CHAPTER IV

MODELS

4.1 Model Assumptions

The model is based on following assumptions

1) The controlling reaction at the metal surface is metal dissolution or ferrous ion formation and this reaction couples with hydrogen evolution.

$$Fe = Fe^{2+} + 2e^- \tag{4.1}$$

$$2H^+ + 2e^- = H_2 \tag{4.2}$$

2) Ferrous ion from reaction (4.1) will be hydrolysed to hydroxide of ion as given below

$$Fe^{2+} + H_2O = Fe(OH)^+ + H^+ \tag{4.3}$$

$$Fe^{2+} + 2H_2O = Fe(OH)_2 + 2H^+ \tag{4.4}$$

$$Fe^{2+} + 3H_2O = Fe(OH)_3^- + 3H^+ \tag{4.5}$$

3) Hydrogen from the reaction 4.2 moves through the metal in an outward direction

4) Half of the ferrous species from reaction (4.1) and reaction (4.3) to reaction (4.5) will form magnetite at metal-oxide interface. The other half is assumed to diffuse through the oxide film.

5) The concentration of ferrous species at the metal surface is 10% supersaturated. As it is in a supersaturated condition, nucleation of magnetite occurs.

$$3Fe^{2+} + 4H_2O = Fe_3O_4 + 8H^+ + 2e^- \tag{4.6}$$

$$2H^+ + 2e^- = H_2 \tag{4.7}$$
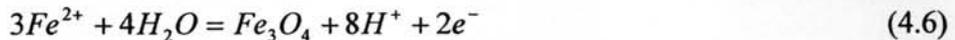
6) Hydrogen formed from reaction (4.7) coupling with the magnetite formation reaction diffuses outwards through the oxide film.

7) Hydrogen molecules and ferrous species will diffuse through pores of the oxide film outwardly to the oxide-solution interface. At oxide-solution interface, these species will move to the bulk solution by a mass transfer mechanism.

However, the mass transfer of hydrogen occurs so fast that the concentration of hydrogen at the oxide-solution interface equals its concentration in the bulk solution.

8) The mass transfer rate of hydrogen ion at oxide-solution interface to the bulk fluid is very fast. Therefore, the concentration of hydrogen ion at oxide-solution interface equals its concentration in the bulk solution. However, hydrogen ion concentration changes across the oxide film. Therefore, the concentration at the metal surface and at the oxide-solution interface is different.

9) Lithium hydroxide (LiOH) is applied to adjust pH in the primary coolant circuit. LiOH is a strong base and the LiOH completely dissociates.

10) Both the electrochemical corrosion and an electrochemical potentials at the oxide-solution interface affect the system significantly. They affect the hydrogen ion transportation through the oxide film, the magnetite solubility, and the dissolution rate constant of magnetite.

11) The potential at the metal surface and the potential at the metal-oxide interface are the same.

12) The concentration of all species at the metal surface is the same as at the oxide-solution interface.

13) The particle size of the spalling oxide is based on a reciprocal distribution of particle size (Lang, 2000).

4.2 Modelling

This model simulates the thinning phenomenon of the outlet feeder. The outlet feeder S08 was considered in this work. Operating conditions in outlet feeder S08 are listed in Table 4.1. In the present computation, the outlet feeder is assumed to be a straight pipe. The concentration of iron in the bulk solution at the entrance is assumed saturated at 265°C, the operating temperature within inlet feeders.

Table 4.1 Operating condition in outlet feeder S08

Temperature	310°C
Coolant velocity (cm/s)	1619
pH at 25°C	10.2
Hydrogen concentration (cc/kg)	5

In the modelling, the mathematical expressions are based on the above assumptions. The computational steps in the program are as following.

1. Load input data such as operating condition, dimension of pipe, and spalling oxide size distribution.

2. Calculate concentration in the system at 310°C: Li^+, Li^+ and $LiOH$, and H^+.

3. Calculate concentration of ferrous species (Fe^{2+}, $Fe(OH)^+$, $Fe(OH)_2$, and $Fe(OH)_3^-$) in the bulk system which is saturated at 265°C.

4. Calculate saturated concentration of ferrous species at 310°C in the bulk solution.

5. Initialize concentration of each species at interfaces.

6. Activity coefficients for ion species are calculated. The concentration of each species is adjusted.

7. Initialize some parameters: magnetite dissolution rate constant (k_d), potential at metal surface or metal-oxide solution interface (Em/o), and potential at the oxide-solution interface (Eo/s).

8. Do Loop computation for the following steps. The number of loop computations is the amount of exposure time.

9. Compute potential at each interface

10. Compute corrosion rate

11. Adjust hydrogen ion at the metal surface with the effect of potential across the oxide film

12. Adjust the magnetite dissolution rate constant at the oxide-solution interface with the effect of potential at the oxide-solution interface.

13. Adjust the magnetite solubility at the oxide-solution interface with the effect of potential at the oxide-solution interface.

14. Compute concentration of ferrous species at the oxide-solution interface

15. Compute concentration of ferrous species at the metal surface.

16. Calculate H_2 concentration at the metal surface.

17. Display output data.

4.2.1 Concentration Calculation

pH and hydrogen ion are related as indicated the Eqn. (4.8) and the hydrogen ion depends on dissociation of water.

$$pH = -\log H^+ \tag{4.8}$$

Dissociation of water is given by Marshall and Franck (1980) as

$$\log K_w = -14.9378 + 0.0424044t - 2.10252 \times 10^{-4} t^2$$
$$+ 6.22026 \times 10^{-7} t^3 - 8.73826 \times 10^{-10} t^4 \tag{4.9}$$

$$K_w = \frac{[H^+][OH^-]}{H_2O} \tag{4.10}$$

To calculate the concentration of lithium ion, Eqns. (4.11) and (4.12) are applied. Dissociation of lithium hydroxide is given by Eqn. (4.11) (EPRI, 1990)

$$\log K_{LiOH} = -0.7532 - 0.0048t + 6.75 \times 10^{-6} t^2 \tag{4.11}$$

$$K_{LiOH} = \frac{[Li^+][OH^-]}{[LiOH]} \tag{4.12}$$

Ferrous ion is not stable in the pH range of the operating condition. It will be hydrolyzed to the hydroxides of ferrous species as shown in reaction (4.3) to reaction (4.5). Equilibrium constants for these hydrolysis reactions are given by Eqns. (4.13) – (4.15), Tremaine and Leblanc (1980).

$$\log K_{Fe(OH)^+} = -4 \times 10^{-10} T^4 + 8.101 \times 10^{-7} T^3$$
$$- 6.296 \times 10^{-4} T^2 + 0.2308T - 41.55 \tag{4.13}$$

$$\log K_{Fe(OH)_2} = -4 \times 10^{-10} T^4 + 8.635 \times 10^{-7} T^3$$
$$- 7.373 \times 10^4 T^2 + 0.3115T - 67.82 \tag{4.14}$$

$$\log K_{Fe(OH)_3^-} = -4.7\times10^{-10}T^4 + 1.050\times10^{-6}T^3$$
$$-9.358\times10^{-4}T^2 + 0.4132T - 97.47 \tag{4.15}$$

$$K_{Fe(OH)^+} = \frac{m_{Fe(OH)^+}\gamma_1 m_{H^+}\gamma_1}{m_{Fe^{2+}}\gamma_2} \tag{4.16}$$

$$K_{Fe(OH)_2} = \frac{m_{Fe(OH)_2} m_{H^+}\gamma_1}{m_{Fe^{2+}}\lambda_2} \tag{4.17}$$

$$K_{Fe(OH)_3^-} = \frac{m_{Fe(OH)_3^-}\gamma_1 m_{H^+}\gamma_1^3}{m_{Fe^{2+}}\gamma_2} \tag{4.18}$$

Activity coefficients for ion species (γ_1 and γ_2) can be estimated from Debye-Hückel theory and Debye-Hückel equations (EPRI, 1990)

$$DHC = 0.5027 - 9.028\times10^{-4}t + 3.315\times10^{-5}t^2$$
$$-1.709\times10^{-7}t^3 + 3.29\times10^{-10}t^4 \tag{4.19}$$

$$I.S. = \frac{1}{2}\Sigma(z\cdot c) \tag{4.20}$$

$$\log\gamma_1 = -\frac{DHC*\sqrt{I.S.}}{1+\sqrt{I.S.}} \tag{4.21}$$

$$\log\gamma_2 = -\frac{4DHC\sqrt{I.S.}}{1+\sqrt{I.S.}} \tag{4.22}$$

where: DHC = Debye-Hückel constant

I.S. = Ionic Strength

z = Charge of ionic species

c = Concentration of ionic species

Concentrations of all species at oxide-solution interface are assumed to be the same as the bulk solution. At the metal-oxide interface, the concentrations of ferrous species are presumed to be supersaturated in order that the nucleation of magnetite can occur at this interface. The initial total ferrous species concentrations can be estimated by Eqn. (4.23).

$$\Sigma(FeII)_{m/o} = f\cdot\Sigma(FeII)_{sat,bulk} \tag{4.23}$$

where: f = supersaturated factor, 10%

4.2.2 Electrochemical Equations

The Nernst equation, Eqn. (4.24), is applied to compute the equilibrium potential at each interface.

$$E_{eq} = E^o - \frac{RT}{nF} \ln\left(\frac{a_{Re}}{a_{Ox}}\right)$$ (4.24)

where: E_{eq} = Equilibrium potential (V)

E^0 = Standard potential at 1atm and 1molar concentration (V)

a_{Re} = Activity or concentration of reduced species (molar)

a_{Ox} = Activity or concentration of oxidized species (molar)

At the metal surface, there are two reactions: one anodic reaction, reaction (4.1), and one cathodic reaction, reaction (4.2). Equilibrium potential for reaction (4.1) and reaction (4.2) can be calculated by Eqns. (4.25) (4.26), respectively.

$$E_{Fe/Fe^{2+},m/o} = -0.448 + \frac{RT}{2F} \ln\left([Fe^{2+}]\gamma_2\right)$$ (4.25)

$$E_{H^+/H_2,m/o} = -\frac{RT}{2F} \ln\left(\frac{[H_2]}{[H^+]^2}\right)$$ (4.26)

In an undersaturated system like the outlet feeder conditions, the magnetite dissolution reaction, reaction (4.6), and the hydrogen evolution, reaction (4.7), occur at the oxide-solution interface. The equilibrium potentials for both reactions are shown in Eqns. (4.27) and (4.28).

$$E_{Fe^{2+}/Fe_3O_4,o/s} = 1.2944 - \frac{RT}{(2/3)F} \ln\left(\frac{[Fe^{2+}]\gamma_2}{[H^+]^{8/3}\gamma_1^{8/3}}\right)$$ (4.27)

$$E_{H^+/H_2,o/s} = -\frac{RT}{(2/3)F} \ln\left(\frac{[H_2]^{1/3}}{[H^+]^{2/3}}\right)$$ (4.28)

Basically, the standard potential relates to the Gibbs free energy of reaction, Eqn. (4.29). The standard potential is a function of temperature since the Gibbs free energy of reaction is a function of temperature. However, the standard potential of hydrogen evolution is equal to zero at all temperatures. The standard

potential of the corrosion reaction, reaction (4.1), at 310°C is -0.448 volts and the standard potential of magnetite formation, reaction (4.6), is 1.2944 volts.

$$E^o = -\Delta G^o nF \tag{4.29}$$

where ΔG^0 = Standard Gibb free energy

E^0 = Standard potential at 1atm and 1molar concentration (V)

F = Faraday's constant, 96487 (Coulomb/mol)

n = Number of electron

Normally, the single reaction could be considered to go both forward and backward. When the rate of the forward reaction equals rate of the backward reaction, exchange current density is obtained. The exchange current density can be estimated from either Eqn. (4.30) or Eqn. (4.31).

$$i_o = k_f C_{Ox} nF \exp\left(\frac{-(1-\beta)nfE_{eq}}{RT}\right) \tag{4.30}$$

$$i_o = k_b C_{Re} nF \exp\left(\frac{\beta nFE_{eq}}{RT}\right) \tag{4.31}$$

The exchange current density for reactions (4.1) and (4.2) at the metal surface can be calculated from Eqns. (4.32) and (4.33), respectively. Eqns. (4.34) and (4.35) can be used to calculate the exchange current density of reactions (4.6) and (4.7), respectively.

$$i_{o,Fe/Fe^{2+},m/o} = k_1 C_{Fe^{2+}} 2F \exp\left(\frac{-(1-\beta)2FE_{Fe/Fe^{2+},m/o}}{RT}\right) \tag{4.32}$$

$$i_{o,H^+/H_2,m/o} = k_2 C_{H^+} 2F \exp\left(\frac{-(1-\beta)2FE_{H^+/H_2,m/o}}{RT}\right) \tag{4.33}$$

$$i_{o,Fe^{2+}/Fe_3O_4,o/s} = k_3 C_{Fe^{2+}} \frac{2}{3} F \exp\left(\frac{\beta(2/3)FE_{Fe^{2+}/Fe_3O_4,o/s}}{RT}\right) \tag{4.34}$$

$$i_{o,H^+/H_2,o/s} = k_4 C_{H^+} \frac{2}{3} F \exp\left(\frac{-(1-\beta)(2/3)FE_{H^+/H_2,o/s}}{RT}\right) \tag{4.35}$$

The mixed potential or potential at each interface is the potential at the point that the rate of anodic reaction equals rate of the cathodic reaction. In this case, the amount of the anodic current density and the cathodic current density is the

same as indicated in Eqn. 4.36. The current density can be estimated by the Butler-Volmer equation, Eqn. (4.38).

$$i = \Sigma i_a = -\Sigma i_c \tag{4.36}$$

$$\therefore \Sigma i_a + \Sigma i_c = 0 \tag{4.37}$$

$$i = i_o\left[\exp\left(\frac{\beta nF(E - E_{eq})}{RT}\right) - \exp\left(\frac{-(1-\beta)nF(E - E_{eq})}{RT}\right)\right] \tag{4.38}$$

For the anodic reaction;

$$i_a = i_{o,a}\left[\exp\left(\frac{\beta nF(E - E_{eq,a})}{RT}\right) - \exp\left(\frac{-(1-\beta)nF(E - E_{eq,a})}{RT}\right)\right]$$

$$\tag{4.39}$$

For the cathodic reaction;

$$i_c = i_{o,c}\left[\exp\left(\frac{\beta nF(E - E_{eq,c})}{RT}\right) - \exp\left(\frac{-(1-\beta)nF(E - E_{eq,c})}{RT}\right)\right]$$

$$\tag{4.40}$$

The Butler-Volmer equation is applied to calculate the anodic current and the cathodic current at each interface as shown in Eqns. (4.39) and (4.40). The summation of both currents is equal zero as indicated in Eqn. (4.37). The Newton-Raphson method indicated in Eqn. (4.41) is the numerical method applied in the model to estimate potential at each interface. According to the Newton-Raphson method, the summation of current is the function "f", where f' is the derivative of the function f, and potential is the parameter "x". The calculation for potential or x at each time period will be done when x in the n iteration is equal to x in the (n-1) iteration.

$$x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})} \tag{4.41}$$

The current at the metal surface is equals to the anodic current of reaction (4.1) as shown in Eqn. (4.42). This current is also called corrosion current.

$$i_{corr} = i_{Fe/Fe^{2+}} = i_{o,Fe/Fe^{2+},m/o} \left[\exp\left(\frac{\beta 2F\left(E_{m/o} - E_{Fe/Fe^{2+},m/o}\right)}{RT} \right) - \exp\left(\frac{-(1-\beta)2F\left(E_{m/o} - E_{Fe/Fe^{2+},m/o}\right)}{RT} \right) \right] \quad (4.42)$$

4.2.3 Computation for Corrosion Rate

The correlation between the corrosion current and the corrosion rate is shown in Eqn. (4.43) following Faraday's law.

$$CR = \frac{i_{corr}}{nF} = \frac{i_{corr}}{2F} \quad (4.43)$$

The corrosion process involves several mechanisms such as diffusion through the oxide film, mass transfer to the bulk solution, and magnetite dissolution or precipitation. The concentration of ferrous species change across the oxide film relates to these mechanisms.

Balance Fe(II) at the oxide-solution interface;

$$Out = In + Generation \quad (4.44)$$

$$MassTransfer = Diffusion + Dissolution \quad (4.45)$$

At the metal surface, it is assumed that the amount of ferrous species not forming magnetite diffuses through the oxide film. This relates to the corrosion rate as following.

$$Diffu\sin g = 0.476(1.101 + \phi)CR \quad (4.46)$$

From Eqn. 4.45 and Eqn. 4.46;

$$h(C_{o/s} - C_b) = 0.476(1.101 + \phi)CR + k_d F^*(C_{sat} - C_{o/s}) \quad (4.47)$$

Note that the mass transfer coefficient, h, refers to the work of Berger and Hua (1977). Berger and Hua (1977) give the relationship in dimensionless numbers: Sherwood number, Schmidt number, and Reynolds number.

$$Sh = 0.0165\,Re^{0.86}\,Sc^{0.33} \quad (4.48)$$

$$Re = \frac{dv\rho}{\mu} \quad (4.49)$$

$$Sc = \frac{\mu}{\rho D} \quad (4.50)$$

$$Sh = \frac{hd}{D} \tag{4.51}$$

Solve for $C_{o/s}$;

$$C_{o/s} = \frac{0.476CR(1.101 + \phi) + hC_b + k_d F^* C_{sat}}{(h + k_d F^*)} \tag{4.52}$$

Apply Fick's law to the amount of diffusing ferrous species through the oxide film;

$$\frac{D_{Fell}\phi}{\tau\delta}(C_{m/o} - C_{o/s}) = 0.476(1.101 + \phi)CR \tag{4.53}$$

Solve for $C_{m/o}$;

$$C_{m/o} = 0.476(1.101 + \phi)CR \cdot \frac{\tau\delta}{D_{Fell}\phi} + C_{o/s} \tag{4.54}$$

It is assumed that the hydrogen molecules at the oxide-solution interface is the same as in the bulk solution because the mass transfer of hydrogen to the bulk solution is very fast. However, the concentration of hydrogen at the metal-oxide interface changes as the magnetite precipitates at the metal-oxide interface. Only hydrogen evolution from the magnetite precipitation is assumed to diffuse outwards through the oxide film. Therefore, the equation to compute the concentration of hydrogen is obtained from Eqn. (4.55).

$$C_{H_2, m/o} = (1 - \phi)CR \cdot fraction \cdot \frac{\tau\delta}{D_{H_2}\phi} + C_{H_2, o/s} \tag{4.55}$$

$$fraction = \frac{MW_{metal}}{\rho_{metal}} \cdot \frac{\rho_{oxide}}{MW_{oxide}} \tag{4.56}$$

4.2.4 The Effect of Electrochemical Potential

The hydrogen ion gradient across the oxide film is due to the effect of potentials at the metal surface and at oxide-solution interface.

Based on Stokes-Einstein equation;

$$\frac{C_{H^+, m/o}}{C_{H^+, o/s}} = 1 - \frac{z_{H^+}F(E_{m/o} - E_{o/s})}{RT} \tag{4.57}$$

As the dissolution of magnetite is the reduction reaction, the effect of the potential on dissolution rate constant is given by in Eqn. (4.58).

$$k_{d,adjust} = k_d \exp\left(\frac{-(1-\beta)nFE}{RT}\right) \tag{4.58}$$

The Nernst equation is applied to adjust magnetite solubility according to Eqn. (4.59). Eqns. (4.16) - (4.18) are applied to calculate other ferrous species saturation. The overall amount of ferrous species is considered the concentration at saturation or solubility.

$$C_{Fe^{2+},sat} = C_{H^+}^{8/3} \exp\left((1.2944 - E_{o/s})\frac{(2/3)F}{RT}\right) \tag{4.59}$$

4.2.5 Spalling of Oxide

The magnetite is considered a protective film for the metal surface and it was found that the inner oxide layer was more compact than the outer oxide layer. Therefore, the inner oxide layer is more protective than the outer oxide layer. In the unsaturated solution and high fluid velocity system that occurs in the outlet feeder, only the inner oxide layer was observed.

The oxide thickness is affected by the corrosion rate, oxide dissolution or precipitation, and oxide spalling off at the oxide-solution interface. The spalling time is estimated by the Eqn. (4.60) or Eqn. (4.61) depending on the solution condition. The spalling time indicates the time that the oxide particle need to be spalled off. A short spalling time means that an oxide particle is easily spalled off.

For a saturated solution;

$$t_{sp} = \frac{s \cdot d_{oxide}}{v^2} \tag{4.60}$$

For an unsaturated solution;

$$t_{sp} = \frac{s \cdot d_{oxide}}{v^2 \phi \cdot k_d F^*\left(C_{sat} - C_{o/s}\right)} \tag{4.61}$$

The size of oxide particle depends on velocity and is based on the reciprocal distribution of the oxide particle size (Lang, 2000).

It is assumed that the volume of the corroded metal equals the volume of magnetite precipitation on metal surface. Therefore, the oxide growth rate on the metal or at the bottom of the oxide can be obtained in the unit of micron as shown in Eqn. (4.62).

$$OxGrowth_{bottom} = CR \times \frac{MW_{metal}}{\rho_{metal}} \times 10^4 \qquad (4.62)$$

At the oxide-solution interface or at the top of the oxide, the precipitation or dissolution of oxide, depending on the solution condition, plays a role in determining the oxide film thickness. If the solution in saturated, the oxide precipitation occurs and the oxide growth rate is positive as shown in Eqn. (4.63).

$$OxGrowth_{top} = \frac{1}{3} k_p F^\bullet \left(C_{o/s} - C_{sat} \right) \cdot \frac{1}{\left(1 - \phi_o \right)} \qquad (4.63)$$

If the solution is unsaturated, the magnetite dissolves to the solution. If there is no outer oxide, the surface of the inner oxide will dissolve according to Eqns. (4.64) and (4.65). In the other hand, the magnetite on the outer oxide surface will dissolve if there is outer oxide and the porosity of outer oxide will be used in the calculation as indicated in Eqns. (4.66) and (4.67). Even the inner or outer oxide dissolves, it affects the growth of oxide film. Dissolution of the oxide makes the oxide film thinner.

$$InnerOxGrowth_{top} = \frac{1}{3} k_d F^\bullet \left(C_{sat} - C_{o/s} \right) \cdot \frac{1}{\left(1 - \phi_i \right)} \qquad (4.64)$$

$$InnerOxGrowth_{top} = -\frac{1}{3} k_d F^\bullet \left(C_{o/s} - C_{sat} \right) \cdot \frac{1}{\left(1 - \phi_i \right)} \qquad (4.65)$$

$$OuterOxGrowth_{top} = \frac{1}{3} k_d F^\bullet \left(C_{sat} - C_{o/s} \right) \cdot \frac{1}{\left(1 - \phi_o \right)} \qquad (4.66)$$

$$OuterOxGrowth_{top} = -\frac{1}{3} k_d F^\bullet \left(C_{o/s} - C_{sat} \right) \cdot \frac{1}{\left(1 - \phi_o \right)} \qquad (4.67)$$

4.3 Parameters in the Model

All parameters used in the model are shown in Table 4.2.

Table 4.2 Parameters used in the model

Diffusivity of diffusing H_2, cm^2/s	10^{-4}
Diffusivity of diffusing iron species, cm^2/s	4.1×10^{-4}
Inner spalling constant	0.0289
Outer spalling constant	0.01
Inner porosity	0.10
Outer porosity	0.30
Tortuosity	1.15
Reaction rate constant ($Fe = Fe^{2+} + e^-$) at metal surface, cm/s	10^{-5}
Reaction rate constant ($H^{2+} + 2e^- = H_2$) at metal surface, cm/s	2.4×10^{-9}
Reaction rate constant ($Fe_3O_4 = Fe(OH)_2$) on oxide film, cm/s	1×10^{-5}
Reaction rate constant ($H^{2+} + 2e^- = H_2$) on oxide film, cm/s	1×10^{-5}
Dissolution rate constant, cm/s	1.1×10^{-7}

4.4 Nomenclature

a_{Ox}	Activity or concentration of oxidized species (molar)
a_{Re}	Activity or concentration of reduced species (molar)
C_b	Bulk concentration
$C_{m/o}$	Concentration at metal-oxide interface
$C_{o/s}$	Concentration at oxide-solution interface
C_{Ox}	Concentration of oxidized species
C_{Re}	Concentration of reduced species
C_{sat}	Solubility
CR	Corrosion rate
c	Concentration

d	Diameter of pipe (cm)
d_{oxide}	Spalling oxide particle
D_{H2}	Diffusivity of hydrogen molecule
D_{FeII}	Diffusivity of ferrous species
DHC	Debye-Hückel constant
E_{eq}	Equilibrium potential (V)
E^0	Standard potential at 1atm and 1molar concentration (V)
f	Supersaturated factor, 10%
f	Newton Raphson function
F	Faraday's constant, 96487 Coulomb/mol
F*	Surface area factor
h	Mass transfer coefficient
i	Current density (Coulomb/cm^2)
i_a	Anodic current density (Coulomb/cm^2)
i_c	Cathodic current density (Coulomb/cm^2)
i_{corr}	Corrosion current density (Coulomb/cm^2)
i_o	Exchange current density (Coulomb/cm^2)
I.S.	Ionic Strength'
k_b	Rate constant of backward reaction (cm/s)
k_d	Magnetite dissolution constant (cm/s)
k_f	Rate constant of forward reaction (cm/s)
k_p	Magnetite precipitation constant (cm/s)
k_1	Rate constant for reaction Fe to Fe^{2+} on metal surface
k_2	Rate constant for hydrogen evolution reaction on metal surface
k_3	Rate constant for magnetite dissolution/precipitation on oxide film
k_4	Rate constant for hydrogen evolution reaction on oxide film
$K_{Fe(OH)+}$	Hydrolysis constant of Fe^{2+} to Fe(OH)$^+$
$K_{Fe(OH)2}$	Hydrolysis constant of Fe^{2+} to Fe(OH)$_2$
$K_{Fe(OH)3-}$	Hydrolysis constant of Fe^{2+} to Fe(OH)$_3^-$
K_{Li}	LiOH dissociation constant
K_w	Water dissociation constant
MWmetal	Molecular weight of iron metal

MWoxide	Molecular weight of oxide
n	Number of electron
R	Gas constant, 8.314 ($J\ mol^{-1}\ K^{-1}$)
Re	Reynolds number
s	Spalling constant
Sc	Schmidt number
Sh	Sherwood number
t	Temperature (°C)
t_{sp}	spalling time
T	Temperature (K)
v	Velocity of coolant (cm/s)
z	Charge of ionic species
β	Symmetry coefficient, 0.5
γ_1	Activity coefficient of ion charge +/-1
γ_2	Activity coefficient of ion charge +/-2
ρ	Density of coolant (g/cm^3)
ρ_{metal}	Density of metal (g/cm^3)
ρ_{oxide}	Density of oxide (g/cm^3)
μ	Viscosity of coolant (g/cm s)
τ	Oxide tortuosity
ϕ	Oxide porosity
ϕ_i	Inner oxide porosity
ϕ_o	Outer oxide porosity
δ	Oxide thickness
ΔG^0	Standard Gibb free energy