Phase Field Modelling of Gas Migration in Bentonite Based Barrier Materials

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1 Introduction

Distribution of Nuclear Power Plants
(From Wikipedia)
1 Introduction

Multi-barrier system of KBS-3 repository

(From Harrington, J., and Horseman, S. 2003)
Gas Generation

Gas Transport

0

Metal Corrosion
Water Radiolysis
Bio-Degradation

Gas Generation

Gas Diffusion
Two Phase Flow
Dilatancy Control Flow
Macro-fracture Flow

*Images from Marschall et al. (2005)
2 Conceptual Coupled HM-PF Model

Gas injection end

Gas breakthrough

Volume dilation
Increase of total stress

Gas outflow end

Preferential pathways

Saturated state
Build up of water pressure

Void exchange
Water transfer

Fracture healing

Experimental result (Horseman et al. (1999))

(From Wiseall et al. 2015)
Couplings Between Different Physical Field

(Modified from Guo, G. & Fall, M. 2019)
3 Numerical Model and Implementation

➢ Phase Field Method

\[
\gamma (d, \nabla d) = \frac{1}{2l} d^2 + \frac{l}{2} |\nabla d|^2
\]

\[
(1 - d) H_M^+ - \left( d - l^2 \nabla^2 d \right) = 0
\]

\[
H_M^+ = \max_{\tau \in [0,t]} \left\{ \frac{\psi_0^{\epsilon +}}{\psi_{cr}} - 1 \right\}
\]
Mechanical Model

\[ \nabla g(d) \sigma^+ (\varepsilon) + \sigma^- (\varepsilon) - \bar{p} I + \rho g = 0 \]

\[ \sigma^{\pm} (\varepsilon) = \sum_{a=1}^{3} \left[ \lambda \langle tr(\varepsilon) \rangle_{\pm} + 2 \mu \langle \varepsilon_a \rangle_{\pm} \right] \mathbf{n}_a \otimes \mathbf{n}_a \]

Replace

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<td>fcon.Si11+fcon.Di11+fcon.ei11+f</td>
<td>N/m²</td>
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Hydraulic Model

\[ v_k^D = - \frac{k_{kr}}{\mu_k} \left( \nabla p_k - \rho_k g \right) \]

\[ \rho_k \phi \left( \frac{S_k}{K_k} - \frac{\partial S_e}{\partial c} \right) \frac{\partial p_k}{\partial t} + \nabla \cdot (\rho_k v_k^D) \]

\[ = -S_k \rho_k \frac{\partial \varepsilon_v}{\partial t} - \rho_k \phi \frac{\partial S_e}{\partial p} \frac{\partial p_k}{\partial t} \]

\[ k_{fi} = C_{ki} k_{pi} \]

\[ k_{f} = \frac{1}{2} S_w^2 (3 - S_w) \]

\[ k_{f} = S_g + \frac{3}{2M} S_g \left( 1 - S_g^2 \right) \]

\[ S_{fe} = 1 + \left( \frac{p_c}{P_{fgev}} \right)^n \]

\[ T(d) = \frac{1}{2} \left\{ \tanh \left[ \theta_i (d - d_c) \right] - \tanh (-d_c \theta_i) \right\} \]

* (From Guo, G. & Fall, M. 2019)
Solver Settings

Study 1

- Step 1: Time Dependent

Solver Configurations

- Solution 1 (sol1)
  - Compile Equations: Time Dependent
  - Dependent Variables 1

- Time-Dependent Solver 1
  - Direct
  - Advanced
  - Fully Coupled 1

- Segregated 1
  - Segregated Step 1
  - Segregated Step 2
  - Segregated Step 3

Results at previous time step

\[ x^i=0(x = p_g, p_w, u, d) \]

Segregated step 1

Solve \( p_g^{i+1}, p_w^{i+1}, u^{i+1} \) based on \( d^i \)

Segregated step 2

Solve \( H_M^{+(i+1)} \) based on \( u^{i+1} \)

Segregated step 3

Solve \( d^{i+1} \) based on \( H_M^{+(i+1)} \)

\[ i = i + 1 \]

Convergence?

- NO
- YES

Done

(Modified from https://www.comsol.com/blogs/improving-convergence-multiphysics-problems/)
4 Simulation Results

➢ Meshing and boundary conditions

(Modified from Guo, G. & Fall, M. 2019)

➢ Fracture trajectory (Phase field) in the heterogeneous domain

Preferentially propagate through areas of low resistance
➢ Distribution of gas pressure (scaled by its degree of saturation)

➢ Distribution of water pressure

➢ Preferential gas flow in the developed fracture

➢ Rise of water pressure during fracturing process
4 Conclusions

➢ The developed coupled HM-PF model is successfully implemented into COMSOL by using Solid Mechanics Module, Darcy’s Law Module, Coefficient Form PDE, Domain ODEs and DAEs and the Previous Solution Node.

➢ The developed model has satisfactorily described some HM behaviors observed in experiments, such as the development of preferential pathways, the localized gas flow and the rise of water pressure.
References


Thank you for your attention!