Simulation Model of Molten Salt Corrosion Using COMSOL

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1. Introduction

Molten salt reactor(MSR) system is one of the Generation-IV reactor system. MSR system use liquid molten salt as coolant and fuel in normal pressure and high temperature. Therefore, MSR system has superior thermal efficiency and stability. However, molten salt is very highly corrosive material. So, in long-term operation, corrosion is main problem.

2. Background

In MSR system, fluoride salts are mainly used. FLiNaK molten salt(46.5LiF-11.5NaF-42KF mol%) is representative fluoride salt. In most high temperature environments, materials derive their corrosion resistance from the formation of a protective surface film of an oxide of Cr, Al, or Si. However, in molten fluoride salt these passive oxide films are chemically unstable, and corrosion is driven largely by the thermodynamically driven dissolution of alloying elements into the molten salt environment. There is no resistance film, corrosion occur uniformly by free energy difference of fluoride compounds. Metals that have high negative free energies of fluoride formation are generally more prone to corrosion, that is, they are more likely to form a fluoride compound and dissolve in the salt[1]. For a basic fluorination reaction of a solid metal M is given by

$$xM(solid) + yF_2(gas) = M_xF_{2y}(liquid)$$
(1)

The corrosion of a pure metal M (Ni, Co, Fe, or Cr) in an alkali fluoride, i.e., Me-fluoride (Me being, for example, Li, Na, K) is given by

$$xM + yMeF = M_xF_y + yMe \tag{2}$$

In this study, we develop simulation model including these reactions using COMSOL.

3. Model

This model used Tertiary Current Distribution physics in COMSOL. This physics describes the current and potential distribution in an electrochemical cell taking into account the individual transport of charged species (ions) and uncharged species in the electrolyte due to diffusion, migration and convection using the Nernst– Planck equations.

The electrode kinetics for the charge transfer reactions can be described by using arbitrary expressions or by using the predefined Butler–Volmer and Tafel expressions.

Ohm's law is used in combination with a charge balance to describe the flow of currents in the electrodes. The charge transfer reactions can be defined as boundary conditions or as sources or sinks within a domain in order for the case of porous electrodes[2].

FLiNaK molten salt was used as electrolyte. And Hastelloy-N was used as structural materials. Corrosion potential was referenced fig. 1.



Fig. 1 Redox potentials of various redox couples as function of temperature in fluoride salts.[3]

4. Result and Conclusion

According to other studies, Cr corrosion is main corrosion. However, in model result, Fe corrosion current is most high and Cr is next. The reason for this would be not considering microscale effects or application incorrect corrosion potential. If the model is modified correctly, it is expected that temperature effects, impurity corrosion, and composition effects can be considered.

REFERENCES

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