Implementation of Damage Model to TOUGH2-MP/FLAC3D Coupled Code

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1. Introduction

In the case of a repository for radioactive waste, corrosion of metallic materials under anoxic conditions will lead to the formation of hydrogen. If the rate of gas production exceeds the rate of gas diffusion within the pores of the barrier, gas will continue to accumulate until its pressure becomes sufficiently large for it to enter the surrounding material. In the case of plastic clays and in particular bentonite, classic concepts of porous medium twophase flow are inappropriate and continuum approaches to modelling gas flow may be questionable. However, the detail of the dilatant mechanisms controlling gas entry, flow and pathway sealing are unclear and such features may impair barrier performance, in particular, acting as preferential flow paths for the movement of radionuclides. Because of that, development of new and novel numerical representations for the quantitative treatment of gas in clay-based repository systems are therefore required. In this study, the damage model is adopted to model the gas migration phenomena, and implemented to TOUGH2-MP/FLAC3D coupled code for hydro-mechanical modeling.

2. Numerical code

TOUGH2-MP and FLAC3D were used to perform thermal-hydraulic-mechanical interaction analysis. TOUGH2-MP is an abbreviation of TOUGH2 Massively Parallel, and is the parallel version of TOUGH2 software. TOUGH2 has a strong point in multiphase/multi-component flow analysis and heat transfer analysis. In case of TOUGH2-MP, parallel analysis is made possible and the analysis speed is dramatically improved. FLAC3D is a code that has strengths in the mechanical analysis of soil and rock. The algorithm of the TOUGH2-MP/FLAC3D coupling analysis module is shown in Fig. 1.

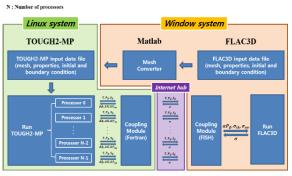


Fig. 1. TOUGH2-MP/FLAC3D coupling module algorithm.

3. Damage model [1]

Tang et al. proposed a flow-stress damage (FSD) coupling model of saturated rocks by taking into account the growth of existing fractures and the formation of new fractures [1].

In elastic damage mechanics, the elastic modulus of the element may degrade gradually as damage progresses, and the elastic modulus of the damaged element is defined as follows:

$$E = (1 - D)E_0$$
 (1)

where D represents the damage variable, and E and E_0 are the elastic moduli of the damaged and undamaged elements, respectively.

When the tensile stress in an element reaches its tensile strength f_i , the damage variable can be described as:

$$D = \begin{cases} 0 & \varepsilon_{t_0} \le \varepsilon_3 \\ 1 - \frac{f_{t_r}}{E_0 \varepsilon_3} & \varepsilon_{t_u} \le \varepsilon_3 \le \varepsilon_{t_0} \\ 1 & \varepsilon_3 \le \varepsilon_{t_u} \end{cases}$$
(2)

where f_{tr} is the residual tensile strength, and ε_3 is tensile principal strain.

To describe the element damage under a

compressive or shear stress condition, we choose the Mohr–Coulomb criterion as the second damage criterion. The damage variable under uniaxial compression is described as:

$$D = \begin{cases} 0 & \varepsilon_1 \le \varepsilon_{c0} \\ 1 - \frac{f_{cr}}{E_0 \varepsilon_1} & \varepsilon_{c0} \le \varepsilon_1 \end{cases}$$
(3)

where f_{cr} is the residual compressive strength, and ε_3 is tensile principal strain.

Fig. 2 shows elastic damage constitutive law for elements under uniaxial compressive stress and tensile stress.

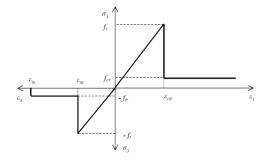


Fig. 2. Elastic damage constitutive law for elements under uniaxial compressive stress and tensile stress.

4. Implementation to TOUGH2-MP/FLAC3D

This section describes the numerical implementation of the FSD model in the framework of the TOUGH2-MP/FLAC3D coupled code. Stress analysis, based on the effective stress principle, is carried out to obtain the stress field. The coupled FS model is used to analyse the coupling problem between flow and stress, and the coupled FD model is used to analyse the coupling problem between flow and stress and strength of the damaged elements will be reduced whereas their porosity and permeability will increase accordingly.

For porosity change, we assume the solid volume is constant. That means porosity increase in proportion to the volumetric strain as described below:

$$\phi = \frac{V_p}{V} = \frac{V_p + \Delta V}{V_0 + \Delta V} = \frac{V_p + \varepsilon_v V_0}{(1 + \varepsilon_v) V_0} \qquad \left(\varepsilon_v = \frac{\Delta V}{V_0}\right) \quad (4)$$

where V_0 is the initial total volume and V_p is the

pore volume.

In this case, permeability is assumed porosity dependent model as described below [2, 3]:

$$k = k_0 \exp\left[A\left(\frac{\phi}{\phi_0} - 1\right)\right] \tag{5}$$

where k_0 is initial (zero stress) intrinsic permeability, ϕ_0 is initial porosity, and A is the empirical factor.

5. Conclusions

In this study, the damage model is adopted to model the gas migration phenomena, and implemented to TOUGH2-MP/FLAC3D coupled code for hydro-mechanical modeling. Elastic modulus is varied according to damage variable D, and porosity and permeability is changed based on the volumetric strain. In the future, we plan to conduct the validation process using the laboratory test results for the damage model of TOUGH2-MP/FLAC3D.

ACKNOWLEDGEMENTS

This research was supported by the Nuclear Research and Development Program of National Research Foundation of Korea (NRF) funded by the Minister of Science, ICT and Future Planning.

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