# Modelling of Sulphide Induced Copper Corrosion in Deep Geologocial Repository With Expected Condition

Nakkyu Chae<sup>1</sup>, Sungyeol Choi<sup>1</sup>, and Heui-Joo Choi<sup>2</sup>

<sup>1</sup>Department of Nuclear and Quantum Engineering, Korea Advanced Institute of Science and Technology, Daejeon, KS015, Republic of Korea

<sup>2</sup>Department of Radioactive Waste Disposal Research, Korea Atomic Energy Research Institute, Daejeon,

KS015, Republic of Korea

coskrrb2002@kaist.ac.kr

# 1. Introduction

Deep geological repository is an important issue in Korea and world. Recently, the land and environmental court in Nacka, Sweden, concluded that the KBS-3 model is not safe enough due to corrosion problems. In Korea and other countries have a similar concept as KBS-3 model. We have to concentrate on the corrosion problems on canisters in the deep geological repository. Hence, in this work we focus on the copper corrosion with sulphide in the deep geological repository with an expected condition (anaerobic). We calculated the expect corrosion depth with several scenarios.

## 2. Method

#### 2.1 Model description

Deep geological repository is located in 500m depth of underground. After the deep geological repository closed, condition expected to be anaerobic condition [1]. Sulphide could be only exist in sulphide ions (HS<sup>-</sup>) without oxygen conditions (O<sub>2</sub> < 0.001 ppb) [1]. During the anaerobic condition, the sulphide ions (HS<sup>-</sup>) will be the dominant corrosion specie. The overall reaction of sulphide ions with copper is equation (1).

$$2Cu+HS^{-}+H_2O \rightarrow Cu_2S+H_2+OH^{-}$$
(1)

In this study, we assumed the fully saturated condition in bentonite and transport is rate determining step of corrosion. We use COMSOL Multiphysics (Numerical analysis program use Finite Element Method, PDE module) to predict the corrosion depth until 10,000 years.

# 2.2 Kinetic and Transport-rate determining step

In deep geological repository system with fully saturated bentonite and anaerobic condition, copper corrosion rate will be determined by transport rate of sulphide (HS<sup>-</sup>). Various literatures relate with copper corrosion with sulphide suggest that transport rate of sulphide (transport) is much slower than sulphide and copper reaction rate (kinetic) [1]. Hence, overall rate determining step of copper corrosion with sulphide is transporation of sulphide (diffusion in bentonite). We used the assumption in our model by equation (2). Equation (3) is steady state analytic solution that will be compared with COMSOL results.

$$\frac{\partial C}{\partial t} = \nabla \cdot (D\nabla C) \tag{2}$$

$$C(r) = \frac{C_1 \ln(\frac{b}{r}) + C_2 \ln(\frac{r}{a})}{\ln(\frac{b}{a})}$$
(3)

#### 2.3 Scenario

Bentonite and Host rock interface is sulphide (HS<sup>-</sup>) source for copper corrosion. Upper and bottom are impermeable conditions. Sulphides are immediately react with copper at the canister surface as they are transported.



### 3. Case results

Fig. 1. Result of sulphide concentration in bentonite.



Fig. 2. Result of copper corrosion depth compare between COMSOL (transient state) and Matlab(steady state with analytical solution).

## 4. Conclusion

The result of transient state with COMSOL is similar to analytical solution calculated by Matlab. We saw the possibilities of COMSOL to solve the transient state. The maximum corrosion depth after 10,000 years with COMSOL is 7.4466 x  $10^{-5}$ [m] and analytical solution is 7.2698 x  $10^{-5}$ [m]. From this model we will develop our model for copper corrosion in anticipated condition.

### REFERENCES

- F. King et al., "An Update of the State-of-the-art Report on the Corrosion of Copper under Expected Conditions in a Deep Geological Repository.", 246, 2012.
- [2] Smith, J.M., "The Corrosion and Electrochemistry of Copper in Aqueous, Anoxic Sulphide Solutions, PhD thesis, University of Western Ontario.", 2007.