanical analysis. In (Javeri & 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. Main objective of the present scoping analysis is to develop a procedure, which allows to study coupled hydrologic-mechanical processes at least in an elementary but in a reasonable manner.

HYDROLOGICAL ANALYSIS WITH TOUGH2

The computer code TOUGH2/EOS7 (Pruess 1990 and 1991) 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 at the interface 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 restrains. 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:

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

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 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 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 of FLAC3D is determined as:

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

In 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 problem, other interpolation scheme should 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:

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

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, 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, following functions are introduced:

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

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

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

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

a, b, c : 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 liquid phase may be corrected:

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

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 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: upper 400 m represents a barrier rock, 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 repository are simulated by a single non decaying solute. The homogeneous gas generation in the repository is represented by hydrogen formation rate in three time segments:

$0 \leq t \leq 1000$ years: linear increase from 0 to Q_{Gas} ,

$1000 \leq t \leq 5000$ years: $Q_{\text{Gas}} = 45$ kg/year,

$5000 \leq t \leq 6000$ 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 liquid phase is given by:

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

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

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

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

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

$$p_{\text{cap}} = p_b(1 - S_{\text{Liquid}})/S_{\text{Gas, Res}}, \quad \text{if } (1 - S_{\text{Gas, Res}}) \leq S_{\text{Liquid}} \leq 1,$$

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

$$p_b = 0.56 k^{-0.346}, \quad k \text{ in m}^2, \quad p_b \text{ in Pa.}$$

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 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 Mohr-Coulomb formulation. Using pressure distribution from of 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 stress 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:

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

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

Fig. 4 shows the pressure distributions of case HC31 in 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 x-direction away from the repository but not in y-direction, as the width in y-direction is relatively small. Because of relatively low permeability and high capillary pressure of the host rock the gas saturation remains below 1 % beyond 100 m from the repository in 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 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 (Javeri and Mielke 2001):

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

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

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 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 complete 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 $1\text{E-}19$ to $2.29\text{E-}19$ m². One can expect that these maximum values could not be exceeded, even if 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 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:

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

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 postulated stress-porosity-permeability relationship, the impact of coupled processes is moderate in case HMC31, which can be enveloped 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 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 following cases are defined.

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

$$\varphi = 0.01 \text{ and } k = 1 \cdot 10^{-19} \text{ m}^2.$$

Case MS31: Geomechanical analysis: Case MS31 is 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 & Mielke 2001):

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

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

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

$$D = 0.18 \text{ 1/day}, \quad A = 6495 \text{ K}, \quad \theta = 298 \text{ K}, \quad \sigma_{\text{ref}} = 1 \text{ MPa}.$$

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:

$$\varphi = 0.01 \exp[5 \cdot 10^{-8} (1/\text{Pa}) \Delta\sigma_{\text{mean,eff}}],$$

$$k = (1.0 \cdot 10^{-11} \text{ m}^2) \varphi^4.$$

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 derived from experimental observations (Hunsche 1993):

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

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

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

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

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

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

$$\phi_i = \phi_{max,i}(\text{case HMS31}), \quad k_i = k_{max,i}(\text{case HMS31}).$$

As the maximum pressure in repository exceeds the lithostatic pressure of 12 MPa, a failure of mechanical stability of rock salt can not be excluded (Fig. 13). Case HMS31 can be reasonably enveloped 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 mechanic code FLAC3D is described and applied to analyze three dimensional gas and nuclide transport in a isothermal repository for radioactive waste in a deep geological formation like clay rock or rock salt. The scoping coupled hydrologic-mechanical 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 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

REFERENCES

Hunsche, U., *Failure behavior of rock salt around underground cavities*, Proc. 7th Symp. on Salt, Vol. 1, 59-65, Elsevier Science Publ., Amsterdam, 1993.

Itasca consulting Group, *FLAC3D, Fast Lagrangian Analysis of Continua in 3 Dimensions, Version 2.1, User's Guide*, Minneapolis, Minnesota, USA, 2002.

Javeri, V., *Scoping analysis of combined gas and nuclide transport including variable brine fraction and rock convergence in a two dimensional repository*, Proc. Int. Conf. on Radioactive waste Disposal (DisTec 2000), 465-470, Germany 2000.

Javeri, V., B. Baltes, *Analysen zum Gas- und Stofftransport in der Geosphäre eines vereinfachten Endlagersystems*, Report GRS-A-2904, Gesellschaft für Anlagen- und Reaktorsicherheit, Germany, 2001.
<http://www.akend.de>

Javeri, V., H. Mielke, *Bewertung und Analysen zur mechanischen Stabilität und Integrität eines Endlagers im Salinar*, Report BMU-2002-585, Schriftenreihe Reaktorsicherheit und Strahlenschutz, Der Bundesminister für Umwelt, Naturschutz und Reaktorsicherheit, Bonn, Germany, 2001.

Pruess, K., *TOUGH2-A general purpose numerical simulator for multiphase fluid flow*, LBL-29400, Lawrence Berkeley National Lab., USA, 1990.

Pruess, K., *EOS7, An equation of state module for the TOUGH2 simulator for two phase flow of saline water and air*, Report LBL-31114, USA, 1991.

Rutqvist, J. et al., A modeling approach for analysis of coupled multiphase fluid flow, heat transfer and deformation in a fractured porous rock, *Int. J. of Rock Mech. & Mining Sciences*, 39, 429-442, 2002.

Table 1. Modeling parameters

Property	Value
Volume of repository	1E5 m ³
Density of liquid phase	$\rho_{\text{Water}}(p,T)$
Dynamic viscosity of liquid phase	$\mu_{\text{Water}}(p,T)$
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 m ² /s
Porosity of barrier and host rock	0.05
Permeability of barrier and host rock	1E-19 m ²
Porosity of repository	0.4
Permeability of repository	1E-12 m ²
Residual liquid saturation, $S_{\text{Liq,Res}}$	0.2
Residual gas saturation, $S_{\text{Gas,Res}}$	0.05
Mechanical properties	
Dry rock density	2000 kg/m ³
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

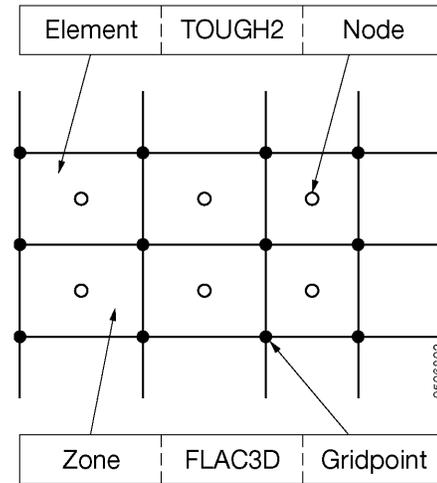


Figure 1. Identical mesh for TOUGH2 and FLAC3D

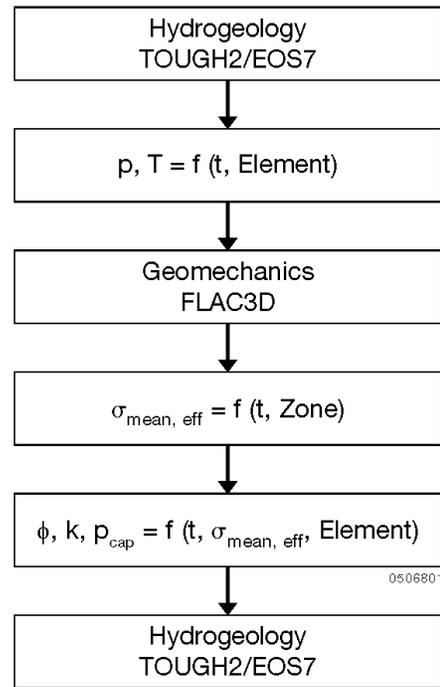
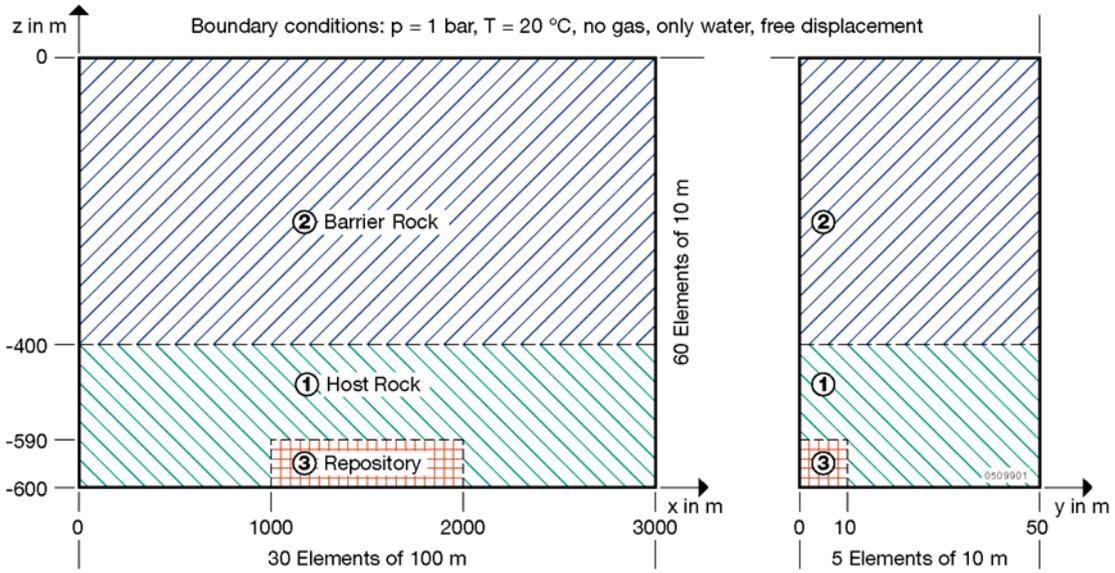


Figure 2. Linear coupling of TOUGH2 and FLAC3D



Initial conditions: $T = 20\text{ °C}$, no gas, $p = p(z)$, $1 \cdot 10^7$ kg solute only in repository
 total stress in vertical direction: lithostatic pressure,
 total stress in horizontal direction: $0.8 \cdot$ (total stress in vertical direction)

Boundary conditions: All boundary surfaces except top surface: impermeable, no normal displacement

Figure 3. Three dimensional model of a repository

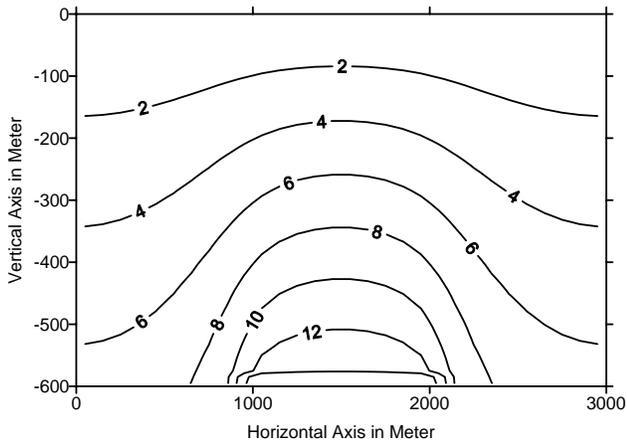


Figure 4. Pressure (MPa) at $y = 5$ m and $t = 5000$ years in case HC31

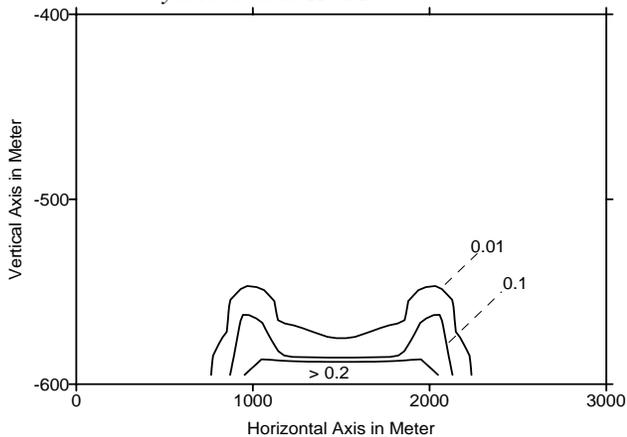


Figure 5. Gas saturation at $y = 5$ m and $t = 5000$ years in case HC31

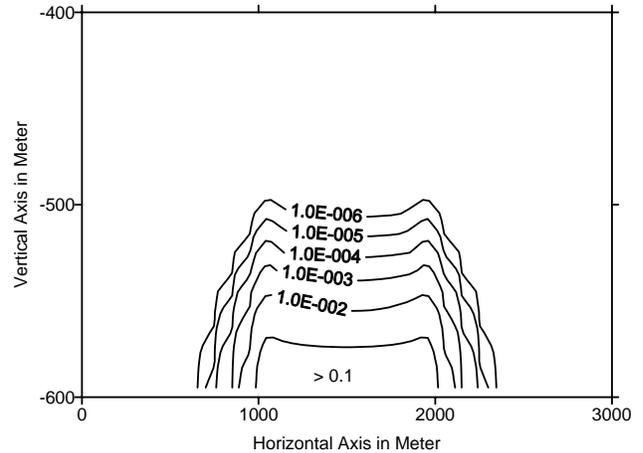


Figure 6. Solute mass fraction in liquid phase at $y = 5$ m and $t = 5000$ years in case HC31

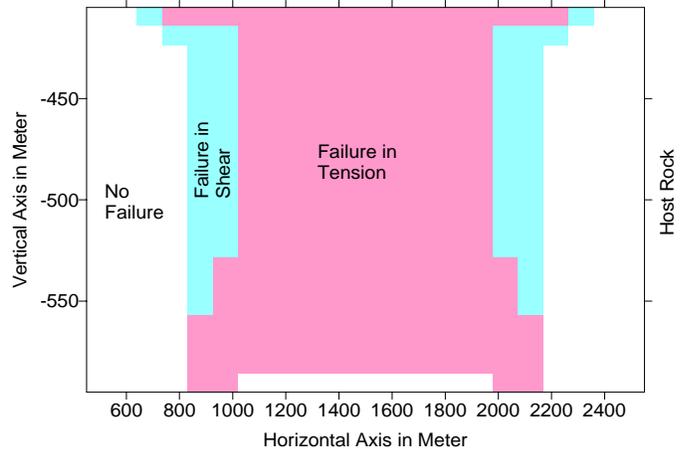


Figure 7. Failure state in case MC31

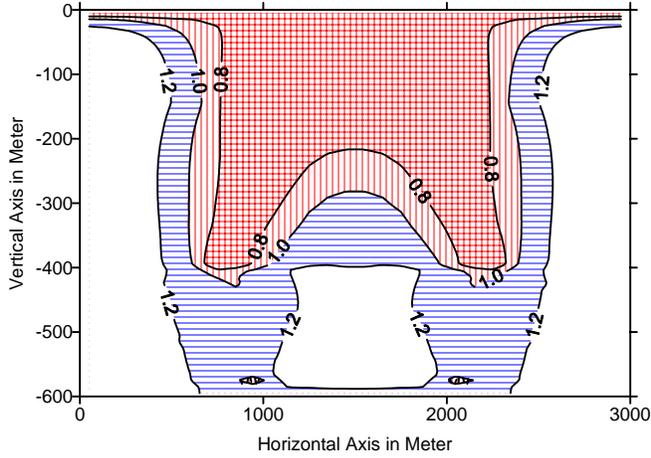


Figure 8. Factor of safety regarding hydro-fracturing at $y = 5$ m and $t = 5000$ years in case HMC31

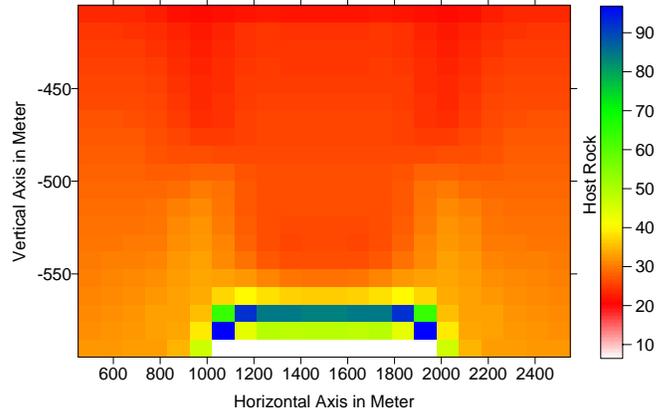


Figure 11. Factor of safety regarding dilatancy at $y = 5$ m and $t = 10000$ years in case MS31

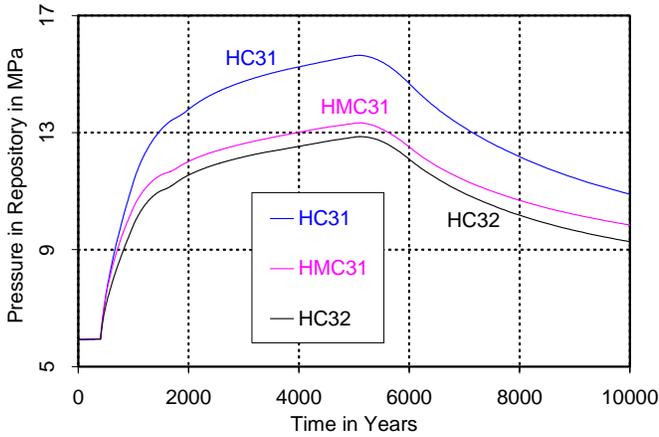


Figure 9. Pressure at the center of repository in clay

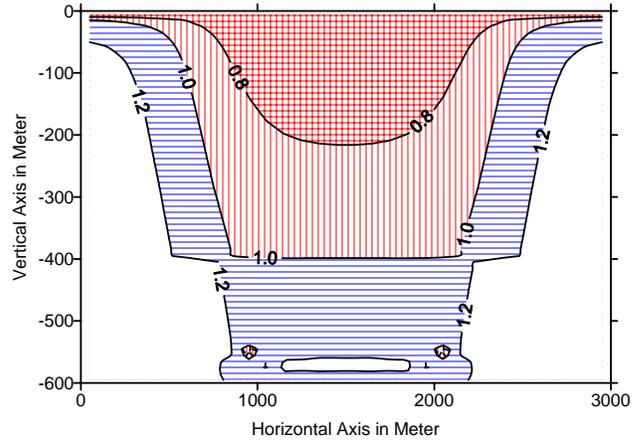


Figure 12. Factor of safety regarding hydro-fracturing at $y = 5$ m and $t = 5000$ years in case HMS31

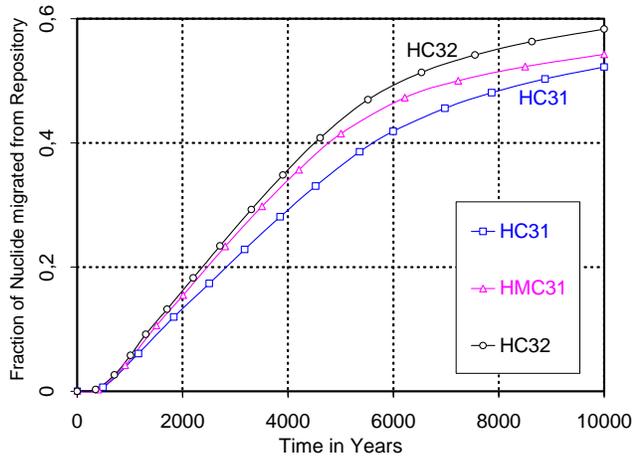


Figure 10. Fraction of nuclide migrated from repository in clay

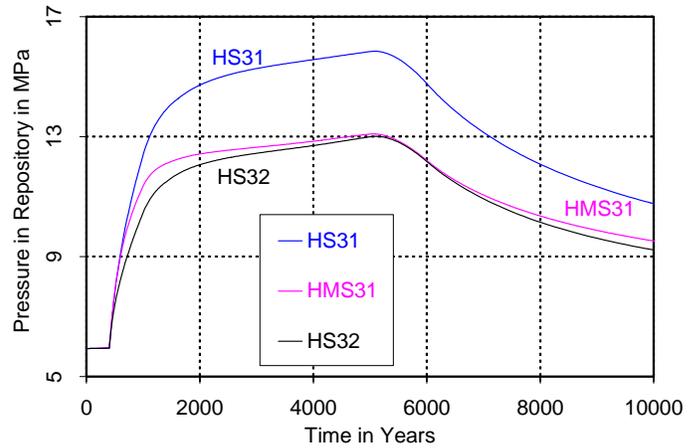


Figure 13. Pressure at the center of repository in salt