Development of a Mechanical Analysis System Considering Chemical Transitions of Barrier Materials

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ABSTRACT

An analysis system for the long-term mechanical behavior of barrier materials (MACBECE: Mechanical Analysis system considering Chemical transitions of BEntonite-based and CEment-based materials) was developed in order to improve the reliability of the evaluation of the hydraulic field that is one of the important environmental conditions in the safety assessment of the TRU waste disposal in Japan. The MACBECE is a system that calculates the deformation of barrier materials using their chemical property changes as inputs, and subsequently their hydraulic conductivity taking both their chemical property changes and deformation into consideration. This paper provides a general description of MACBECE and the results of experimental analysis carried out using MACBECE.

INTRODUCTION

A disposal concept of TRU wastes in Japan involves emplacement of the waste in large underground vaults, where a cement-based material is used as a back fill or a structural material, and a bentonite-based material as a buffer enclosing the backfill or structure. The performance assessment for this disposal concept indicates that I-129 and C-14 which are soluble and are non-sorptive are the key nuclides that have significant radiological impact on human health and that the groundwater flow has significant effect on migration of these nuclides.

Meanwhile, engineered barriers, such as a back fill and a buffer, may be altered chemically by the reaction between cement and bentonite in the long term, leading to a change in hydraulic characteristics and mechanical properties. For example, it is assumed that calcium ion may leach out of cement-based materials, and its porosity may be increased, which may increase a hydraulic conductivity, and change mechanical properties such as rigidity and strength. With regard to bentonite-based materials, it is assumed that calcium ion supplied from cement-based materials may result in alteration into Ca-bentonite from Na-bentonite, which increases permeability and changes in mechanical properties such as swelling property. It is also assumed that the change in the mechanical properties may cause the deformation of the barrier materials that could result in change in the permeability.

With considerations described above, it will be necessary to develop a system which could evaluate long-term transition of hydraulic field of the near-field taking into account the changes in the barrier material properties in order to achieve a more reliable safety assessment, and thus the developed MACBECE is expected to serve as a key element of the evaluation system (Fig.1). The development of MACBECE was funded by Japan Nuclear Cycle Development Institute (present, Japan Atomic Energy Agency).

DESCRIPTION OF MACBECE

Fig.1 shows the flow diagram of the MACBECE that is a FEM based long-term mechanical behavior analysis system.

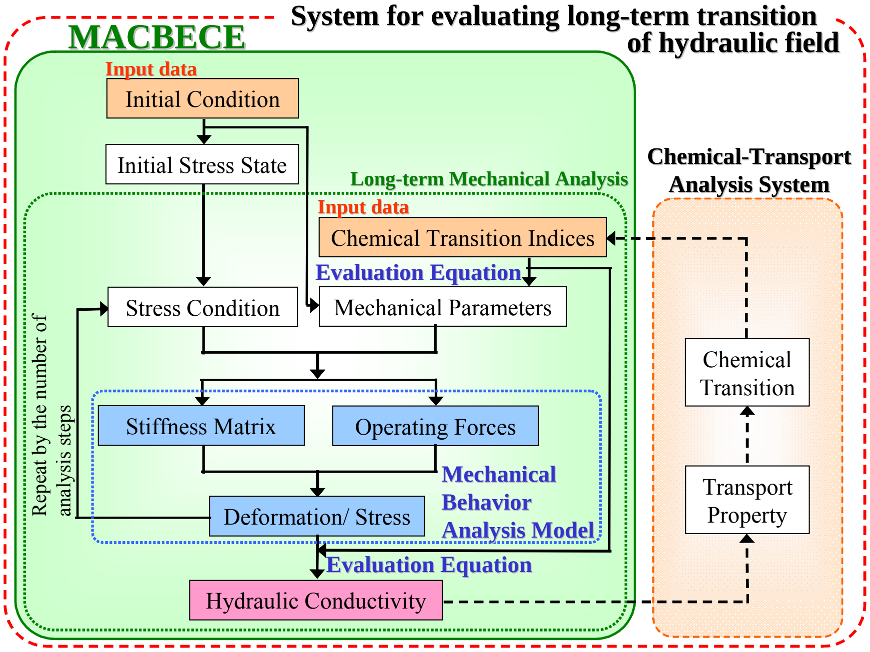


Fig.1. Flow diagram of MACBECE

At first, initial conditions in the MACBECE are set as those after a disposal tunnel is re-saturated and then the initial stress field is calculated in consideration of the weight per unit volume, initial properties of each barriers, and the swelling pressure of the bentonite-based materials, etc.

Then the change of the mechanical properties of each barrier material and the operating forces for the deformation of the materials are calculated using indices as inputs, which represent chemical transition in the materials (hereafter referred to as chemical transition indices). The deformation and the stress state can be obtained by solving the balance of the mechanical properties and operating forces. And the distribution of hydraulic conductivity is calculated based on the chemical property changes as well as the obtained displacement. This computational flow is repeated by the number of the analysis steps (i.e., the number of sets of chemical transition indices).

Although not described in Fig.1, the effect of rock creep deformation around a disposal tunnel can also be roughly evaluated by giving a forced displacement as a boundary condition.

In the sections below, firstly, outline of the chemical transition of barrier materials is described and the representative chemical properties, i.e., 'chemical transition indices', are explained. Secondly, mechanical behavior analysis model for each barrier (i.e., bentonite-based and cement-based) material is described. Thirdly, equations for mechanical parameter evaluation that formulate the relations between parameters and the chemical transition indices are described, and then equations for hydraulic-conductivity evaluation for each barrier materials are described. Finally, the results of the experimental analysis are presented.

CHEMICAL TRANSITIONS OF BARRIER MATERIALS

The long-term chemical transition of bentonite-based material considered in this study includes cation exchange, dissolution of a smectite and formation of secondary minerals, and change in the pore water chemistry. The cation exchange by Ca ions (alteration into Ca-bentonite), dissolution of a smectite and formation of secondary minerals by high alkaline solution due to the dissolution of cement-based material, which is caused by chemical reaction with underground water, are the phenomena that have been observed in experiments or suggested by analyses to have high possibility of occurrence [e.g. 1]. And the change in the pore water chemistry is assuming the case that the composition of near field ground-water may change from those in fresh water to those in seawater, and the swelling capability of bentonite-based materials are influenced by the equivalent ionic concentration [e.g. 2].

The long-term chemical transition of cement-based material considered in this study includes the leaching of Ca ions and formation of secondary minerals. These transitions are phenomena considered to have high possibility of occurrence based on the mineralogical analysis of old concrete structures [3], experiments and analyses [4].

The indices representing these chemical property changes used in this study are shown in Table I.

Table I. Chemical Transition Indices

Barrier materials	Chemical transition phenomena	Chemical transition indices
Bentonite-based materials	Cation exchange	Exchangeable sodium percentage: ESP
	Dissolution of smectite Formation of secondary minerals	Smectite partial dry density: ρ_{sme} [Mg/m^3] Smectite void ratio: e_{sme} Porosity: θ_b
	Change in porewater chemistry	Equivalent ionic concentration: C_i [eq/l]
Cement-based materials	Leaching of Ca	Leached Ca percentage: L_C
	Formation of secondary minerals	Porosity: θ_c

Here, the definitions of the chemical transition indices are as follows;

$$ESP = \frac{Na}{CEC} \quad (0 \le ESP \le 1) \tag{Eq.1}$$

Na : Equivalent concentration of exchangeable sodium ions [meq/100g]

CEC : Cation exchange capacity [meq/100g]

$$\rho_{sme} = \frac{W_{sme}}{V_v + V_{sme}} \ [\mathrm{Mg/m^3}] \tag{Eq.2}$$

$$e_{sme} = \frac{V_v}{V_{sme}} \tag{Eq.3}$$

W_{sme} : Weight of smectite [Mg]

V_V , V_{sme} : Volume of void, smectite [m^3]

$$C_i = \sum C_j Z_j \ [\mathrm{eq.l}] \tag{Eq.4}$$

C_j : Molar concentration of cation j in the solution [mol/l]

Z_j : Valence of cation j in the solution

$$Lc = \frac{LCa}{Ca_0} \qquad \text{(Eq.5)}$$

LCa : Leached quantity of Ca
Ca_0 : Initial quantity of Ca

MECHANICAL BEHAVIOR ANALYSIS MODEL

Bentonite-based Materials

Bentonite-based materials are considered to deform according to the stress balance with other barrier materials while exerting its characteristic nature of swelling property. The model used in this study focusing on the swelling property of the bentonite is an extended version of the elasto-(visco)plastic constitutive equation by Sekiguchi and Ota [5,6] which was coded as a constitutive equation for natural sedimentary clay, and has been used many times so far and proven. Focusing attention on the fact that swelling behavior is in the elastic region, Sasakura et al. extended the applicability of the model to express the swelling of the bentonite by using appropriate bulk modulus K (Fig.2 (a)) [7]. Furthermore, an upper limit for the swelling index is defined when over-consolidation ratio OCR exceeds a certain value (OCR_b) so that it can be applied to a wide range of swelling. The elastic coefficient tensor is shown in the Eq.6.

$$E_{ijkl} = (K_s - \frac{2}{3}G_s)\delta_{ij}\delta_{kl} + G_s(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \qquad \text{(Eq.6)}$$

K_s : Extended bulk modulus ($K_s = \frac{1+e_0}{\kappa}P'$)
e_0 : Initial void ratio
P' : Effective mean stress
κ : Swelling index
G_s : Extended shear modulus ($G_s = \frac{3}{2}\frac{1-2\nu'}{1+\nu'}K_s$)
ν' : Effective Poisson’s ratio
δ_{ij} : Kronecker delta

Then, the swelling index κ, which corresponds to the tangent gradient of the swelling curve (Fig.2 (a)) of the bentonite, are shown as follows.

$$\kappa = \kappa_0 + \xi \cdot OCR \cdot \exp\{\xi(OCR-1)\} \quad (1 < OCR < OCR_b) \qquad \text{(Eq.7)}$$
$$\kappa = \kappa_0 + \xi \cdot OCR_b \cdot \exp\{\xi(OCR_b-1)\} \quad (OCR > OCR_b)$$

where, OCR is the over-consolidation ratio ($OCR = P'_0/P'$), ξ and OCR_b are material constants (hereafter called osmotic swelling parameters), κ_0 is the initial swelling index. ξ, OCR_b, κ_0 can be obtained from swelling characteristics of the materials.

The decrease in the swelling capability due to alteration or change in the environmental conditions can be expressed by changing ξ and OCR_b. On the other hand, the change of the stress state and deformation of the engineered barriers due to the swelling pressure change associated with the alteration/change of the environmental conditions cannot be expressed simply by changing physical properties at a corresponding time-step, since Sekiguchi and Ota model uses incremental values (i.e., incremental force, incremental strain, etc.) to solve the problem. In MACBECE, deformation due to the reduction of the swelling pressure associated with the alteration is evaluated by applying equivalent force that compensates the reduction of ‘balanced swelling pressure’ from the previous analysis step. With regard to the balanced swelling pressure, the parameter evaluation equation is described later.

Cement-based Materials

Cement-based materials (i.e., mortar or concrete) are considered to deform by the swelling pressure of buffer material or by rock pressure while reducing rigidity and strength according to the progress of calcium leaching (Fig.2 (b)). As a constitutive equation to express this behavior that seems similar to the strain softening behavior, a nonlinear elasticity model [8] was incorporated to MACBECE. The incorporated model is an incremental analysis technique that has good consistency with the constitutive equation for bentonite. The stress-strain relation of cement-based materials in a certain degraded state is modeled as a bilinear relation using the elastic modulus and compressive strength at the state. And the Mohr-Coulomb's failure criterion is applied for the failure criterion, and an iterative method for redistribution of stress is applied for the strain softening behavior due to the reduction of the strength and the rigidity associated with the chemical deterioration. In the method for the study, minimum principal stresses are made constant as shown in Fig. 2(b).

Assumed deformation behaviors were classified into three steps; (1) the deformation by the self-weight and by the increase of swelling pressure due to re-saturation (corresponding to the analysis of initial stress in Fig.1), (2) deformation due to the reduction of rigidity, and (3) deformation by the reduction of strength and rigidity. Equivalent nodal forces are formulated according to the following equations respectively.

(1) Deformation by the self-weight and increase of the swelling pressure

$$\{F_0\} = \int_V [B]^T \{\sigma_s\} dV \qquad \text{(Eq.8)}$$

(2) Deformation due to the reduction of rigidity

$$\{F_c\} = \int_V [B]^T [D_i] \{\varepsilon\} dV \qquad \text{(Eq.9)}$$

$$\{\varepsilon\} = \left[[D_i^{-1}] - [D_{i-1}^{-1}] \right] (\sigma)$$

(3) Deformation by the reduction of strength and rigidity

$$\{F_e\} = \int_V [B]^T \{\Delta\sigma\} dV \qquad \text{(Eq.10)}$$

$[B]$: Displacement - strain matrix

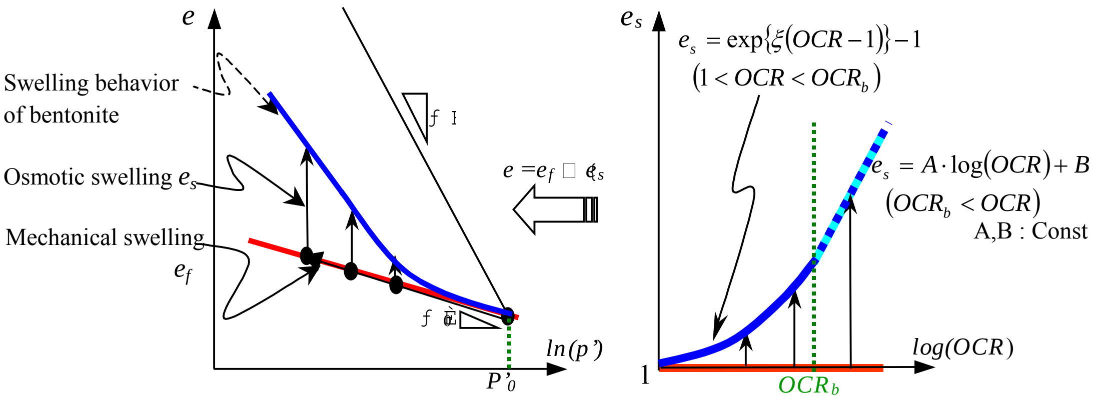
σ_s : Swelling pressure of bentonite

$[D_{i-1}]$: Stress-strain matrix calculated from the elastic modulus E at the analysis step i-1

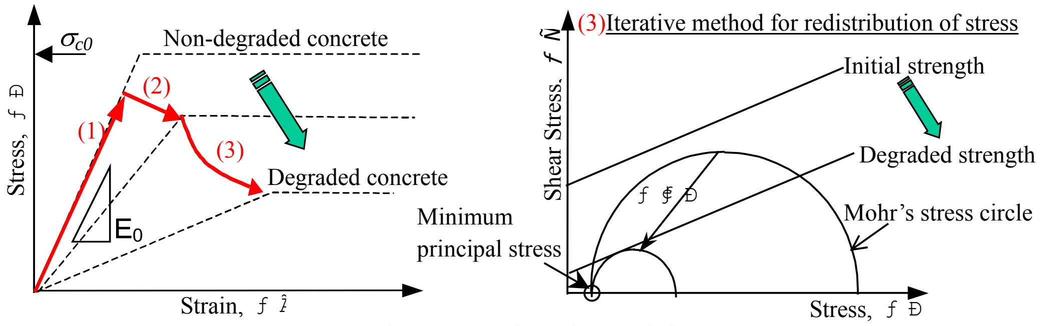
$[D_i]$: Stress-strain matrix calculated from the elastic modulus E at the analysis step i

σ , ε : Stress and strain of cement-based material

$\Delta\sigma$: Excess stress of cement-based materials (Fig.2 (b))



(a) Bentonite-based materials



(b) Cement-based materials

Fig.2. Concept of mechanical behavior analysis model

MECHANICAL PARAMETERS EVALUATION EQUATION

Bentonite-based Materials

For the bentonite-based materials, key mechanical parameters required for the aforementioned mechanical behavior analysis model, laboratory tests referred in setting the parameters for the analysis, and treatment in the analysis are listed in Table II. A general trend has been confirmed by the past experiments that the swelling capability of bentonite-based materials decreases as the alteration into Ca-bentonite progresses (ESP is decreases), as mixing ratio of silica-sand increases, or as equivalent ionic concentration increases [e.g. 2,7,9].

Table II. Key Mechanical Parameters for Bentonite-based Materials

	Referred laboratory tests	Treatment in the analysis
Compression index λ	Consolidation tests	Set constant
Swelling index κ		(Eq.8)
Initial swelling index κ_0		Set constant
Osmotic swelling parameter ξ		Using developed relationship with chemical transition indices
Osmotic swelling parameter OCR_b		Using developed relationship with chemical transition indices
Critical state parameter M	Triaxial $\overline{CU}$ tests	Set constant
Balanced swelling pressure P_{bal}	Swelling pressure tests	Using developed relationship with chemical transition indices

Among parameters listed in Table II, ξ , OCR_b , and P_{bal} , with which relationships to chemical transition indices are developed, are described as follows.

With regard to the osmotic swelling parameters ξ and OCR_b, the relations with the chemical transition indices were developed by fitting the swelling curve to the existing data of consolidation tests (Eq.11 and Eq.12). With regard to dissolution of smectite, however, no data obtained from consolidation test is available to use directly for such a phenomenon, and therefore, by considering the smectite dissolution as the change of the ratio of the swelling mineral (i.e., smectite) to the other non-swelling minerals, the relationship was developed based on the past results of consolidation test using the silica-sand mixing ratio as a parameter.

$$\xi = -(0.0297 \cdot C_{sand} + 0.0039) \cdot C_i - 0.0272 \cdot C_{sand} + 0.0198 \qquad \text{(Eq.11)}$$

Here, $\xi = 0$ when $\xi \leq 0$.

$$\begin{aligned} OCR_b &= (-2.7644 \cdot ESP + 0.7379) \cdot C_i \\ &\quad + (-15.3017 \cdot ESP + 5.1977) \cdot C_{sand} + 8.1629 \cdot ESP + 1.5050 \end{aligned} \qquad \text{(Eq.12)}$$

C_{sand} : Mixing ratio of silica-sand

$$C_{sand} = 1 - \frac{1}{C_{sme} \cdot (1 + C_{sx})}$$

C_{sme} : Smectite content in the bentonite

C_{sx} : Ratio of non-swelling and swelling (smectite) minerals

$$C_{sx} = \frac{G_{sme} \cdot \left(1 - \frac{\rho_{d0} \cdot C_{sand0}}{G_s} - \frac{G_{sme} \cdot \theta_b}{G_{sme} - \rho_{sme}}\right) + \rho_{d0} \cdot C_{sand0}}{G_{sme} \cdot \frac{\rho_{sme} \cdot \theta_b}{G_{sme} - \rho_{sme}}}$$

G_{sme} : Specific gravities of bentonite minerals and formed secondary minerals

G_s : Specific gravity of silica sand

ρ_{d0} : Initial dry density of bentonite-based materials [Mg/m^3]

C_{sand0} : Initial silica-sand mixing ratio in the bentonite-based materials

With regard to the balanced swelling pressure P_{bal}, the following evaluation equation was derived by taking into consideration the change of ρ_{sme} due to deformation as well as by reviewing the past results of swelling pressure tests in terms ESP, ρ_{sme}, C_i.

$$P_{bal} = g(ESP, \rho'_{sme}) \cdot h(C_i) \cdot f(\rho'_{sme}) \text{ [MPa]} \qquad \text{(Eq.13)}$$

$$f = 0.00126 \cdot \exp(6.0573 \rho'_{sme})$$

$$g = L(ESP) \cdot \{J(\rho'_{sme}) - 1\} + 1$$

$$L = 2.985 \cdot ESP - 0.364$$

Here, $L = 1$ when $L \geq 0$, and $L = 0$ when $L \leq 0$

$$J = 2.1272 \cdot \rho'^{\,2}_{sme} - 6.126 \cdot \rho'_{sme} + 5.3114$$

$$h = -1.698 \cdot C_i + 1$$

Here, $h = 0$ when $h \leq 0$

ρ'_{sme} : Dry density of smectite taking the deformation into consideration [Mg/m^3]

$$\rho'_{sme} = \frac{1}{\dfrac{1}{\rho_{sme}} - \dfrac{\varepsilon_v}{G_{sme}} \cdot \dfrac{e_{sme}}{\theta_b}}$$

ε_v: Volumetric strain determined by mechanical analysis

Cement-based Materials

Key parameters required for the analysis of the long-term mechanical behaviors, laboratory tests referred in setting the parameters for the analysis, and treatment in the analysis are listed in Table III. Results of past tests indicate the general trend that strength and rigidity of cement-based materials decreases as the leaching of Ca progresses (as L_C increases).

The internal frictional angle ϕ, which defines the Mohr-Coulomb’s failure criterion, was set conservatively as 0 and consequently the shear strength was set as the value of a half of the compressive strength. With regard to the Poisson's ratio, since its change associated with the Ca dissolution is not significant [10] and a general value can be applicable within elastic region, the value before the yield point was set as 0.2, and the value after the yield point was set as 0.45 since it will increase rapidly after the yield point.

Table III. Key Mechanical Parameters for Cement-based Materials

	Referred laboratory tests	Treatment in the analysis
Internal frictional angle ϕ	□	Set constant
Cohesion c (Compressive strength σ_c)	Uniaxial compression test using cement past samples degraded by flowing water [a] Vickers hardness test using cement paste samples degraded by immersion [a]	Using developed relationship with chemical transition indices
Elastic modulus E		Using developed relationship with chemical transition indices
Poisson's ratio ν	(Set based on existing papers)	Set constant values for before and after yield point

[a] See Ref.10.

Among parameters listed in Table III, c and E, with which relationships to the chemical transition indices were developed, are described as follows.

As described above, the shear strength (i.e., cohesion) of a cement-based material was defined as the following equation.

$$c = \sigma_c / 2 \text{ [MPa]} \qquad \text{(Eq.14)}$$

σ_c: Compressive strength for cement-based materials [MPa]

Here, the change of the compressive strength of the cement-based material (i.e., mortar and concrete) was set by assuming that the rate of change of the material strength is the same as the cement paste with equivalent W/C. Since the lowest strength (i.e., the strength after 100 % of calcium leached out) was not clear, the Eq.15 was introduced so that the lowest strength could be set up separately.

$$\sigma_c = \sigma_{c0} \cdot \alpha_{Sc} \cdot R_{Sp} \text{ [MPa]} \qquad \text{(Eq.15)}$$

$$\alpha_{Sc} = 1 - L_C \cdot (1 - R_{Sc\_fin} / R_{Sp\_fin})$$

$$R_{Sc\_fin} = \sigma_{c(\min)} / \sigma_{c0}$$

$$R_{Sp} = \exp(-7.91 \cdot \exp(-1.35 \cdot (W/C)) \cdot L_C)$$

Where, R_{Sp} : Ratio of residual strength to initial strength of the cement paste

R_{Sc} : Ratio of residual strength to initial strength of the cement-based materials

α_{Sc} : Correction factor for lowest strength

R_{Sc_fin} : R_{Sc} at $L_C = 1$

R_{Sp_fin} : R_{Sp} at $L_C = 1$

W/C : Water–cement ratio of cement-based materials

σ_{c0} : Initial strength of cement-based materials [MPa]

$\sigma_{c(\min)}$: Strength of cement based materials at $L_C = 1$ [MPa]

Since it is well known, according to the past experimental data [11], that an elastic modulus E has strong correlation with the compressive strength, the elastic modulus for the study is set up from the compressive strength derived by the Eq.15. As for the correlation of the elastic modulus with the compressive strength, the equation which is generally applied to the concrete with low strength [11] is used for concrete, and the regression expression obtained based on the past test result [10] is used for mortar.

$$\text{Concrete: } E = 21000 \cdot (\gamma/2.3)^{1.5} \cdot (\sigma_c/20)^{0.5} \quad \text{[MPa]} \qquad \text{(Eq.16)}$$

$$\text{Mortar} \quad : E = 1999 \cdot \sigma_c^{\;0.610} \quad \text{[MPa]} \qquad \text{(Eq.17)}$$

Where, γ : Unit volume weight (air-dried state) [Mg/m^3]

HYDRAULIC CONDUCTIVITY EVALUATION EQUATION

The equation [12], which is based on the data from permeability test and reviewed in terms of the effect of ESP, e_{sme}, and C_i was adopted for the evaluation of the hydraulic conductivity of bentonite-based materials. Moreover, the change of the e_{sme} due to deformation was also taken into account and then the Eq.18 was obtained for evaluation of the hydraulic conductivity.

$$K = 10^{1.30 \cdot C_i} \cdot e'_{sme}{}^{3.48 \cdot C_i} \cdot K_0 \ \text{[m/sec]} \qquad \text{(Eq.18)}$$

Here , $C_i = 10^{1.49 \cdot ESP - 1.0}$ when $C_i > 10^{1.49 \cdot ESP - 1.0}$

$$K = 10^{1.63 \cdot e'_{sme} - 0.24} \cdot K_0 \ \text{when}\ 10^{1.30 \cdot C_i} \cdot e'_{sme}{}^{3.48 \cdot C_i} > 10^{1.63 \cdot e'_{sme} - 0.24}$$

$$K = 10^{-5} \ \text{when}\ K > 10^{-5}$$

$$K_0 = \begin{cases} (0.91 - 1.57 \cdot ESP + 2.00 \cdot ESP^2) \cdot 10^{-13} \cdot e'_{sme}{}^{7.44 - 5.69 \cdot ESP} & (e'_{sme} \le 7.0) \\ K_0\big|_{e_{sme}=7.0} \cdot \left(\dfrac{e'_{sme}}{7.0}\right)^{11.4} & (e'_{sme} > 7.0) \end{cases}$$

Here, $K_0 = K_0\big|_{ESP=1}$ when $K_0 < K_0\big|_{ESP=1}$

Where, e'_{sme} : Smectite void ratio taking the deformation into consideration

$$e'_{sme} = \left(1 - \frac{\varepsilon_v}{\theta_b}\right) e_{sme}$$

ε_v : Volumetric strain determined by mechanical analysis

Meanwhile, for cement-based materials, the relational equation between the porosity and the hydraulic conductivity proposed based on the data for cement paste [13] was adopted. In defining an equation for the evaluation of hydraulic conductivity, since aggregate as well as cement paste is contained in cement-based materials such as mortar and concrete, the porosity was converted to that of cement paste itself by deducting the volume of the aggregate, and the change of porosity due to deformation was also taken into consideration.

$$k_c = k_p \text{ [m/sec]} \qquad \text{(Eq.19)}$$

Here, $k_c = 10^{-5}$ when $k_c \geq 10^{-5}$

$$k_p = 4.34 \cdot 10^{-9} \cdot \theta_p'^3 / (1 - \theta_p')^2 \text{ [m/sec]} \qquad \text{(Eq.20)}$$

Where, k_c : Hydraulic conductivity of cement-based materials [m/sec]

k_p : Hydraulic conductivity of cement paste [m/sec]

θ_p' : Porosity of cement paste taking the deformation into consideration

$$\theta_p' = (\theta_c - \varepsilon_v)/(1.0 - V_c - \varepsilon_v)$$

ε_v : Volumetric strain determined by mechanical analysis

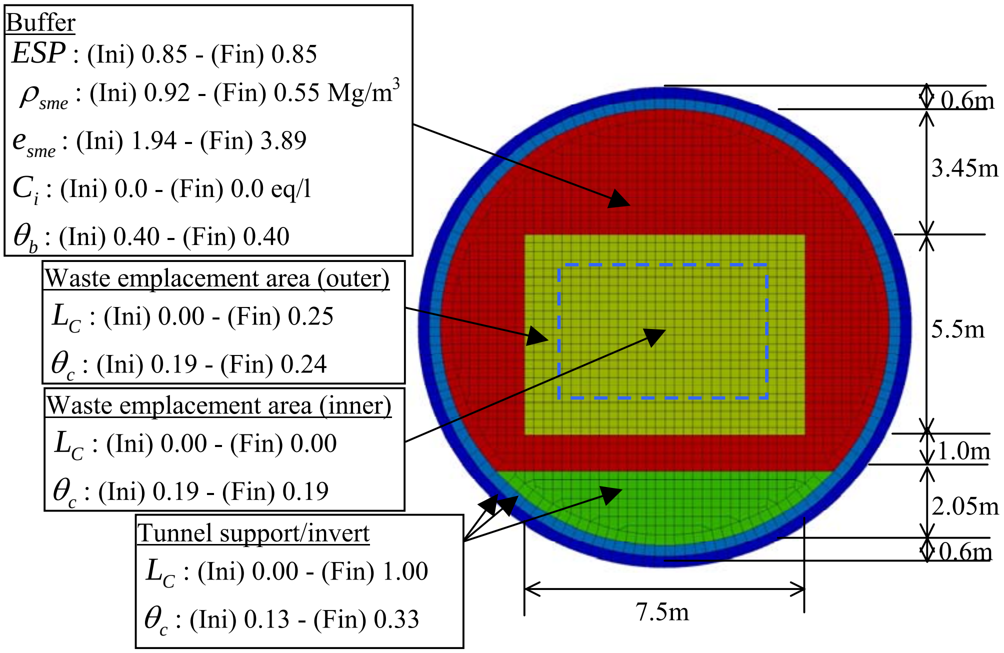
V_c : Volume ratio of the aggregate in cement-based materials

EXPERIMENTAL ANALYSIS

Experimental analysis was carried out using MACBECE.

The diagram of the analytical model is shown in Fig. 3. The chemical transition indices for each barrier material used in the analysis are also shown in the figure. The analysis was carried out using 40 time-steps, in which the parameters were linearly interpolated steps using the values of initial state and final state. For the bentonite-based materials, only the phenomenon that smectite dissolves uniformly in the buffer was considered. And the porosity θ_b was not changed as the analysis condition, which means that it is assumed that same volume of secondary minerals were formed as that of dissolved smectite. For the cement-based material, the different values were used for the extent of dissolution in three parts; inner part and outer part of the waste emplacement area, and tunnel support including inverted concrete. And the porosity θ_c, which was set here, corresponds to leaching of Ca without formation of secondary minerals.

Major physical properties used in the analysis are shown in Table IV and V.



Buffer
ESP : (Ini) 0.85 - (Fin) 0.85
ρ_{sme} : (Ini) 0.92 - (Fin) 0.55 Mg/m^3
e_{sme} : (Ini) 1.94 - (Fin) 3.89
C_i : (Ini) 0.0 - (Fin) 0.0 eq/l
θ_b : (Ini) 0.40 - (Fin) 0.40

Waste emplacement area (outer)
L_C : (Ini) 0.00 - (Fin) 0.25
θ_c : (Ini) 0.19 - (Fin) 0.24

Waste emplacement area (inner)
L_C : (Ini) 0.00 - (Fin) 0.00
θ_c : (Ini) 0.19 - (Fin) 0.19

Tunnel support/invert
L_C : (Ini) 0.00 - (Fin) 1.00
θ_c : (Ini) 0.13 - (Fin) 0.33

Fig.3. Diagram of the analysis model and the chemical transition indices

Table IV. Properties of Bentonite-based Material used in the Analysis

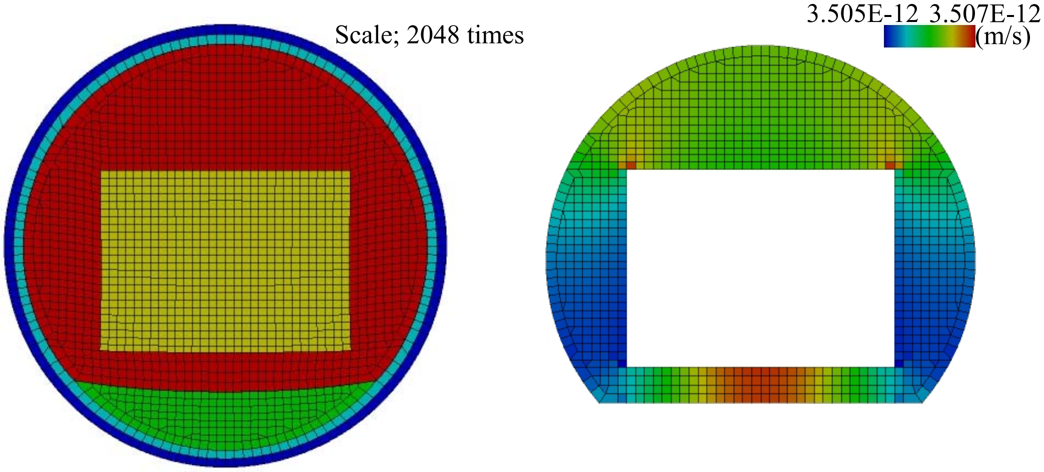
Applied component	Buffer
Initial silica-sand mixing ratio C_{sand0}	0.30
Initial dry density ρ_{d0} [Mg/m^3]	1.6
Compression index λ	0.0842
Swelling index κ	(Eq.8)
Initial swelling index κ_0	0.0086
Osmotic swelling parameter ξ , OCR_b	(Eq.11), (Eq.12)
Critical state parameter M	0.45
Effective Poisson's ratio ν'	0.42
Initial porosity ratio e_0	0.69

Table V. Properties of Cement-based Materials used in Analyses

Applied components	Support/invert	Waste emplacement region
Water/cement ratio W/C	0.45	0.55
Volume ratio of the aggregate V_c	0.67	0.54
Unit volume weight (air-dried state) [Mg/m^3]	2.28	2.09
Initial compressive strength σ_{c0} [MPa]	43	35
Minimum compressive strength $\sigma_{c(\min)}$ [MPa]	0.43	0.35
Internal friction angle ϕ [deg]	0	0
Cohesion c [MPa]	(Eq.14, 15)	(Eq.14, 15)
Elastic modulus E [MPa]	(Eq.16)	(Eq.17)
Poisson's ratio ν	[Before yield] 0.20 [After yield] 0.45	[Before yield] 0.20 [After yield] 0.45

An example of the results is shown in Fig. 4.

As shown in the Fig.4 (a), the result of deformation indicates that the buffer material and the waste emplacement area get depressed into the invert concrete where Ca had been set to leach out by 100% at the final step. As shown in the Fig.4 (b), the hydraulic conductivity of the buffer material in the upper and lower part of the waste emplacement area have risen a little more than that of the case with no deformation (i.e., 3.505E-12m/s which is calculated by Eq.18 using ε_v=0), which means the parts of the buffer material is swelling very slightly. In short, as a whole, long-term deformation is so small that the hydraulic conductivity of the buffer material is in still in the order of 10^{-12} m/s.



(a) Deformation (b) Hydraulic conductivity of the buffer material

Fig.4. Example of the analysis results (at the final step)

CONCLUSION

A code MACBECE was developed, which could be used to evaluate:

1. Changes of mechanical properties of barrier materials,
2. Mechanical behavior of barrier materials, and
3. Transition in hydraulic field.

These evaluations take into account:

1. Cation exchange of bentonite-based materials,
2. Dissolution of smectite and formation of secondary minerals of bentonite-based materials,
3. Change in porewater chemistry of bentonite-based materials, and
4. Leaching of Ca and formation of secondary minerals of cement-based materials.

Experimental analysis demonstrated that, for the assumed disposal tunnel configuration and chemical transitions, the deformation was so small that the buffer materials could keep the hydraulic conductivity in the order of 10^{-12} m/s.

The reliability of the developed MACBECE could be enhanced through the modification/improvement based on the accumulation of data and knowledge in the future.

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