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Task 8 of SKB Task Forces GWFTS and EBS

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Executive summary

This report presents the works performed by the KAERI modeling group on SKB Task 8a–8d. Task 8 is primarily focused on improving the knowledge of the bedrock–bentonite interface with regard to groundwater flow and increasing our ability to model the hydraulic interaction between them. In process of numerical modeling, the far-field represented by stochastic discrete fracture network (DFN) is modeled as homogeneous equivalent porous medium (EPM), in which equivalent permeability is derived from the comparative study between FLAC3D and TOUGH2 codes, and large deterministic fractures or discrete fractures near deposition hole are explicitly embedded into a model. KAERI-simulator (TOUGH2 code coupled with FLAC3D by using MATLAB) is primarily used for analyzing the hydraulic behaviors of bentonite as well as rock mass. Hydration of unsaturated bentonite and the effects of rock fracture on the re-wetting process are identified and properly predicted by TOUGH2 code over the subtasks of Task 8. From the sensitivity analysis it is noted that inflow into probing boreholes is not significantly affected by large deterministic features if they are not directly intersected with the boreholes. The variation in inflow and the bentonite re-saturation are highly influenced by the localized water ingression due to fractures surrounding deposition holes. Thus it is important to identify the site-specific geological features around the deposition hole. In addition, model adjustment and calibration based on the laboratory and field data available data measured in situ are necessary to better reproduce the observations and to increase the reliability of predictive model.

Sammanfattning

I denna rapport presenteras det arbete, relaterat till SKB Task 8a-8d, som har utförts av en modelleringsgrupp från KAERI. Modelleringsuppgiften Task 8 är i huvudsak inriktat på att förbättra kunskapen om gränssnittetet mellan berg och bentonit med avseende på grundvattenflödet samt att öka vår förmåga att modellera den hydrauliska interaktionen mellan dem. När det gäller numerisk modellering, modelleras fjärrfältet, representerat av ett stokastiskt diskret spricknätverk (DFN), som ett homogent ekvivalent poröst medium (EPM), till vilket ekvivalent permeabilitet hämtats från en jämförande studie mellan programkoderna FLAC3D och TOUGH2. Stora deterministiska sprickor eller diskreta sprickor nära deponeringshålen är explicit inbäddade i en av modellerna. KAERI-simulatorn (TOUGH2 kopplad med FLAC3D med hjälp av MATLAB) används främst för att analysera det hydrauliska beteendet för bentonit samt bergmassa. Hydrering av omättad bentonit och effekterna av bergsprickor vid återfuktningsprocessen har identifierats och även predikterats av TOUGH2 i de olika delarna av modelleringsuppgiften Task 8. I känslighetsanalysen noteras det att inflöden i sonderande borrhål inte påverkas signifikant av större deterministiska zoner om de inte direkt skär borrhålen. Variabiliteten i inflöden och bentonitmättnad påverkas starkt av lokala vatten-flöden i de sprickor som omger deponeringshål. Således är det viktigt att identifiera de platsspecifika geologiska egenskaperna runt deponeringshålen. Dessutom är modelljustering och kalibrering baserad på data från laboratoriet och fältdata, som mäts in situ, nödvändiga för att bättre reproducera observationerna och öka tillförlitligheten hos de prediktiva modellerna.

Contents

1 Introduction

1.1 Background

Äspö Task Force is a forum of the international organizations for modeling of groundwater flow and transport of solute transport (GWFT) in fractured rocks. SKB Task 8 primarily focuses on the evaluation of the hydraulic interaction between the bentonite backfill material and near-field host rock. KURT (KAERI Underground Research Tunnel) is a small scale research facility to demonstrate the proposed disposal concept and technologies with regard to the performance of engineered barriers under repository conditions. KURT was expanded at 2015 in KAERI and the phase II program has started simultaneously. The tunnel is a total of 543 m in length in which 6 research modules are included. In parallel with KURT expansion, demonstration and validation of EBS (Engineered Barrier System) from the various in situ tests become more important in the phase II program, especially, by utilizing this facility. Thus, KAERI decided to take part in SKB Task 8 project focusing on the development of predicting model based on BRIE in situ test. KAERI expects that the cooperative research project Task 8 will contribute to the experimental designs of in situ tests and the predictive model development with more reliability.

1.2 Objectives

The overall objective of Task 8 is to enhance the understanding and increase our ability to model the hydraulic interaction between the rock and water unsaturated bentonite on both the scale of an individual deposition hole as well as the scale of deposition tunnel (Vidstrand et al. 2017).

1.3 Scope

Task 8 consists of subtask 8a, 8b, 8c, 8d and 8f with increasing complexity in model. This report summarizes the work performed by KAERI modeling team primarily focusing on the inflow estimation and the variations in saturation and pressure. The simulation results on Task 8f are not currently included in the report. They will be updated after further simulation study. This report does not address the thermal nor the chemical aspect of bentonite in a numerical calculation. The coupled thermal-hydraulic-mechanical numerical modeling is under investigation by anther numerical team in KAERI.

2 Task 8a initial – scoping calculation

2.1 Objectives

As part of scoping calculation, the objective of Task 8a is to enhance understanding on the hydraulic interaction between the initially unsaturated bentonite and surrounding near-field rock with regard to groundwater ingression and to identify the effects of a rock fracture on the hydraulic behaviors of bentonite buffer.

- To determine means of incorporating bentonite in numerical groundwater flow models.
- To evaluate effects of different implementations of the bedrock-bentonite interface in groundwater flow models.

2.2 Approach

Task 8a addresses the hydraulic behaviors of bentonite buffer focusing on the interactions between bentonite and surrounding rock with fracture in the middle of deposition hole. Thus, it is important to describe the re-wetting process of bentonite block numerically and identify the effects of localized water ingression through a fracture on the re-saturation of bentonite. The variations of pressure and saturation in bentonite around the deposition hole are addressed by using TOUGH2 code (Pruess et al. 1999, pp 144–147). 1D axi-symmetric example is, first, solved as an introduction to Task 8a by using TOUGH2 to check the availability of code in use and then compared with the results from Code_Bright (Olivella et al. 1996) and analytic solutions (Börgesson 1985).

2.3 Model setup

Initial degree of saturation of bentonite is 0.36 which corresponds to an initial suction value of 100 MPa. The initial porosity is 0.438 and the corresponding dry density is 1 560 kg/m^3. The tunnel inside is constantly maintained to atmospheric pressure. The pressure at the boundary domain is maintained to 2 MPa as shown in Figure 2-1 below.

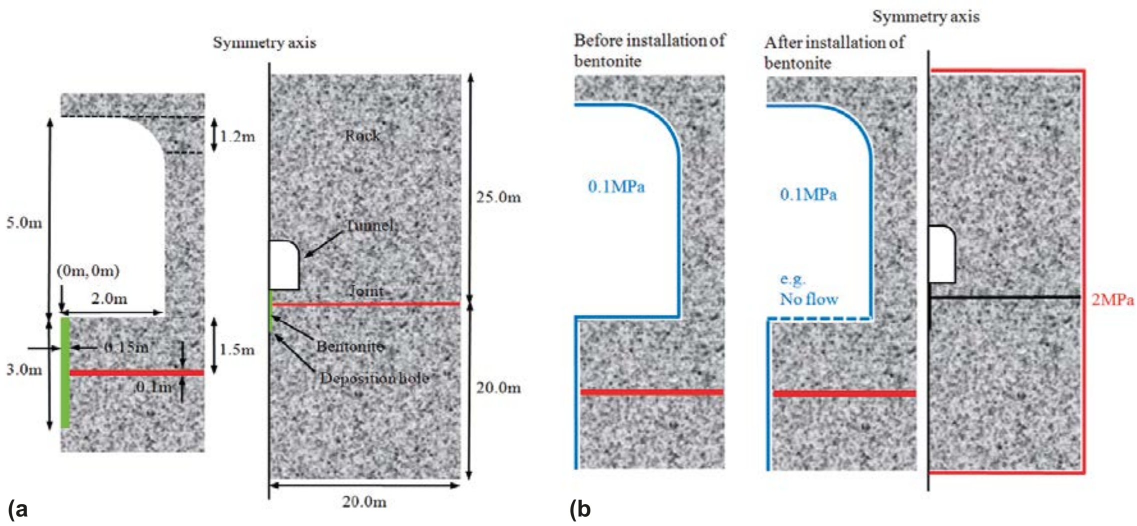


Figure 2-1. Model information of Task 8a: (a) geometry and (b) boundary conditions.

It is assumed that the initial condition is constantly maintained and the groundwater flow at the tunnel floor does not happen after bentonite installation. The initial pressure and temperature in rock matrix are 2 MPa and 20 °C, respectively. The initial gas saturation of rock is set to 0.1 % in two-phase flow. Initial pressure and temperature in bentontie are 0.1 MPa and 20 °C. The initial gas saturation in bentonite is 64 %. While, initial condition of tunnel is set to same as bentonite except that air mass fraction of tunnel is 0.999.

Geometrical set-sup, initial condition, and boundary conditions are presented in Figure 2-1 Material properties used in TOUGH2 code with regard to Task 8a are summarized in Table 2-1. EOS3 module in TOUGH2 was used to analyse the saturation behaviour in which water and air were taken into account. The hydraulic behaviors of bentonite and rock are primarily evaluated with relative permeability and capillary pressure functions in TOUGH2 code. Thus relative permeability and capillary pressure are important input parameters in two-phase flow analysis of unsaturated bentonite. More detailed input parameters for relative permeability and capillary pressure functions are indicated in the report of task description (Vidstrand et al. 2017).

Table 2-1. Material properties for Task 8a in TOUGH2 analysis (Vidstrand et al. 2017).

Material	Input parameter	Value
Intact rock	Hydraulic conductivity	1×10^{-12} m /s
	Porosity	1×10^{-5}
Rock fracture	Transmissivity	5×10^{-10} m^2/s
	Porosity for porous media	1×10^{-3}
Bentonite	Hydraulic conductivity	6.4×10^{-14} m/s
	Porosity	0.438

2.4 Results

1) Comparison with 1D axy-symmetric model and analytic solution

As for scoping calculation of Task 8a, 1D axi-symmetric problem is solved using TOUGH2 code to cross-check numerical approaches and compared with the simulation results from the Code_Bright model and the analytical solution (Crank 1975, pp 71–81).

With regard to bentonite, porosity is 43.8 %, intrinsic permeability is 6.4×10^{-21} m^2. van Genuchten retention curve is used with input parameters of $P_0 = 9.23$ MPa and $\lambda = 0.3$. Cubic power law is used for relative permeability.

The saturation profile from TOUGH2 code is presented with those from Code_Brigh mode and analytical solution in Figure 2-3. In Code-Bright model, full saturation of bentonite is obtained after about one year and degree of saturation is close to 95 % at 300 days. The saturation from TOUGH2 code indicates 94 % after 300 days as shown in Figure 2-3(b). It is, therefore, noted that the results from Code-Bright and TOUGH2 code indicate very close value in case of 1D axi-symmetry condition.

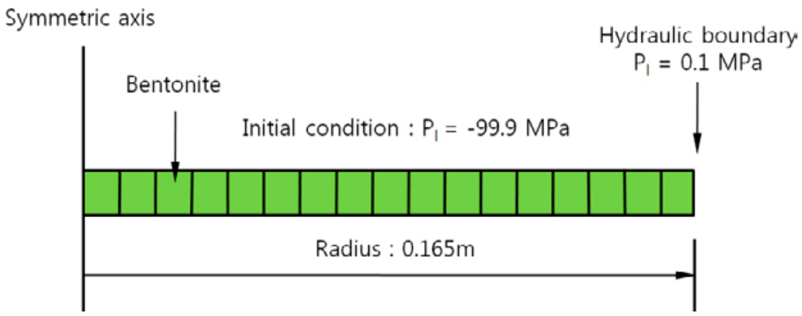


Figure 2-2. *Initial and boundary conditions of a 1D axi-symmetric model.*

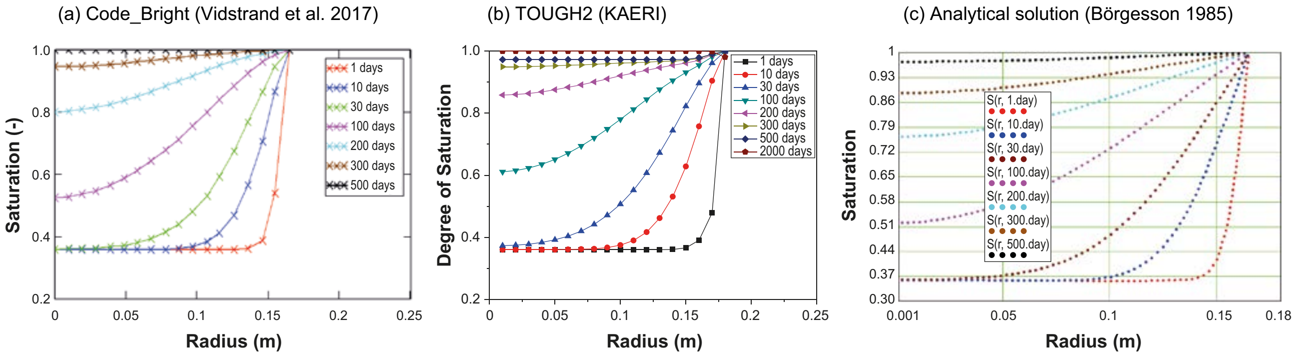


***Figure 2-3.** Radial distribution of liquid saturation in a 1D axi-symmetry model.*

The hydration of bentonite can be described as a diffusion process to some extent. The analytical diffusion solutions for water uptake can also be applied in bentonite resaturation. Standard analytical solution for diffusion (Börgesson 1985) is presented in Figure 2-3(c), which is calculated by Mathcad Ver. 14 in this study. From the analytical diffusion solution, the degree of saturation of bentonite is 89 % after 300 days of hydration. The result is slightly different with other numerical solutions. This is likely attributable to the fact that the diffusivity term is assumed as constant value in diffusion equation although diffusivity term is a function of the degree of saturation, due to the saturation dependence of the retention curve and the relative permeability function (Vidstrand et al. 2017).

2) Variations in pressure and saturation

The hydraulic behaviors of bentonite buffer focusing on the interactions between bentonite and surrounding rock with fracture are investigated using TOUGH2 code as part of a sub-mission of Task 8a. The variations in pressure generated around a tunnel are presented in Figure 2-4 and Figure 2-5. The former indicates the pressure distribution around the tunnel in case of intact rock. The latter shows the pressure variation in case of rock including a fracture at the middle of deposition hole.

It is noted that fast initial drop in pressure due to rock fracture is efficiently recovered to some extent from the part intersected with rock fracture because of the efficient water supply through a fracture. Therefore, more groundwater will be estimated in deposition hole due to rock fracture compared to intact rock.

Figure 2-6 to Figure 2-7 show the saturation variation around the tunnel with time. It is found that the initially unsaturated bentonite intersected with rock fracture shows more rapid resaturation than the case of intact rock.

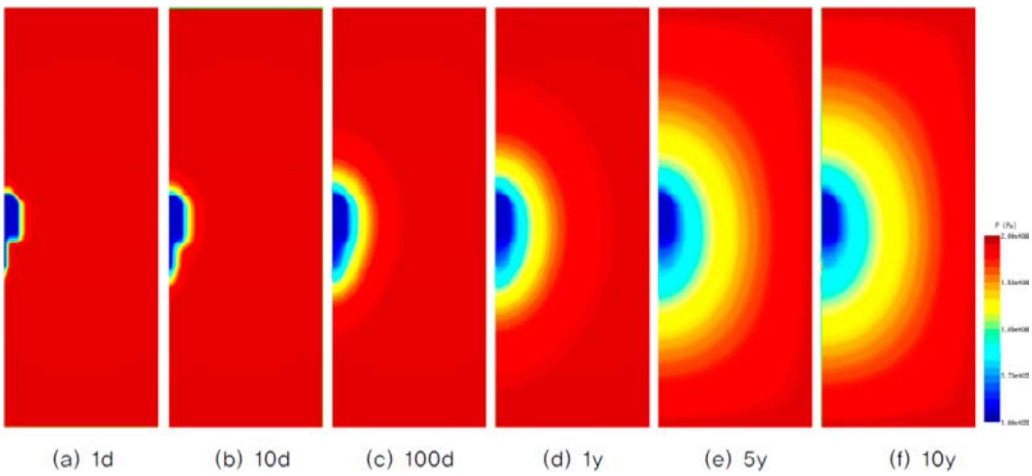


***Figure 2-4.** Water pressure distribution around the tunnel with time (intact rock).*

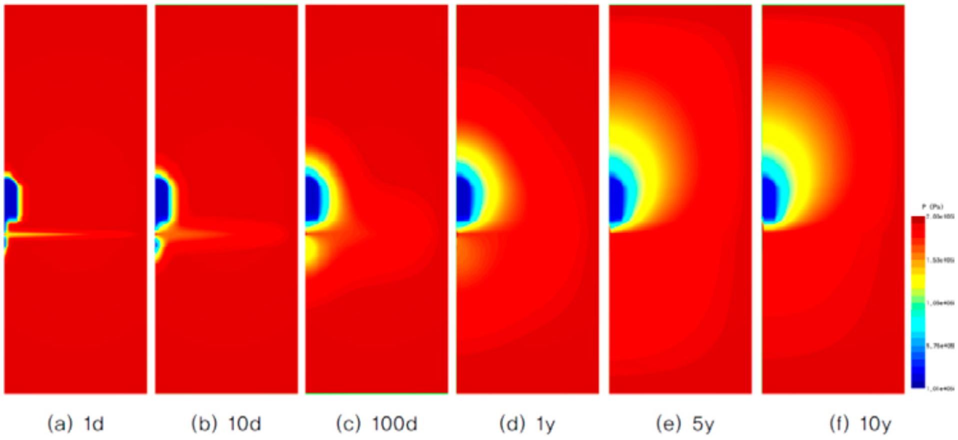


Figure 2-5. *Water pressure distribution around the tunnel with time (rock with fracture).*

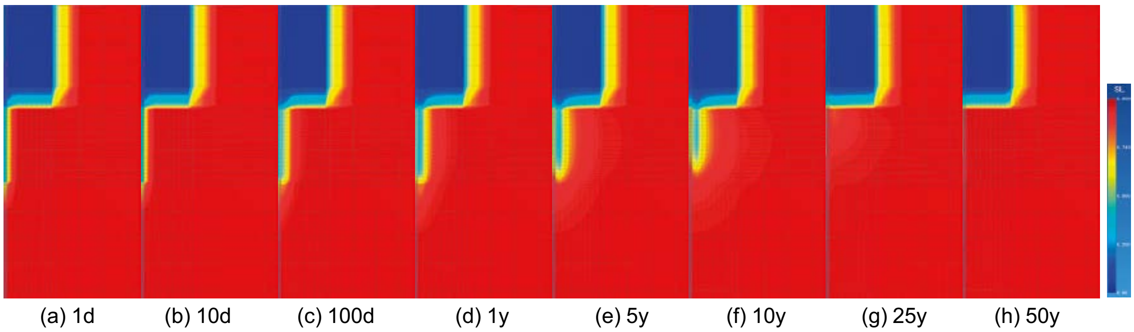


Figure 2-6. *Saturation variation around the deposition hole with time (intact rock).*

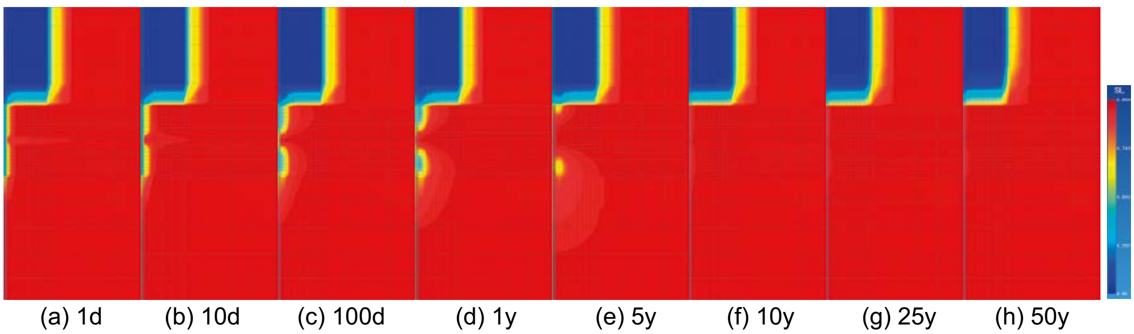


Figure 2-7. *Saturation variation around the deposition hole with time (rock with fracture).*

The radial distribution of saturation around the bentonite buffer is also shown in Figure 2-8 to Figure 2-9. In case of intact rock, more than 25 years is required for the full saturation of bentonite (Figure 2-8). Substantial change in saturation happens especially at the interface between rock and bentonite. The full saturation of fractured rock requires about 2 years at the location contacted with rock fracture. Lower and upper part of bentonite require about 10 years for full saturation.

The overall required time for full saturation across the whole bentonite block is less than about 10 years. The lower part of bentonie block is generally saturated faster than the upper part. This does not mean heterogeneous groundwater ingression into bentonite. That is primarily attributed to the geometric shape of bentonite, that is, a relatively thin and long. The last point to be saturated is in the center of the bentonite at tunnel floor level. Consequently, the re-saturation rate of bentonite contacted with fracture shows 2.5 to 12 times faster than an intact rock.

Except for the location contacted with rock fracture at a 1.5 m depth, the resaturating patterns of bentonite show similar trend each other. The resaturation behavior at 1.5 m depth (Figure 2-9(b)) is very close to that of Figure 2-3 (1D axi-symmetry model), in which corresponds to the case water supply is more than water demand in bentonite.

3) Variations at interface between rock and bentonite

Saturation variation along the axial center lines in bentonite is also visualized in Figure 2-10. Due to the high capillary pressure of bentonite, the desaturation can be noticeable to 3 m away from the center line. Variations in capillary pressure within the bentonite are presented in Figure 2-11.

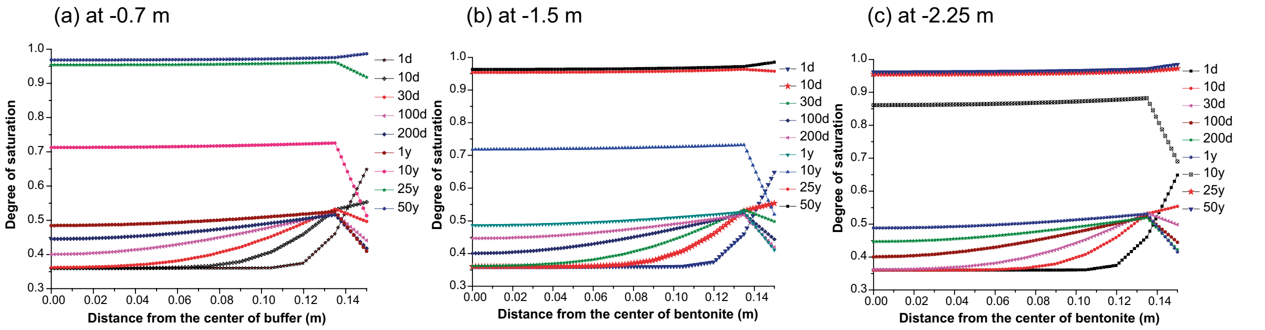


Figure 2-8. *Radial saturation distribution of bentonite in intact rock.*

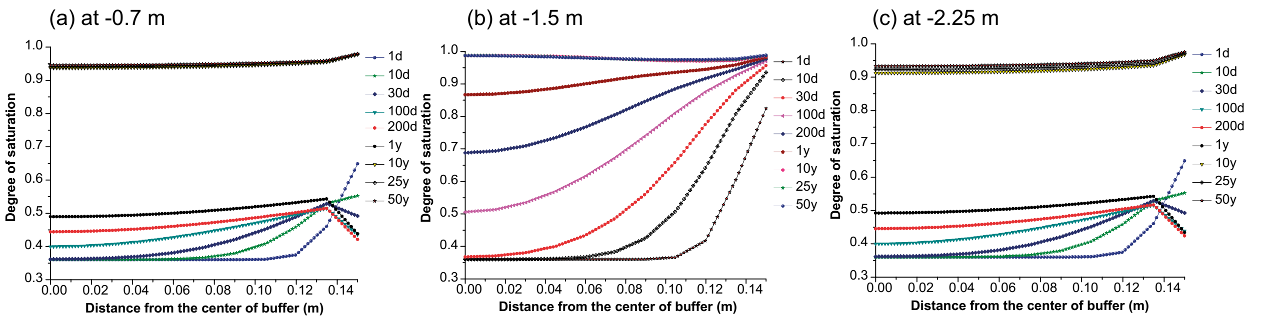


Figure 2-9. *Radial saturation distribution of bentonite in fractured rock.*

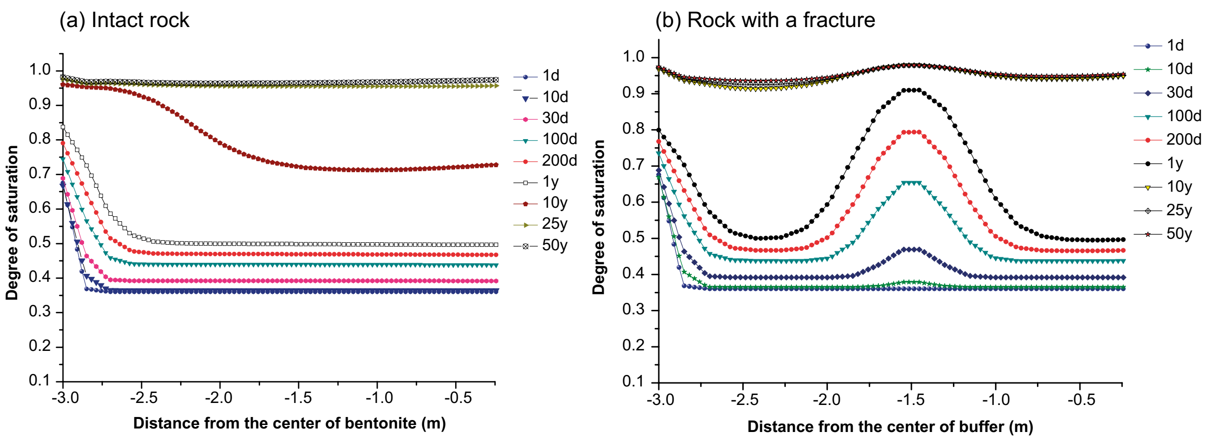


Figure 2-10. *Axial distribution of saturation in the bentonite.*

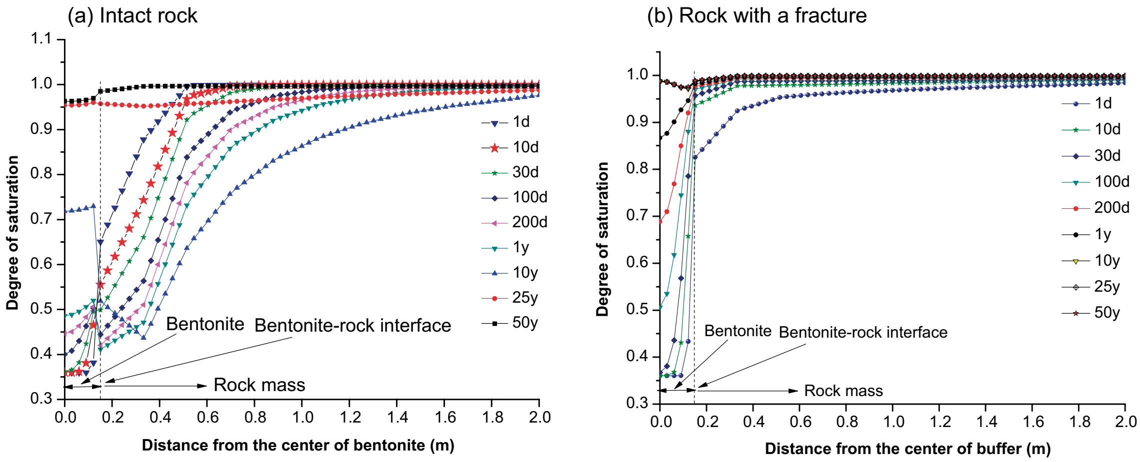


Figure 2-11. Radial distribution of saturation around the bentonite-rock interface (at 1.5 m).

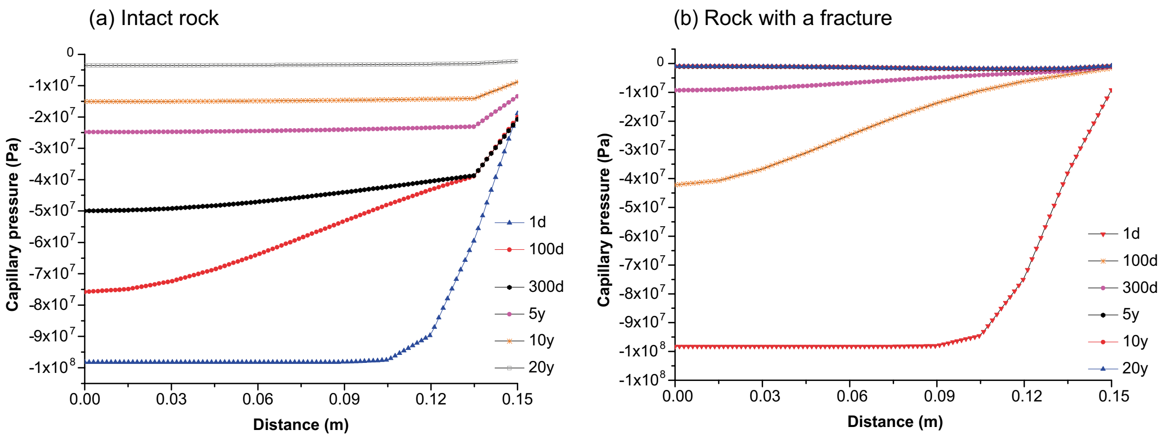


Figure 2-12. Variation of capillary pressure in bentonite.

2.5 Discussion

After installation of bentonite block in deposition hole, the capillary pressure inside the bentonite is initially maintained to −98.5 MPa (Figure 2-12). The pressure generally decreases with time inside the bentonite and significantly decreases at the interface. This is closely related to the sharp increase in saturation at the interface. Considering the initial capillary pressure of unsaturated bentonite is set to 100 MPa as a input parameter, bentontie material is properly implemented into TOUGH2 code.

Based on the numerical results, it is found that the time for full saturation of bentonite is about 2 years right at the vicinity of fracture and about 10 years in the center of the bentonite at tunnel floor level. The overall re-satuation rate for bentonite contacted with a fracture is 2.5 times faster than the case without fracture in deposition hole. Reversed trend in saturation profile is found especially around the rock–bentonite interface when the deposition hole is intact rock. This result is caused from that the water entry is not efficient because of relatively low permeability of intact rock in spite of the initial high capillary pressure of bentonite. The rate of flow across the bentonite-rock interface is controlled by the demand for water by the bentonite.

The results from Task 8a address the localized water entry through a fracture into the bentonite in deposition hole. Saturation, desaturation, pressure change are properly described at the interface of rock and bentontie. This study shows that the hydraulic behavior of unsaturated bentonite material is appropriately identified in this study. From this study, it can be found that hydraulic properties of fractures including location and orientation, especially intersecting the borehole of interest have a large impact on the prediction of bentonite hydration. In addition, the material properties bentonite (specifically permeability and constitutive relations) has also the potential for prominent impact on the bentonite resaturation.

2.6 Conclusions and recommendations

The effects of a rock fracture and high capillary pressure of bentonite on the re-wetting process are identified and appropriately predicted by the TOUGH2 code. The localized hydration of bentontie due to fracture in deposition hole is simulated and compared with the case without fracture from the perspective of the re-saturation and pressure changes especially at the interface of bentonite and rock.

3 Task 8b TASO – scoping calculation

3.1 Objectives

The primary objectives of Task 8b are first to predict inflow into the deposition hole based on the information of deterministic fractures around TASO tunnel, and second to evaluate the effects of artificial fracture which crosses bentonite block at the center of the deposition hole. Most of all, it is necessary to apply site-specific geological conditions and evaluate the impact of rock fractures on flow into deposition holes as well as the re-saturation of bentonite-filled deposition hole. The main objectives of Task 8b are as follows (Vidstrand et al. 2017):

- To predict inflows and inflow characteristics to deposition holes.
- To evaluate the significance of fractures.
- To evaluate effects of the artificial rock fracture along the deposition hole on the wetting of the bentonite.

3.2 Approach

The major differences with Task 8a are that the model domain has changed into 3D from 2D. A hypothetical single rock fracture intersecting deposition hole is taken into account in Task 8b and is assumed to have a thickness of 10 cm. The geometrical framework of Äspö HRL and the geological structure model are specified as CAD layer and imported into the simulation code. Further information on Task 8b such as boundary and initial condition and material specifications is found in the SKB report (Vidstrand et al. 2017). With regard to Task 8b, FracMan & Mafic and TOUGH2 are primarily used for hydraulic analysis. SketchUp Ver. 8 is used for mesh generation.

In this study, the rock matrix is represented by homogeneous continuum model rather than directly incorporating deterministic rock fractures into the numerical study. First of all, for the purpose of obtaining the equivalent permeability of rock mass, it is assumed that inflow from FracMan & Mafic code is identical to that from TOUGH2 code. An imaginary tunnel with a size of 4 m × 1 m × 20 m is taken into account within the same model domain as Task 8b (40 m × 40 m × 40 m) as shown in Figure 3-1. With regard to inflow estimation, a total of four cases are taken into account in the numerical study:

- Case 1: Intact rock.
- Case 2: Deterministic fractures.
- Case 3: Stochastic fractures.
- Case 4: Deterministic fractures + Stochastic fractures.

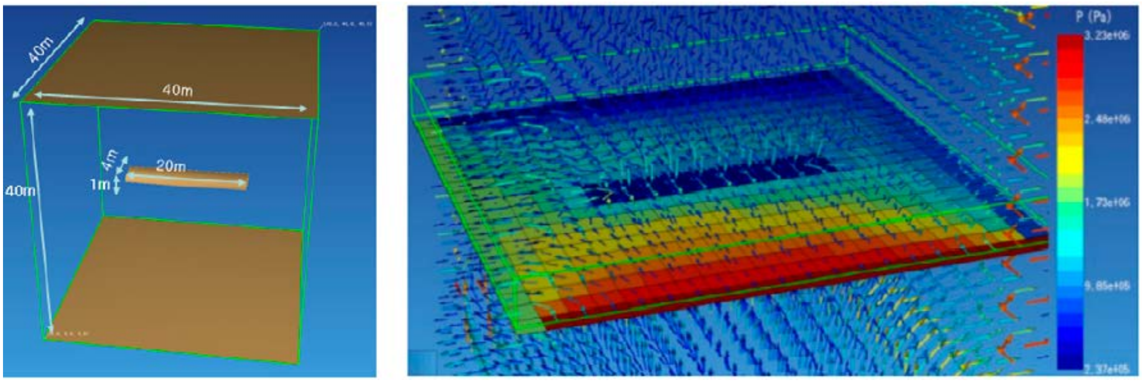


Figure 3-1. *Imaginary tunnel and pressure distribution.*

Saturation and pressure variation are subsequently investigated for the following two cases:

- Case A: Deposition hole without a hypothetical fracture under Case 4.
- Case B: Deposition hole intersected with a hypothetical fracture under Case 4.

Although the original mission in task descriptions (Vidstrand et al. 2017) corresponds to Case 2, additional case studies are performed to compare the modeling results and to evaluate the effects of geological features in rock on the bentonite re-saturation.

3.3 Model setup

A hypothetical single rock fracture is assigned as a circular feature of a diameter of 10 m with its center along with the center axis of the deposition hole. As reference case the single rock fracture should be horizontal and intersect the deposition hole described above at a depth of 1.5 m below the tunnel floor (Figure 3-3).

Pressure distribution on boundary planes is interpolated and averaged from discrete data points in TASO excel file which has been already distributed to members. Tunnel surface is set to atmospheric pressure. The bedrock-bentonite interface is also maintained to atmospheric pressure. The initial degree of saturation is 0.36 which corresponds to an initial suction value of 100 MPa.

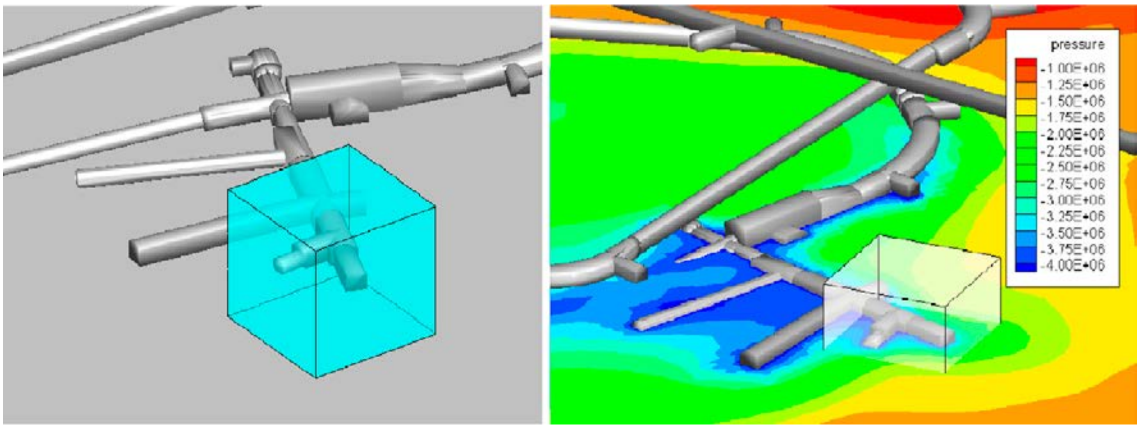


Figure 3-2. *Model domain of Äspö HRL site (a) and initial pressure field (b).*

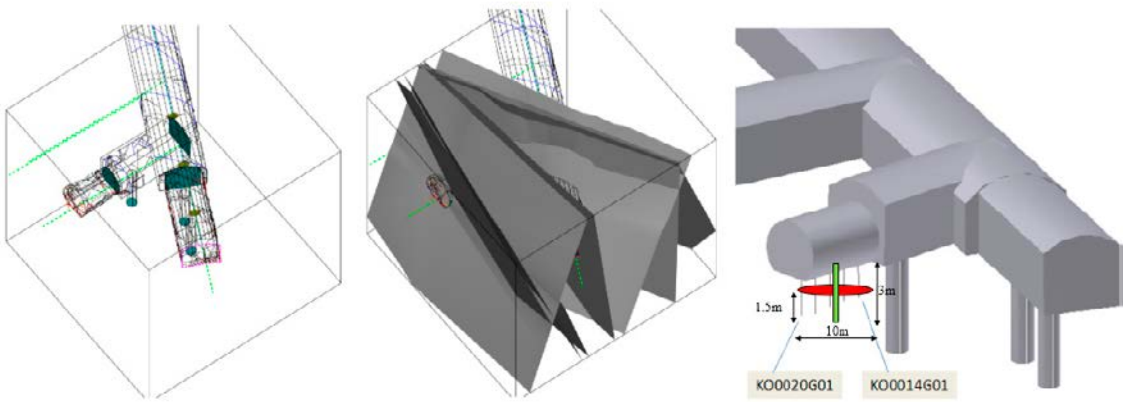


Figure 3-3. *Model geometry of TASO tunnel and deposition holes including geological deterministic fractures.*

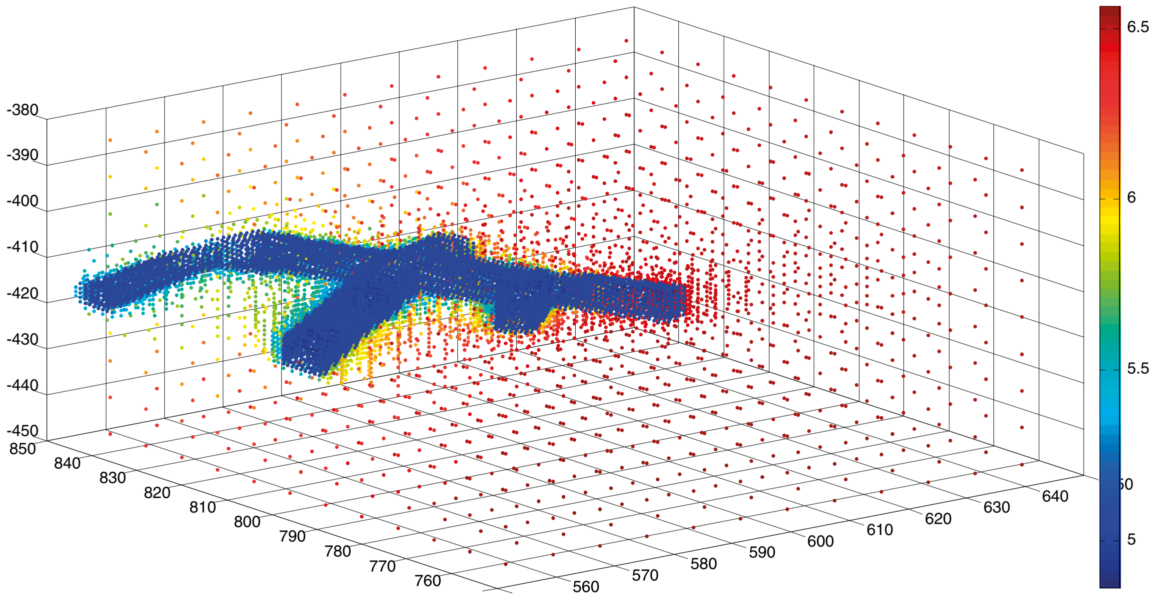


Figure 3-4. Boundary condition from TASO_pressure_salinity_velocity.xls.

Table 3-1. Material properties for Task 8b in TOUGH2 analysis (Vidstrand et al. 2017).

Material	Input parameter	Value
Intact rock	Hydraulic conductivity	1×10^{-12} m/s
	Porosity	1×10^{-5}
	Specific storage	1×10^{-10} m^{-1}
Geological fractures	Transmissivity	5×10^{-8} m^2/s
	Porosity for porous media	1×10^{-3}
	Transport aperture for DFN	1×10^{-5} m
	Storativity	1×10^{-8}
Single rock fracture	Transmissivity	5×10^{-10} m^2/s
	Porosity for porous media	1×10^{-3}
	Transport aperture for DFN	1×10^{-6} m
	Storativity	1×10^{-9}
Bentonite	Hydraulic conductivity	6.4×10^{-14} m/s
	Porosity	0.44
	Specific storage	1×10^{-11} m^{-1}

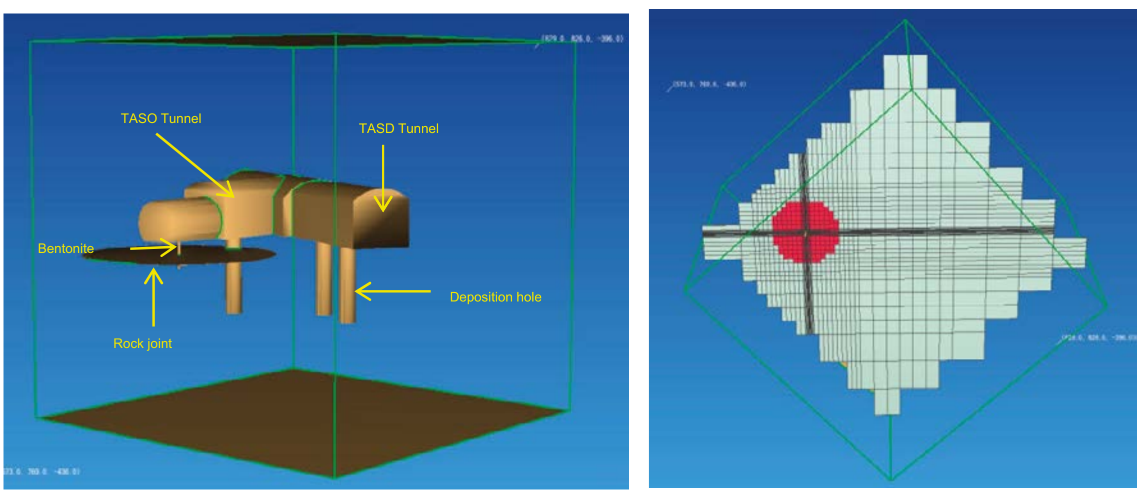


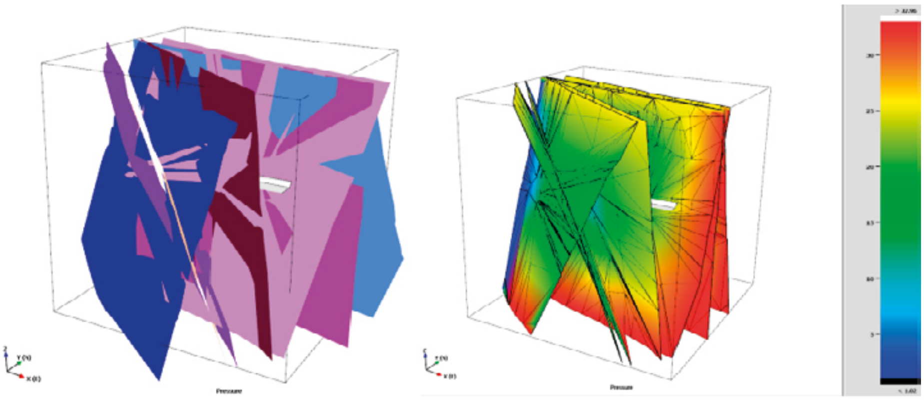
Figure 3-5. Tunnel geometry and element mesh around a hypothetical single rock fracture in TOUGH2 code.

3.4 Results

1) Estimation of equivalent permeability of rock

After the geological features are incorporated in the hydraulic simulation for each case, the groundwater inflows into the imaginary tunnel are subsequently estimated from FracMan and Mafic codes. Regarding the stochastic fractures, the fracture statistics of Task 8c are additionally used in this study.

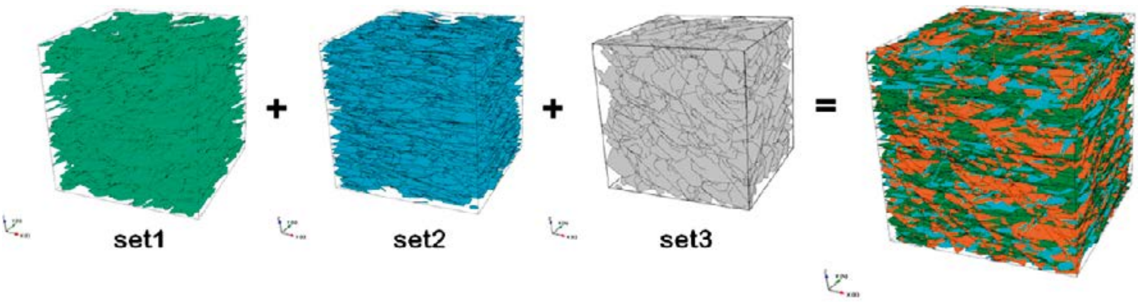
Case 2: Deterministic fractures

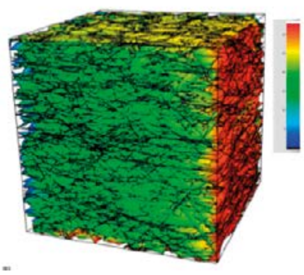


NODAL GROUP	EXTERNAL INFLOW (cu m /sec)	FRACTURE INFLOW (cu m /sec)	MATRIX INFLOW (cu m /sec)	WELL HEAD (m)	WELL INFLOW (cu m /sec)
1	1.924E-05	1.924E-05	0.000E+00		
2	4.253E-05	4.253E-05	0.000E+00		
3	-1.935E-05	-1.935E-05	0.000E+00		
4	9.381E-06	9.381E-06	0.000E+00		
6	-2.548E-05	-2.548E-05	0.000E+00		
7	-2.631E-05	-2.631E-05	0.000E+00		

Figure 3-6. *Pressure distribution and inflow estimation from FracMan & Mafic (Case 2).*

Case 3: Stochastic fractures





NODAL GROUP	EXTERNAL INFLOW (cu m /sec)	FRACTURE INFLOW (cu m /sec)	MATRIX INFLOW (cu m /sec)	WELL HEAD (m)	WELL INFLOW (cu m /sec)
1	1.516E-04	1.516E-04	0.000E+00		
2	2.966E-04	2.966E-04	0.000E+00		
3	-8.429E-05	-8.429E-05	0.000E+00		
4	4.774E-04	4.774E-04	0.000E+00		
5	-3.816E-04	-3.816E-04	0.000E+00		
6	-4.848E-04	-4.848E-04	0.000E+00		
7	2.513E-05	2.513E-05	0.000E+00		

Figure 3-7. *Pressure distribution and inflow estimation from FracMan & Mafic (Case 3).*

Case 4: Deterministic fractures + Stochastic fractures

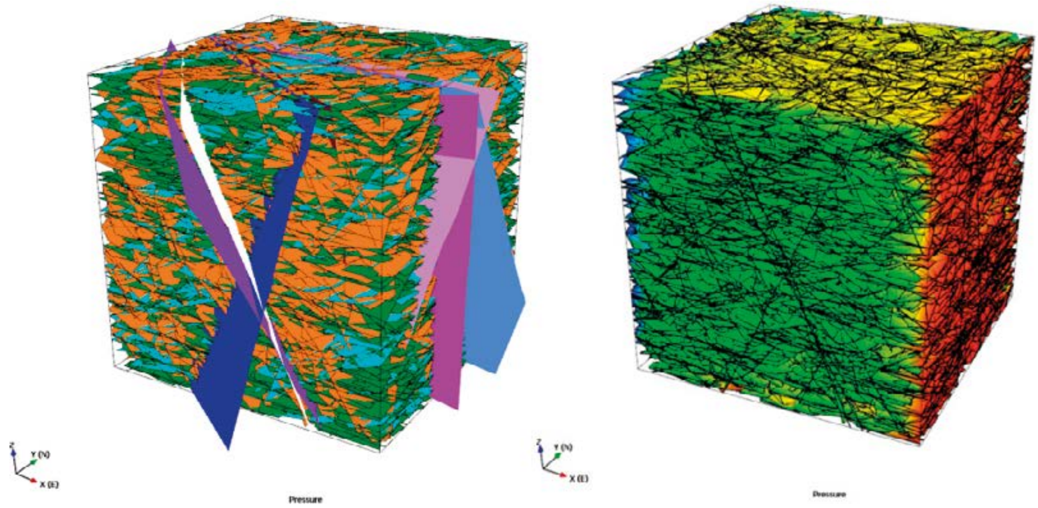


Figure 3-8. *Pressure distribution and inflow estimation from FracMan & Mafic (Case 4).*

When the hydraulic analysis is, for example, performed based on the stochastic fracture data, the inflow into the imaginary tunnel is 8.428E−02 kg/s, which corresponds to the permeability of 1.14E−15 m^2 provided that the hydraulic gradient is constant.

From comparison of inflows calculated from FracMan & Mafic and TOUGH2, the equivalent permeability of rock mass is obtained and listed in Table 3-2, which will be used in homogeneous continuum analysis.

Table 3-2. Estimated equivalent permeability of rock mass.

Type		Inflow (kg/h)	Estimated Eq. perm. (m^2)
Case 2	Deterministic seven fractures	69.66	2.6E−16
Case 3	Stochastic fractures	303.44	1.1E−15
Case 4	Deterministic and stochastic fractures	379.08	1.4E−15

2) Prediction of inflow into deposition hole

Inflow into a deposition hole is estimated for the each case and listed in Table 3-3. It is found in this study that the stochastic fractures have more significant effects on the inflow than seven deterministic fractures. The relatively large amount of inflow is predicted in this study. It is likely attributable to the assumption that stochastic discrete fracture has a permeability of 3.061E−10 m^2 with the aperture of 1E−5 m. This permeability value is typically considered very large. Thus, further study still remains with regard to the parameter uncertainties and sensitivity analysis after changing the permeability of stochastic discrete fracture into more reasonable value.

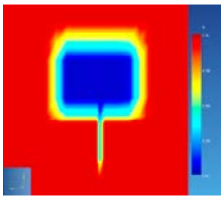
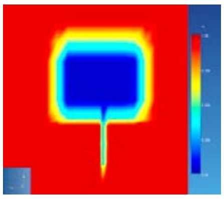
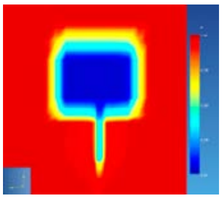
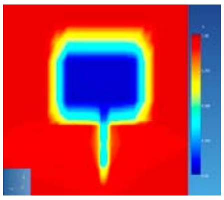
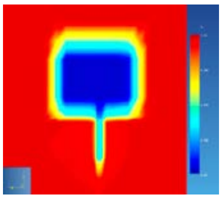
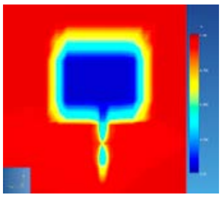
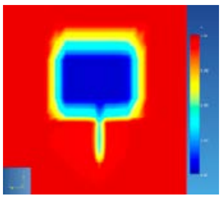
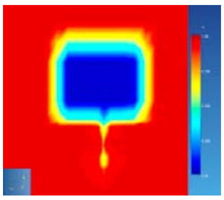
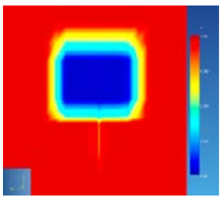
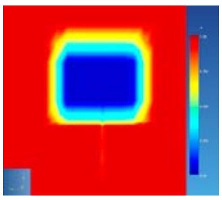
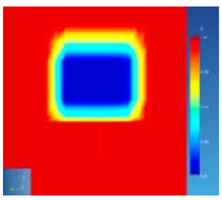
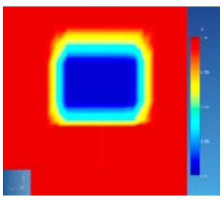
Table 3-3. Estimated inflow into deposition hole.

Parameter	Case 1 Intact rock	Case 2 Deterministic fracture	Case 3 Stochastic fractures	Case 4 Deterministic and stochastic fractures
Inflow (ml/min)	1.92E−2	5.39E−00	15.7E−00	19.1E−00

3) Variation in saturation and pressure around deposition hole

Variations in saturation with time for the Case 4 are presented in Table 3-4 and Figure 3-9 below. The table shows difference in saturation distribution in accordance with whether the rock fracture is taken into account. In addition the pressure distribution around deposition hole at 0.1 year is presented in Figure 3-10 in which horizontal and vertical cutting planes are additionally embedded. The time required to arrive at 99 % of saturation is 2.92 years in case of fractured rock. The case without rock fracture is predicted to be 3.49 years.

Table 3-4. Variation in saturation with time around deposition hole (vertical view).

Elapsed year	Deposition hole (Case A)	Deposition hole with fracture (Case B)
0.0 y		
0.1 y		
0.3 y		
0.5 y		
1.0 y		
2.0 y		

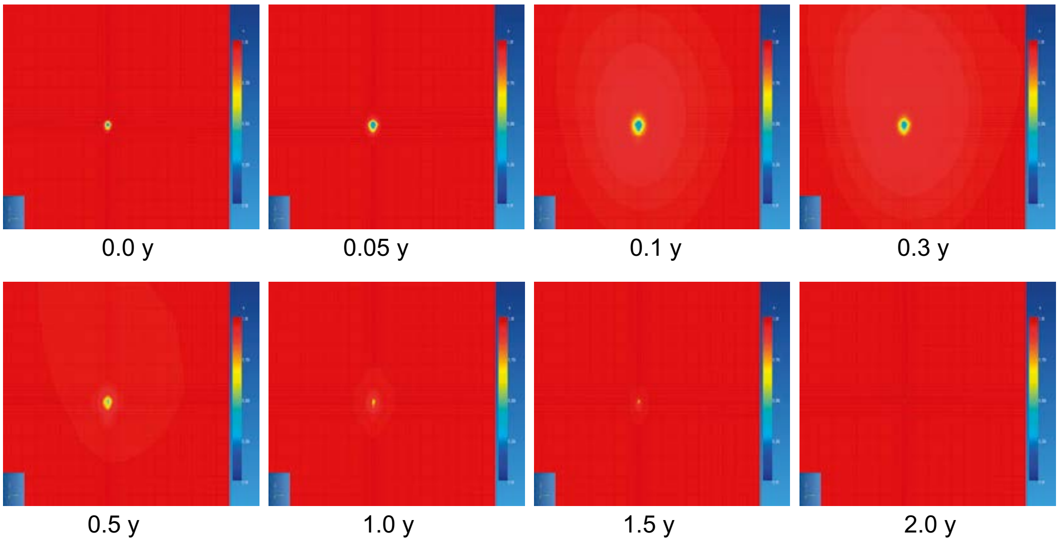
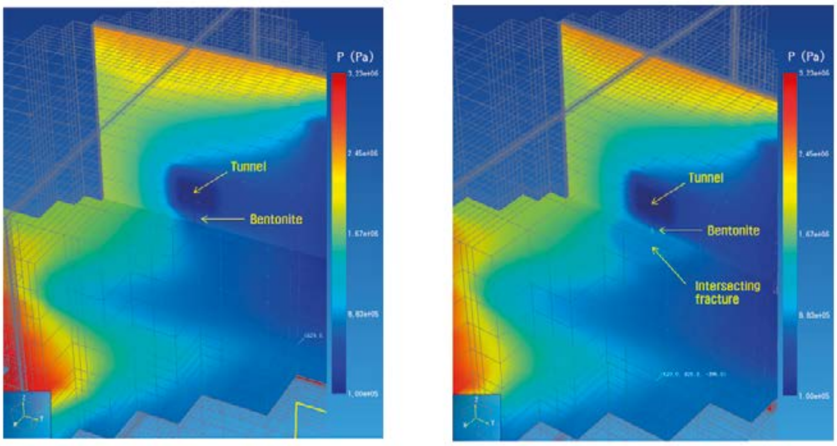


Figure 3-9. *Variation in saturation around deposition hole intersected with fracture (horizontal view).*



(a) Without a fracture

(b) With a fracture

Figure 3-10. *Variation in pressure around deposition hole at 0.1 year.*

3.5 Discussion

Taking into account the a hypothetical single rock fracture gives rise to difference in time required for full saturation, that is, about a half year, which is not a substantial difference from the perspective of long-term performance of bentontie. This is likely caused from that whether bentonite resaturation is limited by the water supply or by the water demand from the bentonite for a variety of fracture configurations.

Although the final time needed to approach full saturation is not different so much, the initial re-wetting behaviors of bentonite are remarkably different with each other because of the localized water entry through a hypothetical fracture.

The effects of major deterministic fractures around TASO tunnel are evaluated by using a concept of equivalent permeability. From Task 8b study, it is found that the stochastic fractures have more significant effects on the inflow than deterministic fractures. But this can include a large uncertainty with regard to estimation inflow because the estimated hydraulic properties are sensitive to the degree to which the current deterministic fractures intersect the tunnel. Moreover, the size of an imaginary tunnel and the range of model domain to be assigned are still remained to be decided from the more reliable background and modeler's experience, which also contributes to the uncertainty of model.

When the deterministic fractures are directly embedded into the model geometry, less inflow is estimated at the deposition hole than the method using equivalent permeability in this study. This has been tested only for less than four deterministic fractures (data not shown here) due to convergence failure beyond four fractures in this study. The application of equivalent permeability concept to major deterministic fractures is regarded as oversimplified approach.

Although the homogeneous continuum model is applied in this study because the TOUGH2 code is sensitive to the sharp contrast in properties across a very short distance such as fractures, it is necessary to develop better method to overcome this problem in TOUGH2. This has been tried in the following sub-Task 8c.

3.6 Conclusions and recommendations

Hydration of bentonite and the effects of rock fracture on the re-wetting process are properly identified even under 3D model domain in which real site-specific information such as geometrical framework, geological structure, and boundary condition is assigned.

The homogeneous continuum model is applied by using equivalent permeability with regard to deterministic fractures in this study. However, it may give rise to the oversimplified model which is less sensitive to changes in material properties and has a large amount of uncertainty. Thus it is necessary that stochastic discrete fracture network is modeled as homogeneous equivalent porous medium, and large deterministic fractures are explicitly embedded into a model geometry.

4 Task 8c BRIE – prediction for central deposition hole

4.1 Objectives

In Task 8c, deterministic rock fractures and stochastic fracture network should be taken into account in addition to Task 8b. Probing boreholes are expanded to a diameter of 0.3 m in which water inflow and bentonit re-wetting should be predicted. Task 8c consists of two parts as follows.

The main objectives of Task 8c are:

- Task 8c1: To predict inflows and inflow characteristics to deposition holes based on the main geological features of the TASO site.
- Task 8c2: To evaluate effects of the fracture locations along the deposition hole on the resulting wetting of the bentonite.

4.2 Approach

The prediction of re-wetting process of bentonite primarily depends on the reliability on measurement of flow into deposition hole. Equivalent porous medium (EPM) with discrete fracture network (DFN) is considered in Task 8c study. Thus stochastic fractures are primarily evaluated by a parameter of equivalent permeability in TOUGH2 . Three deterministic fractures are directly embedded into the model geometry.

Boundary condition and material properties are same to those in Task 8b except for the properties of three deterministic fractures. To take into account fracture statistics for TASO tunnel, FracMan is used to generate DFN. Joint set 1, 2, and 3 are represented by 10685, 19272 and 7381 fractures respectively.

COMSOL is applied for the mesh generation of model geometry including deterministic fractures. FLAC3D is also used for steady-state analysis in prior to TOUGH2 simulation to reduce the possible convergence failure which is usually related to the sharp contrast in properties across a short distance such as fractures. The simulation results from TOUGH2 code are visualized by Tecplot360.

By applying the concept described in Figure 4-1, all the elements are assigned to smeared fracture properties. A large amount of computer resources, however, are generally necessary for numerical calculation in TOUGH2 code.

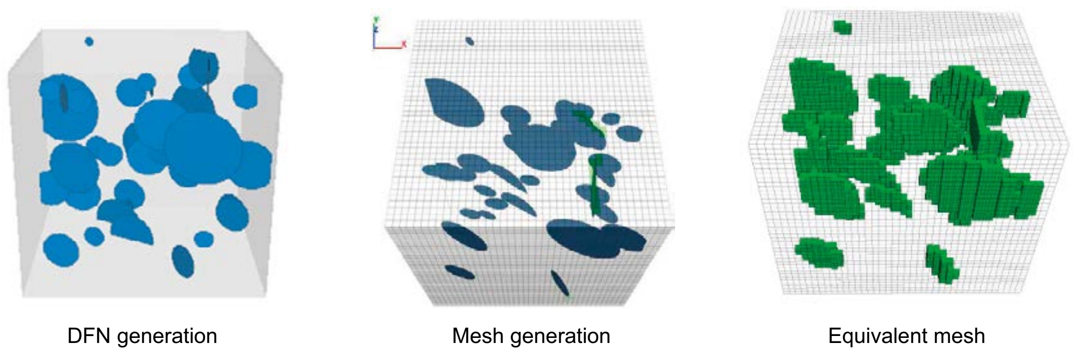


Figure 4-1. *DFN (Discrete fracture network) generation in FLAC3D code.*

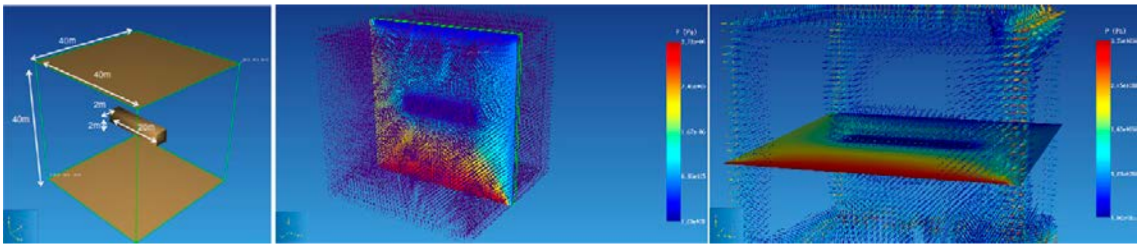


Figure 4-2. Imaginary tunnel and groundwater inflow into tunnel at 0.75 year.

Consequently, additional preprocessing is added before primary numerical calculation. In similar to Task 8b, the imaginary tunnel with a size of 2 × 2 × 20 m is taken into account within a model domain of 40 × 40 × 40 m in which all the element are assigned to smeared fracture properties with regard to stochastic fracture. The equivalent permeability is estimated by assuming that the inflow into an imaginary tunnel calculated from FLAC3D based on the DFN information is same to that from TOUGH2 code under the same geometrical condition. Equivalent permeability of rock mass is obtained in FLAC3D code by applying Smeared Fracture Model as follows:

$$k_e = \frac{k_f \cdot V_f + k_m \cdot V_m}{V_e}$$

k_f: hydraulic conductivity tensor of the fracture

k_m: hydraulic conductivity tensor of the rock matrix

V_e: volume of the element

V_f: volume of the fracture in the element

V_m: volume of the rock matrix in the element

The model assumed that the permeability of element is closely related to that of fracture, in which the amount of increase is proportional to the volume ratio of fracture to rock matrix. When background fractures generated from DFN are intersected in an element, the permeability in an element is increased in accordance with the number of overlapped fractures and intersected distance.

4.3 Model setup

The mode geometry of TASO tunnel including three deterministic fractures and probing boreholes around deposition holes is presented in Figure 4-3. Material properties used in TOUGH2 analysis for Task 8c is listed in Table 4-1. The other material properties and input parameters are same to those used in Task 8b. Total mesh number in Task 8c is 67 002 within a domain of 40 × 40 × 40 m (Figure 4-5).

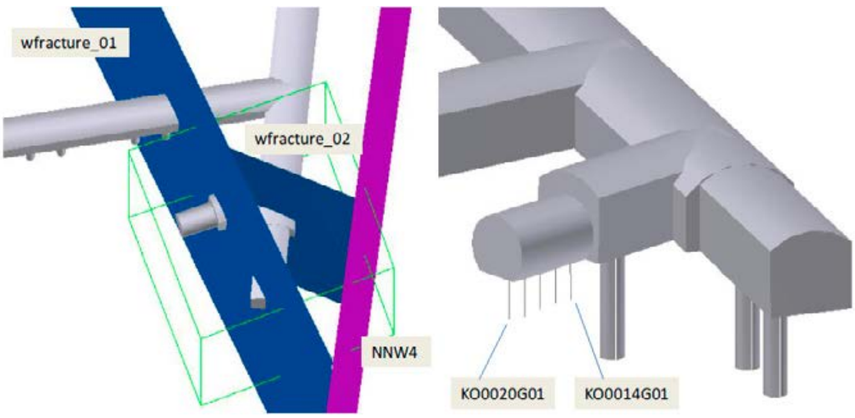


Figure 4-3. Model geometry of TASO tunnel including three deterministic fractures and probing boreholes (Task 8c).

Figure 4-4. *Illustration of probing borehole spacing and naming.*

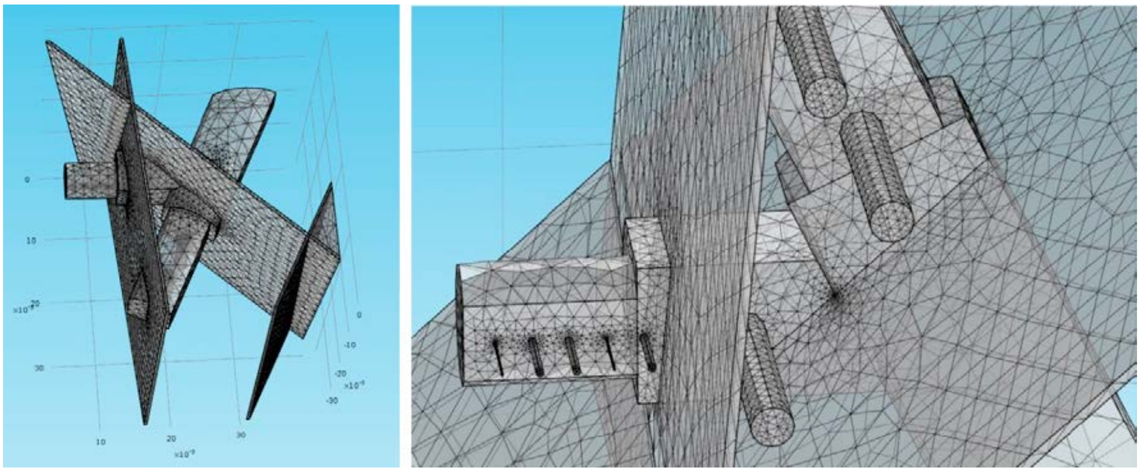


Figure 4-5. *Tunnel mesh information including probing boreholes and three deterministic fractures.*

Table 4-1. Material properties for Task 8c in TOUGH2 analysis (Vidstrand et al. 2017).

Material	Input parameter	Value
Intact rock	Hydraulic conductivity	1×10^{-14} m/s
	Porosity	1×10^{-5}
	Specific storage	1×10^{-11} m^{-1}
Geological wfracture_01	Geological width	1.0 m
	Transmissivity	2×10^{-8} m^2/s
	Porosity for porous media	1×10^{-3}
	Transport aperture for DFN	1×10^{-5} m
	Storativity	1×10^{-8}
Geological wfracture_02	Geological width	0.001 m
	Transmissivity	2×10^{-9} m^2/s
	Porosity for porous media	1×10^{-3}
	Transport aperture for DFN	1×10^{-5} m
	Storativity	1×10^{-8}
NNW4	Geological width	10.0 m
	Transmissivity	6.5×10^{-7} m^2/s
	Porosity for porous media	1×10^{-3}
	Transport aperture for DFN	1×10^{-5} m
	Storativity	1×10^{-7}
Bentonite	Hydraulic conductivity	6.4×10^{-14} m/s
	Porosity	0.44
	Specific storage	1×10^{-6} m^{-1}

Table 4-2. Suggested fracture statistics to be used for the TASO tunnel.

Set	Orientation			Size		Spatial	Intensity
	Trend	Plunge	Fisher konc.	r_0	k_r	Distribution	P_{32} (r_0,∞)
Set 1	280	20	10	0.25	2.6	Poisonian	1.1
Set 2	20	10	15	0.25	2.6	Poisonian	2
Set 3	120	50	10	0.25	2.6	Poisonian	0.75

After DFN is generated from FracMan, the data such as XPosition, YPosition, ZPosition, Dip, Dip direction, Fracture size (diameter) are extracted for each fracture. This information is imported into FLAC3D code by fish function. Then all the elements are assigned to smeared fracture properties. Subsequently, steady state analysis is additionally performed by FLAC3D simulation. By application of an imaginary tunnel, the equivalent permeability is subsequently estimated by comparison the results from FLAC3D and TOUGH2 codes.

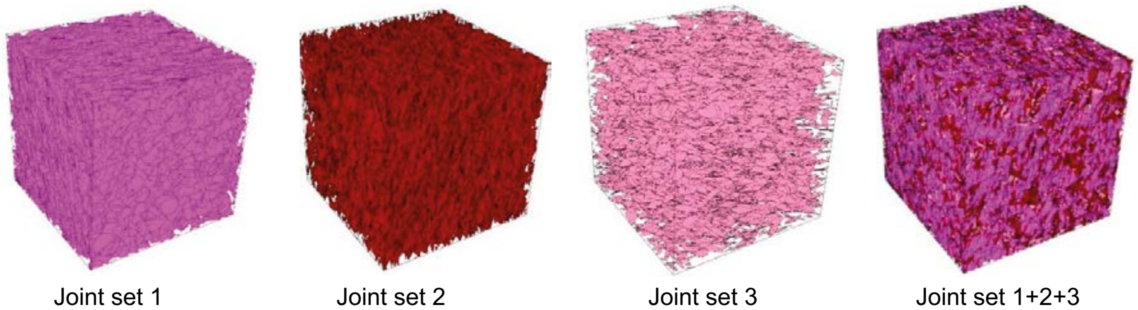


Figure 4-6. *Joint set 1+2+3 from FracMan.*

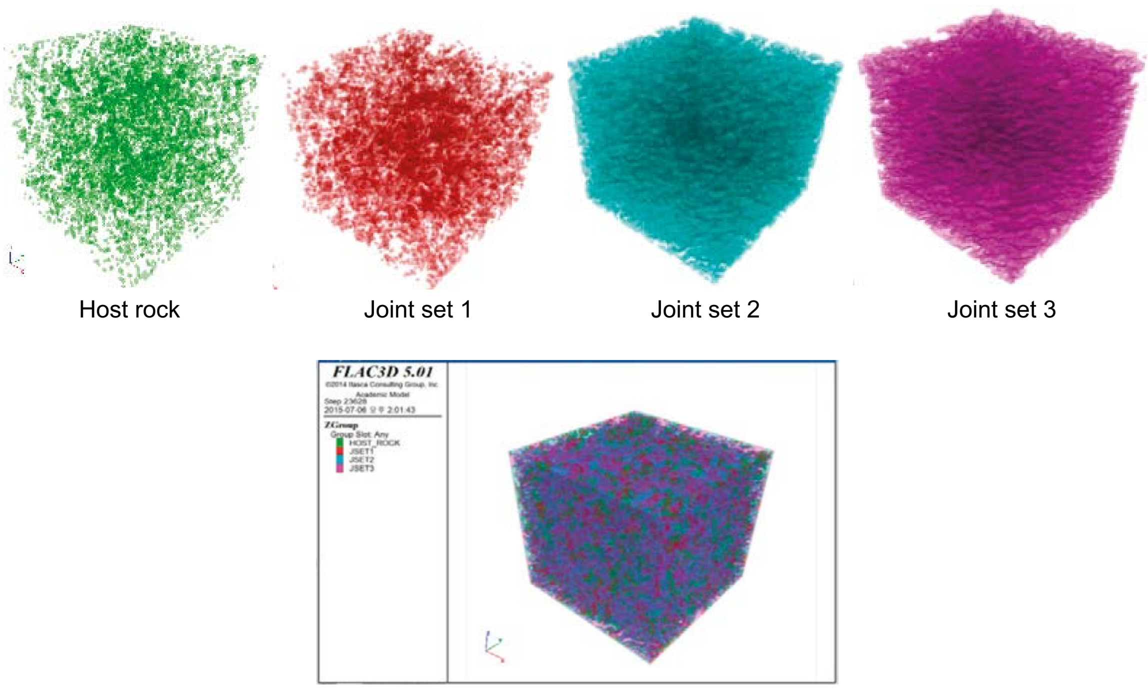


Figure 4-7. *Element information including host rock and joint set 1 + 2 + 3 (DFN and corresponding ZGroup in FLAC3D).*

4.4 Results

1) Estimation of groundwater inflow into probing holes.

The variation of inflow is, first of all, evaluated in according to geological features. After the permeability of DFN joint set is assumed as 1E−10 m^2, the inflow into boreholes are calculated for the cases such as intact rock, intact rock including deterministic fractures, and equivalent porous rock (DFN) including deterministic fractures. The estimated inflows are presented in Table 4-3 and Table 4-4. The borehole of BEN18 and BEN17 are expanded boreholes to 30 cm.

Table 4-3. Inflow into the boreholes after excavation.

Borehole (ml/min)	KO20	KO18	KO17	KO15	KO14
All intact rock	9.72E−05	7.48E−05	6.42E−05	5.55E−05	5.55E−05
Intact rock + deterministic fractures	8.52E−04	1.12E−03	1.12E−03	7.48E−04	1.09E−04
Equivalent porous rock (DFN) + deterministic fractures	8.58E+00	6.39E+00	5.39E+00	4.75E+00	5.07E+00

Table 4-4. Inflow into the over-cored boreholes after excavation.

Over-cored borehole (ml/min)	KO20	BEN18	BEN17	KO15	KO14
All intact rock	8.84E−05	1.50E−04	7.85E−05	4.52E−05	9.28E−05
Intact rock + deterministic fractures	7.50E−04	2.38E−03	1.87E−03	6.64E−04	2.09E−05
Equivalent porous rock (DFN) + deterministic fractures	7.99E+00	1.32E+01	6.85E+00	4.00E+00	9.11E−05

After over-coring the borehole KO18 and KO17, 30 ~ 60 % of inflow increase while causing the inflows slightly decreased in the neighboring boreholes. From this case study, it is found that the background fractures have more dominant effects than deterministic large fractures on inflow estimation.

2) Variations in saturation and pressure around TASO tunnel

The variations in saturation and pressure of bentonite are presented in Figure 4-7 and Figure 4-9 respectively. The degree of saturation in bentonite is 99.2 % after three years. The figures show that full saturations are obtained less than about 5 years.

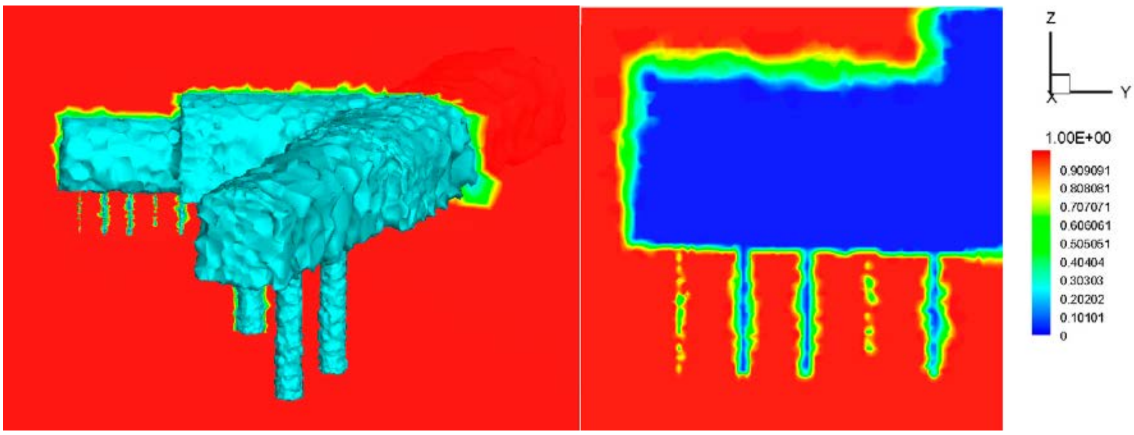


Figure 4-8. *Saturation distribution with geometric model around TASO tunnel.*

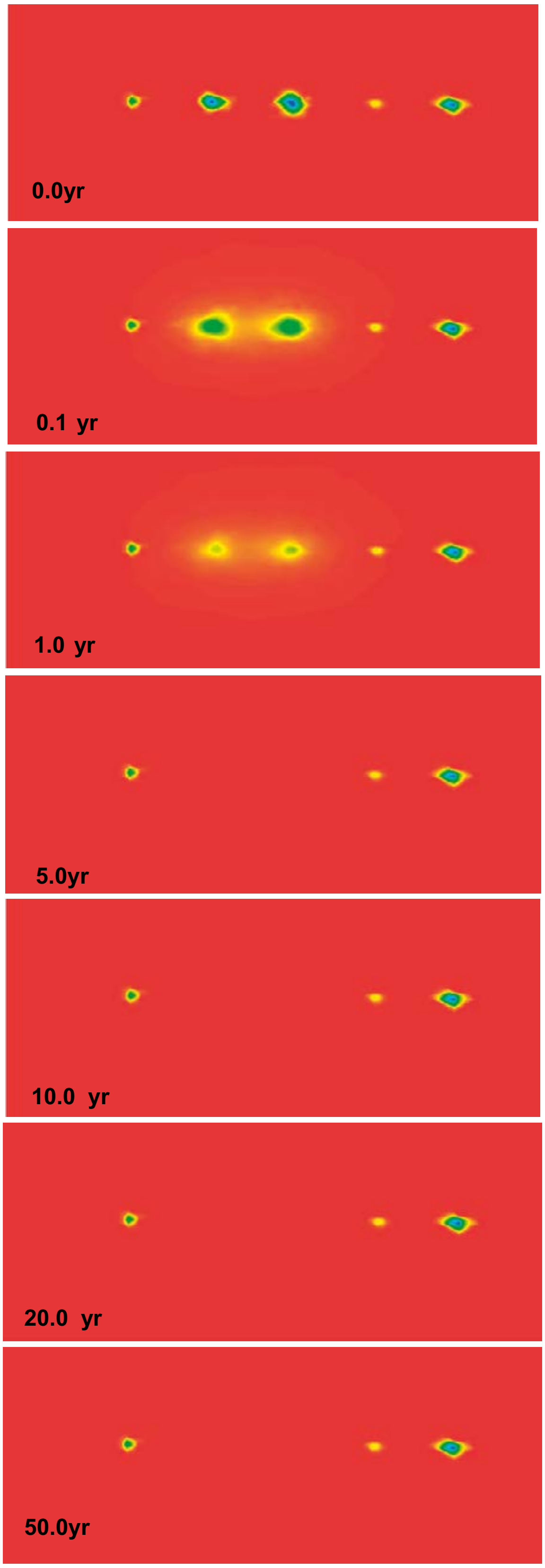


Figure 4-9. *Saturation distribution with time.*

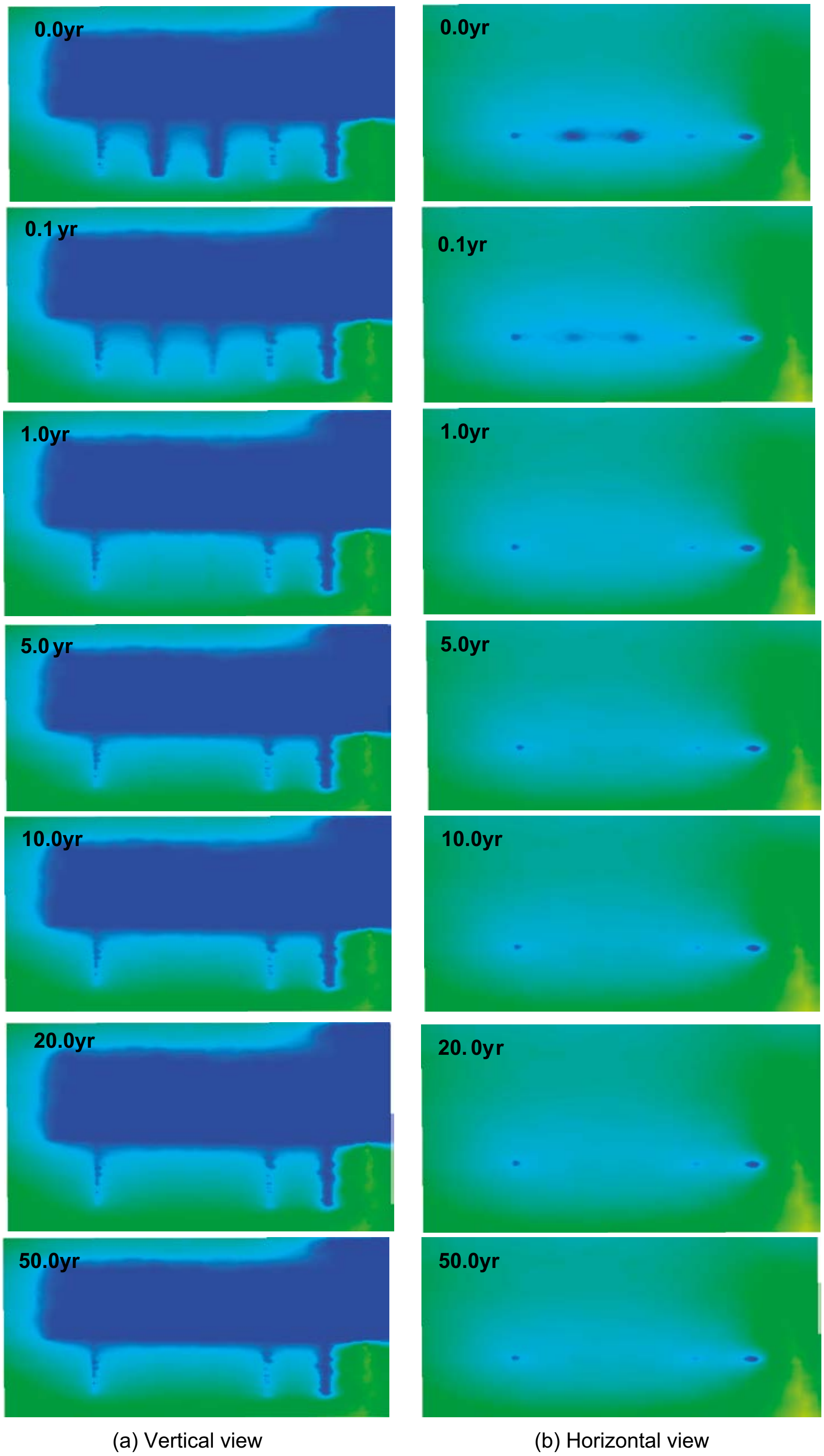


Figure 4-10. *Pressure distribution with time.*

4.5 Discussion

In this study, the rock represented by stochastic discrete fractures is simplified to equivalent porous medium, in which equivalent permeability is primarily taken into account. Geological features in rock mass are very complicated and have some potential affecting the performance behavior of EBS. With regard to the model development, its simplification is inevitable for numerical simulation. This complexity level is difficult to be determined and often requires detailed interpretations to create a solid basis for the simplification. The modeller's insights, preferences, and experiences are also essential factors, along with various constraints and limitations.

Stochastic fractures can be modeled by smeared fractures in Task 8c. Although modeling the fracture by smeared fracture hardly reduce the accuracy of analysis, the direct incorporation of smeared fracture into a model requires a lot of computer resources and time consuming in TOUGH2 code. Thus, equivalent permeability of rock mass is taken into account by smeared fracture model in FLAC3D code. As previously mentioned, however, the size of an imaginary tunnel and the range of model domain to be assigned are still remained to be decided from the more reliable criteria and modeler's experience, which also contributes to the uncertainty of model.

Consequently, it is recommend that the far-field represented by stochastic discrete fracture network (DFN) is simply modeled as homogeneous equivalent porous medium, in which equivalent permeability is obtained from the comparative study between FLAC3D and TOUGH2 codes, and large deterministic fractures or discrete fractures near deposition hole are explicitly embedded into a model. In addition, sensitivity analysis with regard to the aperture distribution, fracture shape, size etc of the stochastic discrete fractures requires further study. The effects of each deterministic fracture on inflow also need to be evaluated.

4.6 Conclusions and recommendations

The inflows into probing boreholes and bentonite re-saturation are predicted based on the geological fracture information around TASO tunnel. It is found that the time required for the full saturation of bentonite is less than five years and the inflow into probing borehole is proportional to the permeability around the rock mass. It is necessary to calibrate the simulation results with the field data from BRIE. From the sensitivity analysis it is noted that inflow into probing boreholes is not significantly affected by large deterministic features if they are not directly intersected with the boreholes.

5 Task 8d BRIE– prediction of inflow and wetting based on detailed characterisation data

5.1 Objectives

Task 8d can be divided into two parts, i.e. Task 8d1 and Task 8d2. Bentonite is not taken into account in the Task 8d1. The simulation conditions are similar to Task 8c. Fractures intersecting probing boreholes and monitoring boreholes are additionally embedded in Task 8d. Additional detailed hydraulic data are included in Task 8d. The main objectives with this exercise are (Vidstrand et al. 2017):

- Task 8d1.
  – To calculate inflows and inflow characteristics to two 76 mm diameter probing boreholes.
  – To calculate inflows and inflow characteristics to two 30 cm diameter open boreholes.
- Task 8d2.
  – To evaluate the resulting wetting of the bentonite installed in the borehole.
  – To evaluate effects of heterogeneous fracture flow and matrix properties on the wetting.

5.2 Approach

Numerical model development is based on the insights and the methodologies gained from previous Task 8c. A lot of computer resources are generally required in TOUGH2 and FLAC3D with regard to application of smeared fracture model to all the elements in model domain. Equivalent permeability, therefore, is estimated from fracture statistics around TASO tunnel by application of an imaginary tunnel (2 × 2 × 20 m) into model domain. Equivalent permeability is obtained by assuming that the inflow estimated from TOUGH2 code is same to that from FLAC3D code in which site-specific DFN is evaluated by applying the smeared fracture model with regard to the hydraulic properties. Three deterministic large fractures and small-scale fractures with large transmissivity ($\log_{10}(T) > -11.6$) intersecting probing borehole are directly embedded to the model geometry of Task 8d. They are assumed to have a thickness of 5 cm

KAERI-simulator (TOUGH2 code coupled with FLAC3D by using MATLAB) is primarily used for analyzing hydraulic behaviors of bentonite including rock mass. COMSOL is used to mesh generation. KAERI-simulator includes TOUGH2 and FLAC3D codes. The former is for hydraulic analysis (T, P_g, S_g) and the other is for stress calculation (σ). Although the mechanical analysis is not included in Task 8, FLAC3D was, firstly, used for geometry generation and initial stabilization (stress and pressure) for increasing numerical stability. The values from FLAC3D were directly used in TOUGH2 simulation as initial values. Additionally, FLAC3D was used for the purpose of monitoring the simulation in process and that post-processing of simulated results, that is, easy to show in form of the graph. When the main simulation starts, the mechanical module of KAERI-simulator was turn off.

5.3 Model setup

The mode geometry is presented in Figure 5-1 below. In contrary to Task 8c, additional monitoring boreholes surrounding probing borehole and site-specific small fractures intersecting probing boreholes are further embedded in Task 8d. Material properties used in TOUGH2 analysis and other input parameters including initial and boundary conditions are same to those used in Task 8c. Total mesh number in Task 8d is 74 184 within a domain of 40 × 40 × 40 m (Figure 5-1).

Site specific-stochastic fracture statistics are given as intensity, size and orientation data, and serve as the basis for the hydraulic properties. DFN generated from FracMan is applied to FLAC3D for equivalent permeability calculation.

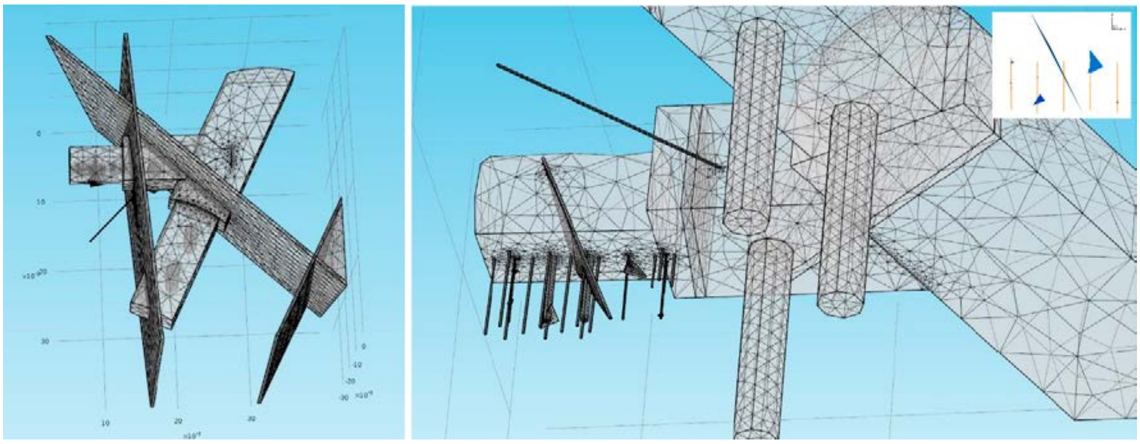
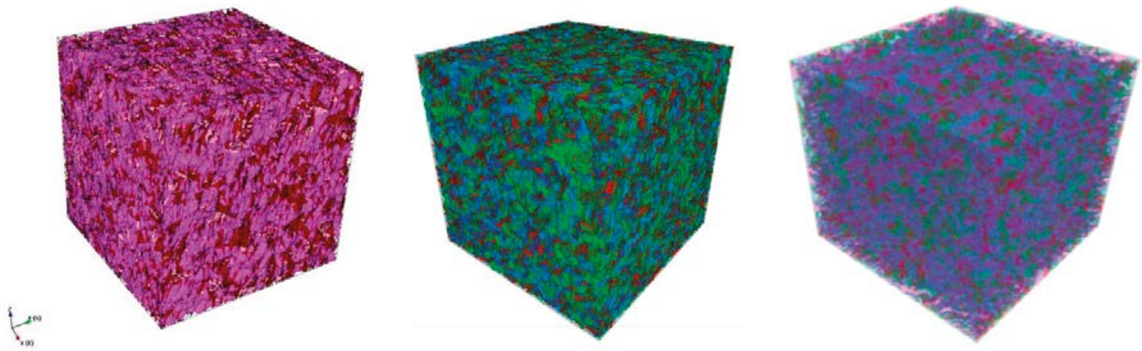


Figure 5-1. *Model geometry for Task 8d.*



(a) DFN from FracMan (b) DFN into FLAC3D (c) EPM with DFN in FLAC3D

Figure 5-2. *DFN generation and EPM (Equivalent Porous Medium).*

5.4 Results

1) Estimation of groundwater inflow into probing holes

When the permeability of intact rock is assumed to be 1.02 × E−21 m^2, the inflow into an imaginary tunnel is calculated as 1.652E−7 kg/sec from FLAC3D. While the inflow from TOUGH2 code is calculated to be 0.911E−7 kg/sec. It should be noted that some difference is found in the estimated flow between TOUGH2 and FLAC3D codes even under the identical input condition without discrete fractures. The value from FLAC3D is consistently 1.813 times larger than that from TOUGH2 code in this study.

TOUGH2 code is possible to take into account the saturation gradient, in particular, at the surface of rock wall. This means that saturation shows a transient profile from the tunnel wall into the rock mass. KAERI team usually assumes the degree of saturation at the tunnel wall is 0.8 ~ 0.85. However, FLAC3D can simulate behaviours only for the cases under the saturated or dry condition provided that the additional modelling technique is not taken into account (i.e. Fish function etc). The rock surface is assumed to be fully saturated in FLAC3D code.

Consequently, the calibration factor between two codes should be taken into account with regard to inflow estimation when using TOUGH2 code. When aperture thickness of discrete fracture is assumed to be a 1E−05 m, the estimated inflow from FLAC3D is presented in accordance with the permeability of joint set in Table 5-1. Equivalent permeability of 1.13E−19 m^2 is selected to be used in this study.

Table 5-1. Equivalent permeability to be used in TOUGH2 by calibration.

Joint set permeability in DFN (m²)	Inflow from FLAC3D (kg/sec)	Calibrated inflow in TOUGH2 (kg/sec)	Equivalent permeability to be used in TOUGH2 (m²)
3.06E−14	1.81E−04	9.96E−05	1.11E−18
3.06E−15	1.82E−05	1.01E−05	1.13E−19
3.06E−16	1.98E−06	1.09E−06	1.22E−20
3.06E−17	3.51E−07	1.93E−07	2.17E−21
3.06E−18	1.84E−07	1.02E−07	1.14E−21
3.06E−19	1.67E−07	9.21E−08	1.03E−21

Based on this information, the inflow into borehole is calculated from TOUGH2 code and listed in Table 5-2. In the borehole of BEN18, relatively large difference is found at inflow estimation between simulation and BRIE data. It is likely that there are some geological features or processes such as impermeable zone around the BEN18 (KO018). As more data became available, the model should be adjusted to better reproduce the observations made in probing boreholes.

Table 5-2. Inflow into boreholes after excavation at 0.1 year.

Borehole	KO20	BEN18(KO18)	BEN17(KO17)	KO15	KO14
Inflow (ml/min)	0.48	1.00	0.95	0.13	0.22
BRIE (ml/min)*	0.01	0.0 (0.01–0.03)**	1.0 (0.12–0.25)**	0.6	0.1

* Inflows from short duration test (approx. 15 min).

** Values in parenthesis indicate inflow into 300 mm diameter open boreholes.

2) Variations in saturation and pressure around TASO tunnel

The required time for full saturation of bentonite is around 100 years or more. These values are much longer than the time from Task 8c (less than 5 years).

Pressure distribution around TASO tunnel is presented in Figure 5-4 with time. The pressure does not show substantial difference with time and remains relatively low value around the boreholes.

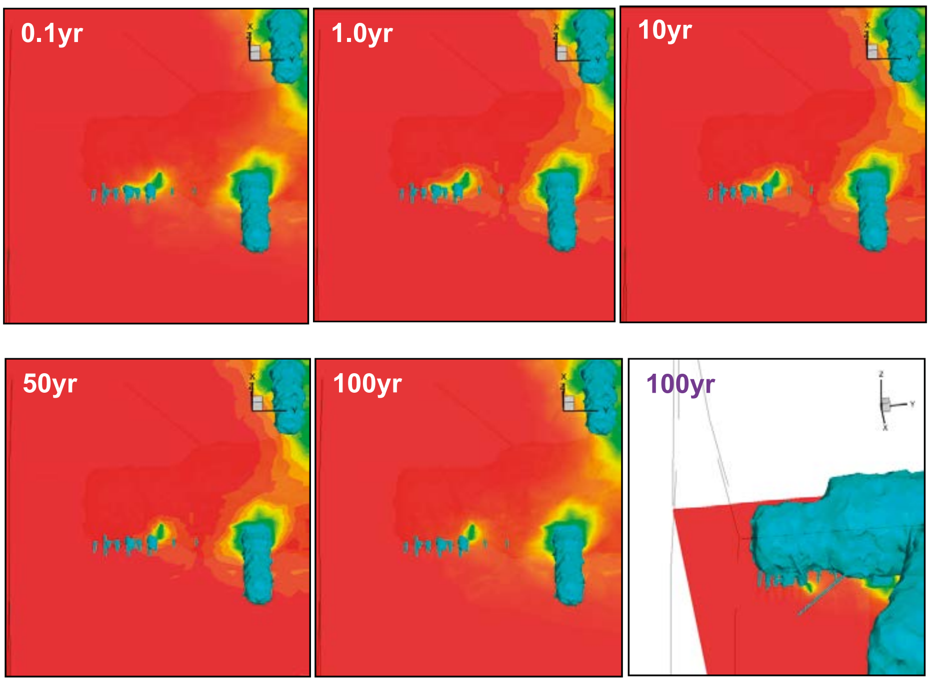


***Figure 5-3.** Saturation distribution at the middle of probing hole (1.5 m below).*

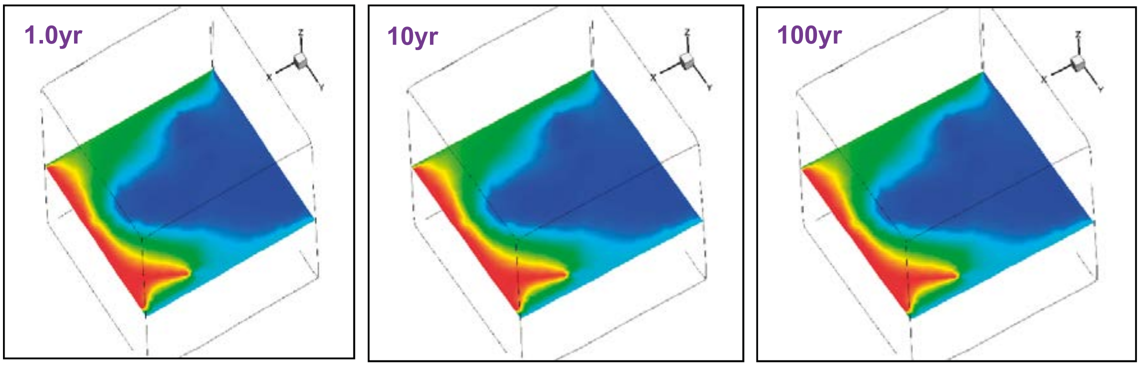


Figure 5-4. *Pressure distribution at the middle of probing hole (1.5 m below).*

5.5 Discussion

The time required for the full saturation of benonite in Task 8d is estimated to be much longer than that in Task 8c although additional fractures are taken into account and the inflow is larger. It is likely that additional boreholes and fractures intersecting tunnel and boreholes results in slow saturation in Task 8d. In particular, various monitoring boreholes surrounding each probing borehole give rise to low pressure distribution.

Although it is recommend that all boreholes should be assumed completely packed-off during the simulations, the modeler team missed this point. This seems the most attributable cause to slow saturation in Task 8d. Thus it is necessary to update from further numerical modeling.

However, it is worthwhile to notice that the borehole KO17 shows very slow saturation profile (Figure 5-3). Even after 100 years, some location does not show fully saturated. This is attributable to the fact that a large fracture is intersected with the tunnel inside which has a constant atmospheric pressure. Subsequently, more information on the geological features near the deposition holes, such as interconnection of fractures is also required for improving prediction of inflow as part of deposition hole characterization.

Even though the numerical study is further carried out after the all the boreholes are completely packed off, it is not likely that the estimated inflow reasonably represents a large difference in measured inflow between KO17 and KO18 under the present model developed in this study. It is, therefore, inevitable that the developed model should be adjusted and calibrated based on the available data measured in situ to better reproduce the observations because fractured rock surrounding deposition hole is inherently complicated system. These model adjustments can be accomplished by updating of transmissivities, inclusion of specific features (adding skin zones and discrete fractures that intersect deposition holes), condition of stochastic simulation to fracture trace maps, and the selection of a particular stochastic realization.

In addition, the material model should be validated and updated based on the BRIE water uptake test and in situ retention curve (van Genuchten) obtained from RH sensors and measured degrees of saturation. The hydraulic process between bentonite and rock is closely related to the water uptake and saturation profile. Thus, it is necessary to further study by updating input parameters in material model for Task 8d and subsequent Task 8f (back-analysis modeling of BRIE).

5.6 Conclusions and recommendations

Even after more site-specific complex features around the deposition hole are additionally taken into account in Task 8d, the modeling approach suggested in this study is still able to capture the general trend of inflow and bentonite hydration. Better prediction of the hydraulic interaction between the near-field rock and bentonite depends on how well the site-specific features around the deposition are identified. Subsequently, more information on the geological features near the deposition holes, such as interconnection with man-made structures is also required for improving prediction of inflow. In addition, model adjustment and calibration based on the available data measured in situ are necessary to better reproduce the observations.

6 Summary and conclusions

6.1 Summary

The general objective of Task 8 is to improve the understanding of bedrock-bentonite interface with regard to groundwater flow, and enhance the ability to model the hydraulic interactions between them. In process of model development, natural system is simplified by assuming that the far-field represented by stochastic discrete fracture network (DFN) is modeled as homogeneous equivalent porous medium (EPM), in which equivalent permeability is derived from the comparative study between FLAC3D and TOUGH2 codes, and large deterministic fractures or discrete small-scale fractures near deposition hole are explicitly embedded into a model geometry. With regard to the comparative study, it is assumed that the inflow estimated from TOUGH2 code is identical to that from FLAC3D code in which site-specific DFN is evaluated by the smeared fracture model.

KAERI-simulator is primarily used for analyzing hydraulic behaviors of bentonite as well as rock mass. COMSOL is applied for mesh generation. FLAC3D is used for not only preliminary inflow calculation but also steady state analysis for increasing numerical stability in prior to TOUGH2 analysis. Hydration of initially unsaturated bentonite and the effects of rock fracture on the re-wetting process are identified and properly predicted by TOUGH2 code over the whole subtasks of Task 8. From the sensitivity analysis it is noted that inflow into probing boreholes is not significantly affected by large deterministic features if they are not directly intersected with the boreholes. The variation in inflow and bentonite re-saturation are highly influenced by the localized water ingression due to fractures intersected with deposition holes. Thus it is important to identify the site-specific geological feature around the deposition hole. In addition, model adjustment and calibration are necessary based on the available data measured in situ to better reproduce the observations and to increase the reliability of predictive model.

6.2 Conclusions

The modeling approach suggested in this study is able to properly describe the inflow variation into deposition hole and the re-wetting process of bentonite in fractured rocks.The inflow and bentonite re-saturation are highly influenced by the localized water ingression through fractures intersected deposition holes. Thus it is important to identify the site-specific geological feature around the deposition hole and appropriately evaluate the impact of rock fracture. Due to heterogeneity and complexity of natural system, the developed model should be adjusted and calibrated with laboratory and field data for better prediction and increasing reliability.

6.3 Evaluation

In parallel with SKB Task 8, In-DEBS (In situ Demonstration of Engineered Barrier System) has been launched at KAERI since 2012. In-DEBS is primarily focused on in situ demonstration of THM (Thermal-Hydraulic-Mechanical) behaviors of EBS and its experiment set-up was installed at KURT in 2015. The lessons learned from Task 8 and BRIE gave guidance to site characterization as well as the experimental design for In-DEBS, in which THM sensor instrumentation and site selection for deposition hole were included. In particular, considerable efforts for understanding localized site-specific features such as water conducting fractures were made before installation of In-DEBS. Currently their effects on the hydraulic behavior of bentonite are being evaluated in the predictive model development.

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