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

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

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

$$xM + yMeF = M_xF_y + yMe \quad (2)$$

If there is impurities in salt, corrosion will be accelerate. Most common impurities is water. It make HF and occur corrosion by HF reduction.

$$HF + e^- = F^- + \frac{1}{2}H_2 \quad (3)$$

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.

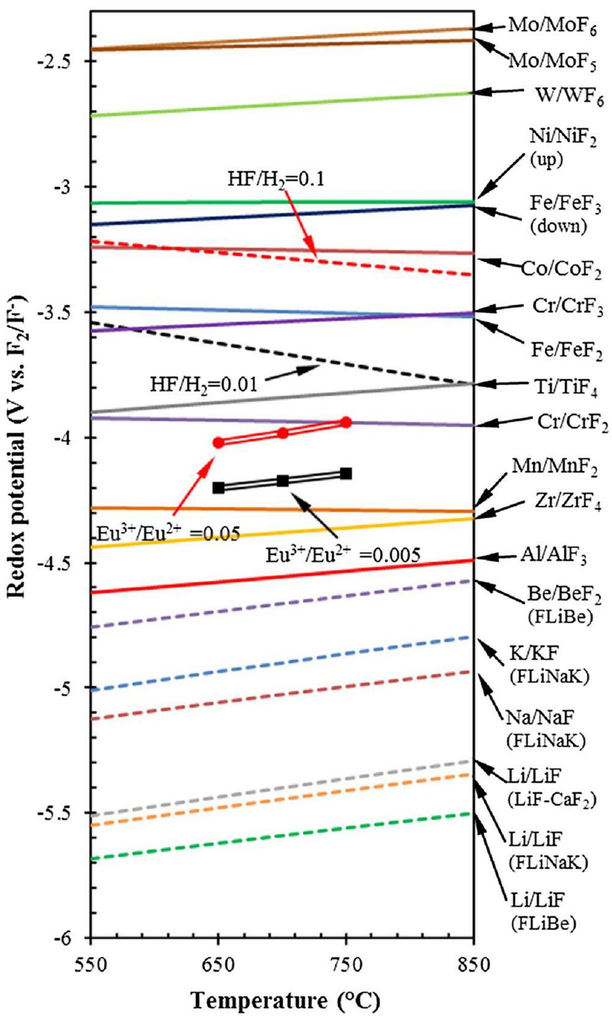

Fig. 1 Redox potentials of various redox couples as function of temperature in fluoride salts.[3]

Table 1: Result by flow velocity

u(m/s)	Average of local current Cr^{2+} (A)	Average of local current Cr^{3+} (A)	Average of local current Fe^{2+} (A)	Average of local current Fe^{3+} (A)	Average of local current Ni^{2+} (A)	Average of total current (A)
0	0.227534	-0.00962	-0.01152	-0.05343	-0.00605	0.146914
0.1	0.339514	-0.006616	-0.01037	-0.11427	-0.06847	0.139796
0.3	0.675656	-0.000326	-0.00666	-0.32187	-0.21763	0.129176
0.5	1.03053	0.005211	-0.00361	-0.54565	-0.3658	0.12069

4. Result and Conclusion

For our result, Cr/Cr^{2+} reaction is main corrosion, and other reactions was reduction reaction. And corrosion rate increased as flow velocity increased. According to redox potential curve, Cr/Cr^{2+} couple was lowest redox potential. Therefore, Cr corrosion was dominant and others was reduced. If flow velocity increased, flux of species was increased. This model was considered only water impurities. If actinides or other impurities was considered, the model would be more realistic.

REFERENCES

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