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APPENDICES

Appendix A Method for Thin Section Preparation (Ancel, 2007)

Thinned samples are needed for obtaining the cross-sectional image of samples. The following method is used to prepare thinned section sample at university of New Brunswick, Fredericton, Canada.

Method for thin section preparation

1. Sample is cut with a slow speed saw in oil – using a diamond wafering blade.
2. Sample for sectioning is cleaned with alcohol and left to dry.
3. Mould is filled with cold mounting epoxy. Label (with sample numbers) is placed in and the mould is allowed to cure 24 hours.
4. Epoxy block is removed from mould and flattened to expose the sample. This is done by rubbing the sample against a flat glass plate using 400 silicon carbide grit and kerosene as lubricant – once the sample is exposed and flat, it is cleaned with alcohol.
5. Next step is making the sample smoother using a flat glass plate with 600 silicon carbide grit and kerosene. Then smooth sample is cleaned with alcohol.
6. Flatten sample is then affixed to a 27 mm x 46 mm petrographic glass slide using Buehler Epo Thin Epoxy and allowed to cure 24 hours.
7. Glass slide with sample glued to it is cut using the slow speed saw (diamond blade – oil lubricant) so that a sample about 300 – 400 microns thick is left.
8. The sample is then ground flat by using Logitech Thin Rock Section Machine System – using 600 silicon carbide grit and oil.
9. The thinned sample is then processed on Logitech Precision Lapping and Polishing Machine by these following steps.
   9.1 Sample is polished using Tex Met PSU Polishing Pod with 3-micron diamond paste and Ethandiol-Alcohol (lubricant) until the surface viewed

under reflective petrographic microscope is suitable. Sample is cleaned with alcohol.

9.2 Sample is polished using Tex Met PSU Polishing Pod with 1-micron diamond paste and Ethandiol-Alcohol (lubricant) until surface is acceptable – checked under reflective petrographic microscope. Sample is cleaned with alcohol.

9.3 Sample is polished using Tex Met PSU Polishing Pod with 0.25-micron diamond paste and Ethandiol-Alcohol (lubricant) until sample's surface is acceptable, checked under reflective petrographic microscope, and then cleaned with alcohol. Thinned sample is prepared.

Appendix B The Standard Color of Some Iron Oxides (Cornell, 2003)

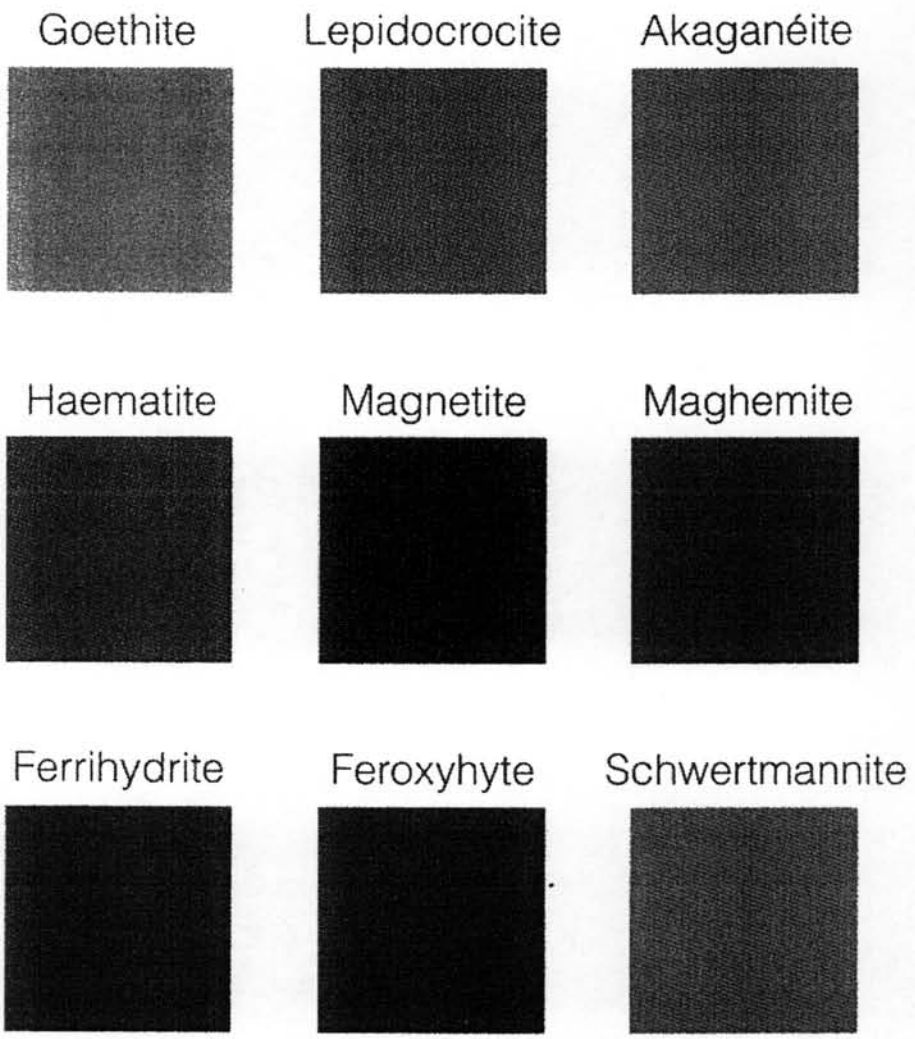

Figure B.1 The standard color of some iron oxides.

Appendix C Energy-Dispersive X-ray Analysis Results

Table C.1 Energy-Dispersive X-ray analysis results for static experiment samples

Samples	Fraction (At %)															
	O	Mg	Al	Si	P	S	Ca	Ti	Zr	Cr	Mn	Fe	Ni	Cu	Zn	Total
Bare coupon	0.00	0.00	0.00	1.42	0.00	0.00	0.00	0.00	0.00	0.00	0.86	97.72	0.00	0.00	0.00	100.00
0 m/s, 15 days																
- Fine grain particles	50.54	0.06	0.12	0.63	0.01	0.00	0.17	0.31	0.00	0.00	0.17	45.31	0.00	2.62	0.03	100.00
- Hexagonal crystalline particles	59.40	1.09	0.51	0.39	0.16	0.00	0.19	17.90	0.00	0.03	0.45	19.58	0.00	0.30	0.00	100.00
0 m/s, 20 days																
- Fine grain particles	52.18	0.49	0.69	1.19	1.24	0.00	0.32	0.92	0.00	0.04	0.29	37.79	0.07	4.78	0.00	100.00
- Hexagonal crystalline particles	59.00	0.55	0.18	0.30	0.23	0.00	0.07	17.26	0.00	0.00	0.52	21.40	0.00	0.49	0.00	100.00
0 m/s, 30 days																
- Fine grain particles	51.10	0.07	0.21	1.78	0.00	0.00	0.04	0.22	0.00	0.06	0.36	44.72	0.00	1.39	0.07	100.00
- Hexagonal crystalline particles	59.88	0.28	0.05	0.05	0.00	0.00	0.02	19.44	0.00	0.00	0.79	19.19	0.00	0.06	0.24	100.00
0 m/s, 50 days																
- Fine grain particles	50.68	0.09	0.13	0.51	0.00	0.00	0.08	0.58	0.00	0.02	0.24	45.60	0.00	1.87	0.18	100.00
- Hexagonal crystalline particles	59.74	0.44	0.14	0.13	0.00	0.00	0.01	19.03	0.00	0.00	0.58	19.46	0.00	0.20	0.24	100.00

Table C.2 Energy-Dispersive X-ray analysis results for flow experiment samples

Samples	Fraction (At %)															
	O	**Mg**	**Al**	**Si**	**P**	**S**	**Ca**	**Ti**	**Zr**	**Cr**	**Mn**	**Fe**	**Ni**	**Cu**	**Zn**	**Total**
Bare tube probe	0.00	0.00	0.00	0.77	0.00	0.00	0.00	0.00	0.00	0.00	0.77	98.46	0.00	0.00	0.00	100.00
5 m/s, 15 days																
- Fine grain particles	51.32	0.14	0.24	0.77	1.08	0.00	0.03	0.02	0.00	0.10	0.18	46.06	0.00	0.00	0.04	100.00
5 m/s, 38 days																
- Fine grain particles	50.60	0.00	0.00	0.40	0.00	0.00	0.00	0.07	0.00	0.02	0.28	48.63	0.00	0.00	0.00	100.00
- Octahedral crystalline particles	50.14	0.00	0.00	0.09	0.00	0.00	0.00	0.22	0.00	0.02	0.28	49.25	0.00	0.00	0.00	100.00
5 m/s, 38 days																
- Fine grain particles	50.11	0.00	0.00	0.23	0.00	0.00	0.00	0.00	0.00	0.10	0.20	40.44	8.93	0.00	0.00	100.00
- Octahedral crystalline particles	50.36	0.00	0.00	0.64	0.00	0.00	0.00	0.00	0.09	0.04	0.16	47.14	1.57	0.00	0.00	100.00
10 m/s, 38 days																
- Fine grain particles	50.57	0.00	0.24	0.55	0.04	0.13	0.22	0.11	0.00	0.13	0.50	47.15	0.36	0.00	0.00	100.00
20 m/s, 234 days																
- Fine grain particles	50.33	0.00	0.00	0.52	0.00	0.00	0.00	0.14	0.00	0.05	0.22	46.33	2.41	0.00	0.00	100.00
- Octahedral crystalline particles	50.34	0.00	0.00	0.14	0.00	0.00	0.00	0.50	0.00	0.16	0.11	39.73	9.02	0.00	0.00	100.00

Appendix D FAC Model Program Code (Orawee, 2007)

''PARAMETERS ''

''' PARAMETERS IN "OUTPUT" '''

" K = Iteration number or hour

" InnerOx = Inner oxide layer (micron)

" OuterOx = Outer oxide layer (micron)

" CR = Corrosion rate (mol/cm2 s)

" CorrCur = Corrosion Current (Amp/cm2)

" MOPot = Potential at Metal surface and Metal-Oxide interface (V)

" OSPot = Potential at Oxide-Solution interface (V)

" CB = Bulk concentration of iron species (mol/kg)

" CW = Concentration of iron species at metal surface (mol/kg)

" CS = Concentration of iron species at Oxide-Solution interface (mol/kg)

" Sat = Saturated concentration of iron species at Oxide-Solution interface (mol/kg)

''' PARAMETERS IN "ELECTROCHEMISTRY" '''

" equilPotentialFe = Equilibrium potential of Fe to Fe2+ rxn at metal surface (V)

" equilPotentialH2_MO = Equilibrium potential of H+ to H2 rxn at metal surface (V)

" equilPotentialMag = Equilibrium potential of magnetite formation at oxide-solution interface (V)

" equilPotentialH2_OS = Equilibrium potential of H+ to H2 rxn at oxide-solution interface (V)

" rxnConstantFe = Reaction rate constant of Fe to Fe2+ rxn at metal surface (cm/s)

" rxnConstantHonMetal = Reaction rate constant of H+ to H2 rxn at metal surface (cm/s)

" rxnConstantMag = Reaction rate constant of magnetite formation rxn at oxide-solution interface (cm/s)

" rxnConstantH2onMag = Reaction rate constant of H+ to H2 rxn at oxide-solution interface (cm/s)

" exchangecurrentFe = Exchange current density of Fe to Fe2+ rxn at metal surface (Amp/cm2)

" exchangecurrentHonFe = Exchange current density of H+ to H2 rxn at metal surface (Amp/cm2)

" exchangecurrentMag = Exchange current density of magnetite formation at oxide-solution interface (Amp/cm2)

" exchangecurrentHonMag = Exchange current density of H+ to H2 rxn at oxide-solution interface (Amp/cm2)

''' PARAMETERS in "Concentration" '''

" mH2 = Concentration of H2 (mol/kg)

" mH = Concentration of H+ (mol/kg)

" mOH = Concentratin of OH- (mol/kg)

" mLi = Concentration of Li+ (mol/kg)

" FeTotal = Concentration of total iron species (mol/kg)

" Fesat = Saturation concentration of iron species (mol/kg)

" mFE2 = Concentration of Fe2+ (mol/kg)

" mFEOH = Concentration of Fe(OH)+ (mol/kg)

" mFEOH2 = Concentration of FE(OH)2 (mol/kg)

" mFEOH3 = Concentration of FE(OH)3- (mol/kg)

" gamma1 = Activity coefficient for ion +/- 1

" gamma2 = Activity coefficient for ion +/- 2

" Inner_SpallingFrequency = Spalling frequency of inner oxide from the spalling distribution

" Outer_SpallingFrequency = Spalling frequency of outer oxide from the spalling distribution

" InnerSize = Spalling size of inner oxide from the spalling distribution

" OuterSize = Spalling size of outer oxide from the spalling distribution

" TC_input = Input temperature (celcius)

" TK_input = Input temperature (kelvin)

" TC = Temperature (celcius)

" TK = Temperature (kelvin)

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" pH25 = pH at 25 celcius
" KW = Dissociation constant of water
" KFE2 = Solubility constant of Fe2+
" KLi = Dissociation constant of LiOH
" IonicStrength = Ionic strength used in Debye-Huckel equation
" DHC = Debye-Huckel constant
" kd_chem = Magnetite dissolution constant (cm/s)
" kd_elect = Magnetite dissolution constant affected by potential (cm/s)
" Area_factor = Area factor affecting dissolution rate
" m = Power in dissolution rate equation
" Incr = Incremental time (second)
" period = Total exposure time (hour)
" velocity = Coolant velocity (cm/s)
" Den = Coolant density (g/cm3)
" mH25 = Concentration of H+ at 25 celcius (mol/kg)
" mOH25 = Concentration of OH- at 25 celcius (mol/kg)
" mLi = Concentration of Li+ (mol/kg)
" mLitotal = Concentration of total Li (mol/kg)
" mt_coeff = Mass transfer coefficient (cm/s)
" DH2 = Diffusivity of H2 (cm2/s)
" DFe = Diffusivity of Fe species (cm2/s)
" porosity_in = Porosity of inner oxide
" porosity_out = Porosity of outer oxide
" tortuosity = Tortuosity of oxide
" R = Gas constant (J/mol K)
" F = Faraday constant (C/mol)
" beta = Symmetry coefficient
" fraction = Ratio of Fe mole in a moleof magnetite
" MW_metal = Molecular weight of iron or metal
" Den_metal = Density of iron or metal (g/cm3)
" MW_mag = Molecular weight of magnetite
" Den_mag = Density of magnetite (g/cm3)
" OSCur = Current density at oxide-solution interface (Amp/cm2)
" Dis_rate = Dissolution rate of magnetite (mol/cm2 s)
" LastCR = Set corrosion rate as the initial (mol/cm2 s)

" MO_Interface = Parameter for electrochemical variables at metal-oxide interface
" OS_Interface = Parameter for electrochemical variables at oxide-solution interface
" MO_Int = Parameter for concentration variables at metal-oxide interface
" OS_Int = Parameter for concentration variables at oxide-solution interface
" Bulk = Parameter for concentration variables in bulk solution
" Results1 = Parameter for output

```
Type Output
  K  As Long
  InnerOx As Double
  OuterOx As Double
  CR As Double
  CorrCur As Double
  MOPot As Double
  OSPot As Double
  CB As Double
  CW As Double
  CS As Double
  Sat As Double
  Spall_in As Double
```

```
  Spall_out As Double
  Hmo As Double
  Hos As Double
  kd As Double
  Eeq1 As Double
  Eeq2 As Double
  Eeq3 As Double
  Eeq4 As Double
  Io1 As Double
  Io2 As Double
  Io3 As Double
  Io4 As Double
  In_SPTime As Double
  Out_SPTime As Double
End Type

'ELECTROCHEMICAL PARAMETERS
Dim Inlet_equilPotentialFe As Double, Inlet_equilPotentialH2_MO As Double,
Inlet_equilPotentialMag As Double, _
  Inlet_equilPotentialH2_OS As Double, Inlet_rxnConstantFe As Double,
Inlet_rxnConstantHonMetal As Double, _
  Inlet_rxnConstantMag As Double, Inlet_rxnConstantH2onMag As Double,
Inlet_exchangecurrentFe As Double, _
  Inlet_exchangecurrentHonFe As Double, Inlet_exchangecurrentMag As Double,
Inlet_exchangecurrentHonMag As Double

Dim Outlet_equilPotentialFe As Double, Outlet_equilPotentialH2_MO As Double,
Outlet_equilPotentialMag As Double, _
  Outlet_equilPotentialH2_OS As Double, Outlet_rxnConstantFe As Double,
Outlet_rxnConstantHonMetal As Double, _
  Outlet_rxnConstantMag As Double, Outlet_rxnConstantH2onMag As Double,
Outlet_exchangecurrentFe As Double, _
  Outlet_exchangecurrentHonFe As Double, Outlet_exchangecurrentMag As Double,
Outlet_exchangecurrentHonMag As Double

'H2 Concentration
Dim Inlet_mH2 As Double, Outlet_mH2 As Double

'BULK CONCENTRATION
Dim Inlet_Bulk_mH2(7) As Double, Inlet_Bulk_mH(7) As Double, Inlet_Bulk_mOH(7) As
Double, Inlet_Bulk_mLi(7) As Double, _
  Inlet_Bulk_mLiTotal(7) As Double, Inlet_Bulk_FeTotal(7) As Double, Inlet_Bulk_Fesat(7)
As Double, Inlet_Bulk_mFE2(7) As Double, _
  Inlet_Bulk_mFEOH(7) As Double, Inlet_Bulk_mFEOH2(7) As Double,
Inlet_Bulk_mFEOH3(7) As Double, Inlet_Bulk_gamma1(7) As Double, _
  Inlet_Bulk_gamma2(7) As Double

Dim Outlet_Bulk_mH2(7) As Double, Outlet_Bulk_mH(7) As Double, Outlet_Bulk_mOH(7)
As Double, Outlet_Bulk_mLi(7) As Double, _
  Outlet_Bulk_mLiTotal(7) As Double, Outlet_Bulk_FeTotal(7) As Double,
Outlet_Bulk_Fesat(7) As Double, _
  Outlet_Bulk_mFE2(7) As Double, Outlet_Bulk_mFEOH(7) As Double,
Outlet_Bulk_mFEOH2(7) As Double, _
  Outlet_Bulk_mFEOH3(7) As Double, Outlet_Bulk_gamma1(7) As Double,
Outlet_Bulk_gamma2(7) As Double

'M/O CONCENTRATION
```

```
Dim Inlet_MO_mH2(7) As Double, Inlet_MO_mH(7) As Double, Inlet_MO_mOH(7) As Double, Inlet_MO_mLi(7) As Double, _
  Inlet_MO_mLiTotal(7) As Double, Inlet_MO_FeTotal(7) As Double, Inlet_MO_Fesat(7) As Double, Inlet_MO_mFE2(7) As Double, _
  Inlet_MO_mFEOH(7) As Double, Inlet_MO_mFEOH2(7) As Double, Inlet_MO_mFEOH3(7) As Double, Inlet_MO_gamma1(7) As Double, _
  Inlet_MO_gamma2(7) As Double

Dim Outlet_MO_mH2(7) As Double, Outlet_MO_mH(7) As Double, Outlet_MO_mOH(7) As Double, Outlet_MO_mLi(7) As Double, _
  Outlet_MO_mLiTotal(7) As Double, Outlet_MO_FeTotal(7) As Double, Outlet_MO_Fesat(7) As Double, Outlet_MO_mFE2(7) As Double, _
  Outlet_MO_mFEOH(7) As Double, Outlet_MO_mFEOH2(7) As Double, Outlet_MO_mFEOH3(7) As Double, Outlet_MO_gamma1(7) As Double, _
  Outlet_MO_gamma2(7) As Double

'O/S CONCENTRATION
Dim Inlet_OS_mH2(7) As Double, Inlet_OS_mH(7) As Double, Inlet_OS_mOH(7) As Double, Inlet_OS_mLi(7) As Double, _
  Inlet_OS_mLiTotal(7) As Double, Inlet_OS_FeTotal(7) As Double, Inlet_OS_Fesat(7) As Double, Inlet_OS_mFE2(7) As Double, _
  Inlet_OS_mFEOH(7) As Double, Inlet_OS_mFEOH2(7) As Double, Inlet_OS_mFEOH3(7) As Double, Inlet_OS_gamma1(7) As Double, _
  Inlet_OS_gamma2(7) As Double
Dim Outlet_OS_mH2(7) As Double, Outlet_OS_mH(7) As Double, Outlet_OS_mOH(7) As Double, Outlet_OS_mLi(7) As Double, _
  Outlet_OS_mLiTotal(7) As Double, Outlet_OS_FeTotal(7) As Double, Outlet_OS_Fesat(7) As Double, Outlet_OS_mFE2(7) As Double, _
  Outlet_OS_mFEOH(7) As Double, Outlet_OS_mFEOH2(7) As Double, Outlet_OS_mFEOH3(7) As Double, Outlet_OS_gamma1(7) As Double, _
  Outlet_OS_gamma2(7) As Double

Dim Printing() As Output


'SPALLING PARAMETERS
Dim Inlet_Inner_SpallingFrequency(125,8) As Double, Inlet_Outer_SpallingFrequency(125,1) As Double, _
  Inlet_InnerSize(125) As Double, Inlet_OuterSize(125) As Double

Dim Outlet_Inner_SpallingFrequency(125, 8) As Double, Outlet_Outer_SpallingFrequency(125, 1) As Double, _
  Outlet_InnerSize(125) As Double, Outlet_OuterSize(125) As Double

'SYSTEM
Dim Inlet_Node As Long
Dim Inlet_Dia(7) As Double, Inlet_Leng(7) As Double
Dim Inlet_velocity(7) As Double
Dim Inlet_Den, Inlet_Vis As Double

Dim Outlet_Node As Long
Dim Outlet_Dia(7) As Double, Outlet_Leng(7) As Double
Dim Outlet_velocity(7) As Double
Dim Outlet_Den, Outlet_Vis As Double

'SYSTEM CONDITION (Temperature/pH)
Dim Inlet_TCinput As Double, Inlet_TKinput As Double
```

```
Dim Inlet_pH25 As Double
Dim Inlet_mH25 As Double, Inlet_mOH25 As Double

Dim Outlet_TCinput As Double, Outlet_TKinput As Double
Dim Outlet_pH25 As Double
Dim Outlet_mH25 As Double, Outlet_mOH25 As Double



'CONSTANT PARAMETERS
Dim Inlet_kd_chem As Double, Inlet_kp_chem As Double, Inlet_spconst_in As Double, Inlet_spconst_out As Double
Dim Inlet_kd_elect(7) As Double, Inlet_kp_elect(7) As Double
Dim Inlet_Area_factor As Double                'Area factor taken into account of magnetite dissolution
Dim Inlet_DH2 As Double, Inlet_DFe As Double, Inlet_porosity_in As Double, Inlet_porosity_out As Double, Inlet_tortuosity As Double
Dim Inlet_mt_coeff(7) As Double
Dim Outlet_kd_chem As Double, Outlet_kp_chem As Double, Outlet_spconst_in As Double, Outlet_spconst_out As Double  'dissolution coefficients, spalling constants for inner and outer
Dim Outlet_kd_elect(7) As Double, Outlet_kp_elect(7) As Double
Dim Outlet_Area_factor As Double               'Area factor taken into account of magnetite dissolution
Dim Outlet_DH2 As Double, Outlet_DFe As Double, Outlet_porosity_in As Double, Outlet_porosity_out As Double, Outlet_tortuosity As Double
Dim Outlet_mt_coeff(7) As Double

'GENERAL VARIABLES
Public R As Double, F As Double, beta As Double
Public MW_metal As Double, Den_metal As Double, MW_mag As Double, Den_mag As Double
Public fraction As Double
Dim Incr As Double 'Incr = incremental time
Dim period As Long

'OUTPUT PARAMETERS
Dim K As Long
Dim StartPot_MO As Double, StartPot_OS As Double

Dim Inlet_CR(7) As Double, Inlet_CorrCur(7) As Double, Inlet_MOPot(7) As Double, Inlet_OSPot(7) As Double
Dim Inlet_InnerOx(7) As Double, Inlet_OuterOx(7) As Double

Dim Outlet_CR(7) As Double, Outlet_CorrCur(7) As Double, Outlet_MOPot(7) As Double, Outlet_OSPot(7) As Double
Dim Outlet_InnerOx(7) As Double, Outlet_OuterOx(7) As Double

Dim Inlet_In_SpallTime(7) As Double, Inlet_Out_SpallTime(7) As Double
Dim Outlet_In_SpallTime(7) As Double, Outlet_Out_SpallTime(7) As Double

Dim Inlet_Eeq1(7) As Double, Inlet_Eeq2(7) As Double, Inlet_Eeq3(7) As Double, Inlet_Eeq4(7) As Double, _
  Inlet_Io1(7) As Double, Inlet_Io2(7) As Double, Inlet_Io3(7) As Double, Inlet_Io4(7) As Double
Dim Outlet_Eeq1(7) As Double, Outlet_Eeq2(7) As Double, Outlet_Eeq3(7) As Double, Outlet_Eeq4(7) As Double, _
  Outlet_Io1(7) As Double, Outlet_Io2(7) As Double, Outlet_Io3(7) As Double, Outlet_Io4(7) As Double
```

```
'Dim Results1(16, 10000) As Output
Dim Results1(25, 10000) As Output, PrintIter As Long 'Maximum worksheet per workbook is 255
Dim IFeedSheet(7) As String
Dim OFeedSheet(7) As String
Dim HFeedSheet(2) As String

Dim DiffGamma1 As Double, DiffGamma2 As Double
Dim ErrGamma As Double 'Error checking for gamma correction
Dim MaxIter As Long 'Maximum iteration for gamma correction

Dim FILEPATH As String

' Constants for KW calculation
Const MF_constant1 As Double = -14.9378
Const MF_constant2 As Double = 0.0424044
Const MF_constant3 As Double = -0.000210252
Const MF_constant4 As Double = 0.000000622026
Const MF_constant5 As Double = -0.000000000873826

'Constants for KLi calculation
Const Li_constant1 As Double = -0.7532
Const Li_constant2 As Double = -0.0048
Const Li_constant3 As Double = 0.00000675

'Constant Fe2+ to Fe(OH)+
Const FeOH_Constant1 As Double = -4.0000000002121E-10
Const FeOH_Constant2 As Double = 8.1013333337064E-07
Const FeOH_Constant3 As Double = -6.2962960002269E-04
Const FeOH_Constant4 As Double = 0.23076341387204
Const FeOH_Constant5 As Double = -41.554229416762

'Constant Fe2+ to Fe(OH)2
Const FeOH2_Constant1 As Double = -4.00000000027982E-10
Const FeOH2_Constant2 As Double = 8.63466666713771E-07
Const FeOH2_Constant3 As Double = -7.37309600026264E-04
Const FeOH2_Constant4 As Double = 0.311498720538374
Const FeOH2_Constant5 As Double = -67.8248276565119

'Constant Fe2+ to Fe(OH)3-
Const FeOH3_Constant1 As Double = -4.6666666670835E-10
Const FeOH3_Constant2 As Double = 1.0496000000844E-06
Const FeOH3_Constant3 As Double = -9.3577453338961E-04
Const FeOH3_Constant4 As Double = 0.41318595841421
Const FeOH3_Constant5 As Double = -97.470892206812

Const DH_constant1 As Double = 0.5027
Const DH_constant2 As Double = -0.0009028
Const DH_constant3 As Double = 0.00003315
Const DH_constant4 As Double = -0.0000001709
Const DH_constant5 As Double = 0.000000000329
'    KFEOH = 10 ^ (-4.0000000002121E-10 * TK ^ 4 + 8.1013333337064E-07 * TK ^ 3 - 6.2962960002269E-04 * TK ^ 2 + 0.23076341387204 * TK - 41.554229416762)
'    KFEOH2 = 10 ^ (-4.00000000027982E-10 * TK ^ 4 + 8.63466666713771E-07 * TK ^ 3 - 7.37309600026264E-04 * TK ^ 2 + 0.311498720538374 * TK - 67.8248276565119)
'    KFEOH3_ = 10 ^ (-4.6666666670835E-10 * TK ^ 4 + 1.0496000000844E-06 * TK ^ 3 - 9.3577453338961E-04 * TK ^ 2 + 0.41318595841421 * TK - 97.470892206812)
```

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```
Public strTemplate2 As String

Sub Compute()
  .
' For Benchmarking
Dim Count As Long
Dim BenchMark As Double

'Dim wbDISTRIBUTION As Workbook

FILEPATH = ThisWorkbook.Path

'Start of calculation
BenchMark = Timer

'SET PrintIter in order to Clear Memory
PrintIter = 0

Workbooks(1).Activate

'DATA LOAD
Sheets("Inlet").Select

  'System Properties
  Inlet_Node = Range("C9").Value
  For i = 1 To Inlet_Node
    Inlet_Dia(i) = Range(Cells(10, i + 2), Cells(10, i + 2)).Value
    Inlet_velocity(i) = Range(Cells(11, i + 2), Cells(11, i + 2)).Value '(cm/s)
    Inlet_Leng(i) = Range(Cells(12, i + 2), Cells(12,i + 2)).Value
  Next i

  Inlet_TCinput = Range("C13").Value '(Celcius)
  Inlet_TKinput = Range("C14").Value '(Kevin)
  Inlet_Den = Range("C15").Value '(g/cm3)
  Inlet_Vis = Range("C16").Value '(g/cm s)
  Inlet_pH25 = Range("C17").Value
  Inlet_mH2 = Range("C25").Value '(mol/kg)

  For i = 1 To Inlet_Node
    Inlet_Bulk_mH2(i) = Inlet_mH2 '(mol/kg)
  Next i


  'Constants
  Inlet_DFe = Range("C29").Value '(cm2/s)
  Inlet_DH2 = Range("C30").Value '(cm2/s)
  Inlet_spconst_in = Range("C31").Value
  Inlet_spconst_out = Range("C32").Value
  Inlet_porosity_in = Range("C33").Value
  Inlet_porosity_out = Range("C34").Value
  Inlet_tortuosity = Range("C35").Value

  For i = 1 To Inlet_Node
  Inlet_mt_coeff(i) = Range(Cells(39, i + 2), Cells(39, i + 2)).Value '(cm/s)
  Next i

  Inlet_kd_chem = Range("C40").Value
```

```
Inlet_kp_chem = Range("D40").Value
Inlet_Area_factor = Range("C41").Value

'Electrochemical Constants
Inlet_rxnConstantFe = Range("C44").Value '(cm/s)
Inlet_rxnConstantHonMetal = Range("C45").Value
Inlet_rxnConstantMag = Range("C46").Value '(cm/s)
Inlet_rxnConstantH2onMag = Range("C47").Value '(cm/s)

'Initial Oxide thickness
For i = 1 To Inlet_Node
Inlet_InnerOx(i) = Range("C28").Value
Inlet_OuterOx(i) = Range("C28").Value
Next i

Sheets("Outlet").Select

'System Properties
Outlet_Node = Range("C9").Value
For i = 1 To Outlet_Node
Outlet_Dia(i) = Range(Cells(10, i + 2), Cells(10, i + 2)).Value
Outlet_velocity(i) = Range(Cells(11, i + 2), Cells(11, i + 2)).Value '(cm/s)
Outlet_Leng(i) = Range(Cells(12, i + 2), Cells(12, i + 2)).Value
Next i

Outlet_TCinput = Range("C13").Value '(Celcius)
Outlet_TKinput = Range("C14").Value '(Kevin)
Outlet_Den = Range("C15").Value '(g/cm3)
Outlet_Vis = Range("C16").Value '(g/cm s)
Outlet_pH25 = Range("C17").Value
Outlet_mH2 = Range("C25").Value '(mol/kg)

For i = 1 To Outlet_Node
Outlet_Bulk_mH2(i) = Outlet_mH2 '(mol/kg)
Next i

'Constants
Outlet_DFe = Range("C29").Value '(cm2/s)
Outlet_DH2 = Range("C30").Value '(cm2/s)
Outlet_spconst_in = Range("C31").Value
Outlet_spconst_out = Range("C32").Value
Outlet_porosity_in = Range("C33").Value
Outlet_porosity_out = Range("C34").Value
Outlet_tortuosity = Range("C35").Value
For i = 1 To Outlet_Node
Outlet_mt_coeff(i) = Range(Cells(39, i + 2), Cells(39, i + 2)).Value '(cm/s)
Next i

Outlet_kd_chem = Range("C40").Value
Outlet_kp_chem = Range("D40").Value
Outlet_Area_factor = Range("C41").Value

'Electrochemical Constants
Outlet_rxnConstantFe = Range("C44").Value '(cm/s)
Outlet_rxnConstantHonMetal = Range("C45").Value
Outlet_rxnConstantMag = Range("C46").Value '(cm/s)
Outlet_rxnConstantH2onMag = Range("C47").Value '(cm/s)
```

```
'Initial Oxide thickness
For i = 1 To Outlet_Node
Outlet_InnerOx(i) = Range("C28").Value
Outlet_OuterOx(i) = Range("C28").Value
Next i

Sheets("General Input").Select
R = Range("C7").Value '(J/mol K)
F = Range("C8").Value '(C/mol)
beta = Range("C9").Value

'Molecular weight and Density
MW_metal = Range("C12").Value
Den_metal = Range("C13").Value '(g/cm3)
MW_mag = Range("C14").Value
Den_mag = Range("C15").Value '(g/cm3)

'Incremental time and Duration
Incr = Range("C18").Value '(seconds)
period = Range("C19").Value '(hours)


'Load Spalling Data
Set wbDISTRIBUTION = Workbooks.Open(FILEPATH & "\Oxide spalling reciprocal distribution.xls")


'Inlet
For A = 1 To 55
Inlet_InnerSize(A) = Range(Cells(A + 3, 11), Cells(A + 3, 11)).Value
Inlet_Inner_SpallingFrequency(A, 1) = Range(Cells(A + 3, 12), Cells(A + 3, 12)).Value
Inlet_OuterSize(A) = Range(Cells(A + 3, 13), Cells(A + 3, 13)).Value
Inlet_Outer_SpallingFrequency(A, 1) = Range(Cells(A + 3, 14), Cells(A + 3, 14)).Value
Next A


'Outlet and Header
For A = 1 To 125
Outlet_InnerSize(A) = Range(Cells(A + 3, 1), Cells(A + 3, 1)).Value
For z = 1 To 7
Outlet_Inner_SpallingFrequency(A, z) = Range(Cells(A + 3, z + 1), Cells(A + 3, z + 1)).Value
Next z
Outlet_OuterSize(A) = Range(Cells(A + 3, 9), Cells(A+ 3, 9)).Value
Outlet_Outer_SpallingFrequency(A, 1) = Range(Cells(A + 3, 10), Cells(A + 3, 10)).Value
Next A


'SET CONSTANTS FOR GAMMA CORRECTION
MaxIter = 1000
' ErrGamma = 0.0000000000001 '1E-13
ErrGamma = 0.0001 '1E-4

'INITIALIZE H2 CONCENTRATION

For i = 1 To Inlet_Node
Inlet_OS_mH2(i) = Inlet_Bulk_mH2(i)
Inlet_MO_mH2(i) = Inlet_Bulk_mH2(i)
```

```
  Next i

  For i = 1 To Outlet_Node
  Outlet_OS_mH2(i) = Outlet_Bulk_mH2(i)
  Outlet_MO_mH2(i) = Outlet_Bulk_mH2(i)
  Next i

'CALCULATE CONCENTRATION OF TOTAL Li

For i = 1 To Inlet_Node
  Call System(Inlet_pH25, Inlet_Bulk_mLiTotal(i), Inlet_Bulk_mLi(i))
Next i


For i = 1 To Outlet_Node
  Call System(Outlet_pH25, Outlet_Bulk_mLiTotal(i), Outlet_Bulk_mLi(i))
Next i

'CALCULATE SATURATED CONCENTRATION
For i = 1 To Inlet_Node
  Call Fesat(Inlet_TCinput, Inlet_TKinput, Inlet_Bulk_mLiTotal(i), Inlet_Bulk_mH2(i),
Inlet_Bulk_Fesat(i), _
        Inlet_Bulk_mLi(i), Inlet_Bulk_mH(i), Inlet_Bulk_mOH(i))
Next i

For i = 1 To Outlet_Node
  Call Fesat(Outlet_TCinput, Outlet_TKinput, Outlet_Bulk_mLiTotal(i), Outlet_Bulk_mH2(i),
Outlet_Bulk_Fesat(i), _
        Outlet_Bulk_mLi(i), Outlet_Bulk_mH(i), Outlet_Bulk_mOH(i))
Next i

'INITIALIZE BULK CONCENTRATION
'Let Fetotal in the bulk is 1.595E-8 mol/kg
For i = 1 To Inlet_Node
  Inlet_Bulk_FeTotal(i) = 0.00000001595
Next i

For i = 1 To Outlet_Node
'  Outlet_Bulk_FeTotal(i) = 0.00000001595
  Inlet_Sat = TL_solubility(Outlet_Bulk_mH(i), Outlet_Bulk_mH2(i),265)
  Outlet_Bulk_FeTotal(i) = Outlet_Bulk_Fesat(i)
Next i

'CALCULATE ACTIVITY COEFF. FOR BULK SYSTEM
For i = 1 To Inlet_Node
  Call BulkSystem(Inlet_TCinput, Inlet_TKinput, Inlet_Bulk_FeTotal(i), Inlet_Bulk_mFE2(i),
Inlet_Bulk_mFEOH(i), _
        Inlet_Bulk_mFEOH2(i), Inlet_Bulk_mFEOH3(i), Inlet_Bulk_mLi(i),
Inlet_Bulk_mH(i), Inlet_Bulk_mOH(i), _
        Inlet_Bulk_gamma1(i), Inlet_Bulk_gamma2(i))
Next i


For i = 1 To Outlet_Node
  Call BulkSystem(Outlet_TCinput, Outlet_TKinput, Outlet_Bulk_FeTotal(i),
Outlet_Bulk_mFE2(i), Outlet_Bulk_mFEOH(i), _
        Outlet_Bulk_mFEOH2(i), Outlet_Bulk_mFEOH3(i), Outlet_Bulk_mLi(i),
Outlet_Bulk_mH(i), Outlet_Bulk_mOH(i), _
```

```
            Outlet_Bulk_gamma1(i), Outlet_Bulk_gamma2(i))
Next i

'DEFINE Supersaturation Value
  supersat = 1.1  'Supersaturated factor

'INITIALIZE CONCENTRATION AT O/S INTERFACE
For i = 1 To Inlet_Node
  Inlet_OS_mH(i) = Inlet_Bulk_mH(i)
  Inlet_OS_mOH(i) = Inlet_Bulk_mOH(i)
  Inlet_OS_mLi(i) = Inlet_Bulk_mLi(i)
  Inlet_OS_FeTotal(i) =  Inlet_Bulk_FeTotal(i) 'FIRST ITERATION - ASSUME O/S [Fe] =
BULK CONCENTRATION
  Inlet_OS_Fesat(i) = Inlet_Bulk_Fesat(i)
  Inlet_OS_gamma1(i) = Inlet_Bulk_gamma1(i)
  Inlet_OS_gamma2(i) = Inlet_Bulk_gamma2(i)
Next i

For i = 1 To Outlet_Node
  Outlet_OS_mH(i) = Outlet_Bulk_mH(i)
  Outlet_OS_mOH(i) = Outlet_Bulk_mOH(i)
  Outlet_OS_mLi(i) = Outlet_Bulk_mLi(i)
  Outlet_OS_FeTotal(i) = Outlet_Bulk_FeTotal(i) 'FIRST ITERATION - ASSUME O/S [Fe] =
BULK CONCENTRATION
  Outlet_OS_Fesat(i) = Outlet_Bulk_Fesat(i)
  Outlet_OS_gamma1(i) = Outlet_Bulk_gamma1(i)
  Outlet_OS_gamma2(i) = Outlet_Bulk_gamma2(i)
Next i

'INITIALIZE CONCENTRATION AT M/O INTERFACE

For i = 1 To Inlet_Node
  Inlet_MO_FeTotal(i) = Inlet_Bulk_Fesat(i) * supersat 'FIRST ITERATION - ASSUME M/O
[Fe] = BULK CONCENTRATION
  Inlet_MO_mH(i) = Inlet_Bulk_mH(i) 'First Iteration; assume M/O [H+] = Bulk [H+]
  Inlet_MO_mOH(i) = Inlet_Bulk_mOH(i)
  Inlet_MO_mLi(i) = Inlet_Bulk_mLi(i)
  Inlet_MO_gamma1(i) = Inlet_Bulk_gamma1(i)
  Inlet_MO_gamma2(i) = Inlet_Bulk_gamma2(i)
Next i

For i = 1 To Outlet_Node
  Outlet_MO_FeTotal(i) = Outlet_Bulk_Fesat(i) * supersat 'FIRST ITERATION - ASSUME
M/O [Fe] = BULK CONCENTRATION
  Outlet_MO_mH(i) = Outlet_Bulk_mH(i) 'First Iteration; assume M/O [H+] = Bulk [H+]
  Outlet_MO_mOH(i) = Outlet_Bulk_mOH(i)
  Outlet_MO_mLi(i) = Outlet_Bulk_mLi(i)
  Outlet_MO_gamma1(i) = Outlet_Bulk_gamma1(i)
  Outlet_MO_gamma2(i) = Outlet_Bulk_gamma2(i)
Next i

'CORRECT ACTIVITY COEFF. AT M/O INTERFACE

'Inlet
  For i = 1 To Inlet_Node
    Do
      Call    composition(Inlet_TKinput,    Inlet_MO_FeTotal(i),    Inlet_MO_mFE2(i),
Inlet_MO_mFEOH(i), _
```

```
                Inlet_MO_mFEOH2(i),     Inlet_MO_mFEOH3(i),     Inlet_MO_mH(i),
Inlet_MO_mOH(i), _
                Inlet_MO_gamma1(i), Inlet_MO_gamma2(i))
      old_gamma1 = Inlet_MO_gamma1(i)
      old_gamma2 = Inlet_MO_gamma2(i)
      Call DebyeHuckel(Inlet_MO_mFE2(i), Inlet_MO_mFEOH(i), Inlet_MO_mFEOH3(i),
Inlet_MO_mH(i), _
              Inlet_MO_mOH(i),        Inlet_MO_mLi(i),        Inlet_MO_gamma1(i),
Inlet_MO_gamma2(i), _
              Inlet_TCinput)
      DiffGamma1 = Abs(Inlet_MO_gamma1(i) - old_gamma1) / ((Inlet_MO_gamma1(i) +
old_gamma1) / 2)
      DiffGamma2 = Abs(Inlet_MO_gamma2(i) - old_gamma2) / ((Inlet_MO_gamma2(i) +
old_gamma2) / 2)
    Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)
  Next i

'Outlet
  For i = 1 To Outlet_Node
    Do
      Call    composition(Outlet_TKinput,    Outlet_MO_FeTotal(i),    Outlet_MO_mFE2(i),
Outlet_MO_mFEOH(i), _
              Outlet_MO_mFEOH2(i),    Outlet_MO_mFEOH3(i),    Outlet_MO_mH(i),
Outlet_MO_mOH(i), _
              Outlet_MO_gamma1(i), Outlet_MO_gamma2(i))
      old_gamma1 = Outlet_MO_gamma1(i)
      old_gamma2 = Outlet_MO_gamma2(i)
      Call            DebyeHuckel(Outlet_MO_mFE2(i),            Outlet_MO_mFEOH(i),
Outlet_MO_mFEOH3(i), Outlet_MO_mH(i), _
              Outlet_MO_mOH(i),       Outlet_MO_mLi(i),       Outlet_MO_gamma1(i),
Outlet_MO_gamma2(i), _
              Outlet_TCinput)
      DiffGamma1 = Abs(Outlet_MO_gamma1(i) - old_gamma1) / ((Outlet_MO_gamma1(i)
+ old_gamma1) / 2)
      DiffGamma2 = Abs(Outlet_MO_gamma2(i) - old_gamma2) / ((Outlet_MO_gamma2(i)
+ old_gamma2) / 2)
    Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)
  Next i

'CORRECT ACTIVITY COEFF. AT O/S INTERFACE

'Inlet
  For i = 1 To Inlet_Node
    Do
      Call    composition(Inlet_TKinput,    Inlet_OS_FeTotal(i),    Inlet_OS_mFE2(i),
Inlet_OS_mFEOH(i), _
              Inlet_OS_mFEOH2(i),     Inlet_OS_mFEOH3(i),     Inlet_OS_mH(i),
Inlet_OS_mOH(i), _
              Inlet_OS_gamma1(i), Inlet_OS_gamma2(i))
      old_gamma1 = Inlet_OS_gamma1(i)
      old_gamma2 = Inlet_OS_gamma2(i)
      Call  DebyeHuckel(Inlet_OS_mFE2(i),  Inlet_OS_mFEOH(i),  Inlet_OS_mFEOH3(i),
Inlet_OS_mH(i), _
              Inlet_OS_mOH(i),        Inlet_OS_mLi(i),        Inlet_OS_gamma1(i),
Inlet_OS_gamma2(i), _
              Inlet_TCinput)
      DiffGamma1 = Abs(Inlet_OS_gamma1(i) - old_gamma1) / ((Inlet_OS_gamma1(i) +
old_gamma1) / 2)
```

```
      DiffGamma2 = Abs(Inlet_OS_gamma2(i) - old_gamma2) / ((Inlet_OS_gamma2(i) +
old_gamma2) / 2)
    Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)
  Next i

'Outlet
  For i = 1 To Outlet_Node
    Do
      Call composition(Outlet_TKinput, Outlet_OS_FeTotal(i), Outlet_OS_mFE2(i),
Outlet_OS_mFEOH(i), _
          Outlet_OS_mFEOH2(i), Outlet_OS_mFEOH3(i), Outlet_OS_mH(i),
Outlet_OS_mOH(i), _
          Outlet_OS_gamma1(i), Outlet_OS_gamma2(i))
      old_gamma1 = Outlet_OS_gamma1(i)
      old_gamma2 = Outlet_OS_gamma2(i)
      Call DebyeHuckel(Outlet_OS_mFE2(i), Outlet_OS_mFEOH(i),
Outlet_OS_mFEOH3(i), Outlet_OS_mH(i), _
        Outlet_OS_mOH(i), Outlet_OS_mLi(i), Outlet_OS_gamma1(i),
Outlet_OS_gamma2(i), _
        Outlet_TCinput)
      DiffGamma1 = Abs(Outlet_OS_gamma1(i) - old_gamma1) / ((Outlet_OS_gamma1(i) +
old_gamma1) / 2)
      DiffGamma2 = Abs(Outlet_OS_gamma2(i) - old_gamma2) / ((Outlet_OS_gamma2(i) +
old_gamma2) / 2)
    Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)
  Next i

'INITIAILIZE Kd
"note: kd_chem input from worksheet
For i = 1 To Inlet_Node
  Inlet_kd_elect(i) = Inlet_kd_chem
'  Inlet_kp_elect(i) = Inlet_kp_chem
Next i

For i = 1 To Outlet_Node
  Outlet_kd_elect(i) = Outlet_kd_chem
'  Outlet_kp_elect(i) = Outlet_kp_chem
Next i
  fraction = (MW_metal / MW_mag) * (Den_mag / Den_metal) * 3 'ratio of Fe mole in a mole
of oxide = 3

'"INITIALIZE MO_Potential; Let MO_Potential = Eeq of Fe/Fe2+ reation

'Inlet  ;Eo = -0.44 V
For i = 1 To Inlet_Node
  StartPot_MO = -0.44 + R * Inlet_TKinput / (2 * F) _
      * Log(Inlet_MO_mFE2(i) * Inlet_MO_gamma2(i) * Inlet_Den) 'conc is in (mol/L)
  Inlet_MOPot(i) = StartPot_MO
Next i

'Outlet  ;Eo = -0.42 V
For i = 1 To Outlet_Node
  StartPot_MO = -0.42 + R * Outlet_TKinput / (2 * F) _
      * Log(Outlet_MO_mFE2(i) * Outlet_MO_gamma2(i) * Outlet_Den) 'conc is in
(mol/L)
  Outlet_MOPot(i) = StartPot_MO
Next i
```

```
'''INITIALIZE OS_Potential; Let OS_Potential = Eeq of Fe3O4/Fe(OH)2 reaction

'Inlet  ;Eo = -1.1486 V
For i = 1 To Inlet_Node
   StartPot_OS = -1.1486 - (R * Inlet_TKinput * Log((Inlet_OS_mFEOH2(i) * Inlet_Den)) / (2 /
3 * F)) _
          + (R * Inlet_TKinput * Log((Inlet_OS_mH(i) * Inlet_OS_gamma1(i) * Inlet_Den) ^
(2 / 3)) _
          / (2 / 3 * F)) 'n=2/3
   Inlet_OSPot(i) = StartPot_OS
Next i

'Outlet  ;Eo = -1.1958 V
For i = 1 To Outlet_Node
   StartPot_OS = -1.1958 - (R * Outlet_TKinput * Log((Outlet_OS_mFEOH2(i) * Outlet_Den))
/ (2 / 3 * F)) _
   .      + (R * Outlet_TKinput * Log((Outlet_OS_mH(i) * Outlet_OS_gamma1(i) *
Outlet_Den) _
          ^ (2 / 3)) / (2 / 3 * F)) 'n=2/3
   Outlet_OSPot(i) = StartPot_OS
Next i

'HYDROGEN ION CONCENTRATION
'''Assume that the initial H+ at MO and OS are the same

'Inlet
For i = 1 To Inlet_Node
   Inlet_MO_mH(i) = Inlet_OS_mH(i)
Next i

'Outlet
For i = 1 To Outlet_Node
   Outlet_MO_mH(i) = Outlet_OS_mH(i)
Next i
"""""ITERATION WITH EXPOSURE TIME
For K = 1 To period

"""INLET
For i = 1 To Inlet_Node

'CALCULATE POTENTIALS
   section = "inlet"
   Call Potential(section, Inlet_TKinput, Inlet_Den, Inlet_rxnConstantFe,
Inlet_rxnConstantHonMetal, _
          Inlet_rxnConstantMag, Inlet_rxnConstantH2onMag, Inlet_MO_mFE2(i), _
          Inlet_MO_mH(i), Inlet_MO_mH2(i), Inlet_MO_gamma1(i), Inlet_MO_gamma2(i),
_
          Inlet_OS_mFEOH2(i), Inlet_OS_mH(i), Inlet_OS_mH2(i), Inlet_OS_gamma1(i), _
          Inlet_OS_gamma2(i), Inlet_MOPot(i), Inlet_OSPot(i), Inlet_CorrCur(i),
Inlet_Eeq1(i), Inlet_Eeq2(i), _
          Inlet_Eeq3(i), Inlet_Eeq4(i), Inlet_Io1(i), Inlet_Io2(i), Inlet_Io3(i), Inlet_Io4(i))

'CALCULATE CORROSION RATE
   Call CorrosionRate(Inlet_CorrCur(i), Inlet_CR(i))

'CALCULATE OXIDE THICKNESS
   Call Oxide(Inlet_InnerOx(i), Inlet_OuterOx(i), Inlet_TCinput, Inlet_TKinput, Inlet_Den,
Inlet_CR(i), Inlet_Bulk_FeTotal(i), _
```

```
        Inlet_MO_FeTotal(i), Inlet_MO_mFE2(i), Inlet_MO_mFEOH(i),
Inlet_MO_mFEOH2(i), Inlet_MO_mFEOH3(i), _
        Inlet_MO_mH2(i), Inlet_MO_mH(i), Inlet_MO_mOH(i), Inlet_MO_mLi(i),
Inlet_MO_gamma1(i), Inlet_MO_gamma2(i), _
        Inlet_OS_Fesat(i), Inlet_OS_FeTotal(i), Inlet_OS_mFE2(i), Inlet_OS_mFEOH(i),
Inlet_OS_mFEOH2(i), Inlet_OS_mFEOH3(i), _
        Inlet_OS_mH2(i), Inlet_OS_mH(i), Inlet_OS_mOH(i), Inlet_OS_mLi(i),
Inlet_OS_gamma1(i), Inlet_OS_gamma2(i), _
        Inlet_kd_chem, Inlet_kd_elect(i), Inlet_kp_chem, Inlet_kp_elect(i), Inlet_Area_factor,
Inlet_porosity_in, _
        Inlet_porosity_out, Inlet_tortuosity, Inlet_DFe, Inlet_DH2, Inlet_mt_coeff(i), section,
Inlet_rxnConstantFe, _
        Inlet_rxnConstantHonMetal, Inlet_rxnConstantMag, Inlet_rxnConstantH2onMag,
Inlet_MOPot(i), Inlet_OSPot(i), _
        Inlet_CorrCur(i))

'CALCULATE OXIDE THICKNESS (SPALLING EFFECT)
  Call Spall(i, section, Inlet_Den, Inlet_velocity(i), Inlet_Inner_SpallingFrequency, _
          Inlet_InnerSize, Inlet_Outer_SpallingFrequency, Inlet_OuterSize, _
          Inlet_OS_Fesat(i), Inlet_OS_FeTotal(i), Inlet_spconst_in, Inlet_spconst_out, _
          Inlet_porosity_in, Inlet_porosity_out, Inlet_tortuosity, Inlet_kd_elect(i), _
          Inlet_kp_elect(i), Inlet_Area_factor, Inlet_InnerOx(i), Inlet_OuterOx(i), _
          Inlet_CR(i), Inlet_In_SpallTime(i), Inlet_Out_SpallTime(i))


'ELECTROCHEMICAL EFFECT
  Call PotentialEffect(section, Inlet_TKinput, Inlet_Den, Inlet_MO_mH(i), Inlet_OS_Fesat(i),
_
        Inlet_OS_FeTotal(i), Inlet_OS_mFEOH2(i), Inlet_OS_mH(i),
Inlet_OS_gamma1(i), _
        Inlet_OS_gamma2(i), Inlet_kd_chem, Inlet_kp_chem, Inlet_kd_elect(i), _
        Inlet_kp_elect(i), Inlet_MOPot(i), Inlet_OSPot(i))
  Call OSSatConcentration(Inlet_TKinput, Inlet_OS_Fesat(i), Inlet_OS_mFE2(i),
Inlet_OS_mFEOH(i), _
          Inlet_OS_mFEOH2(i), Inlet_OS_mFEOH3(i), Inlet_OS_mH(i), _
          Inlet_OS_gamma1(i), Inlet_OS_gamma2(i))


'ADJUST CONCENTRATION
  Call ConcAdjustment(Inlet_TCinput, Inlet_TKinput, Inlet_Den, Inlet_Bulk_FeTotal(i), _
        Inlet_MO_FeTotal(i), Inlet_MO_mFE2(i), Inlet_MO_mFEOH(i), _
        Inlet_MO_mFEOH2(i), Inlet_MO_mFEOH3(i), Inlet_MO_mH2(i),
Inlet_MO_mH(i), _
        Inlet_MO_mOH(i), Inlet_MO_mLi(i), Inlet_MO_gamma1(i),
Inlet_MO_gamma2(i), _
        Inlet_OS_Fesat(i), Inlet_OS_FeTotal(i), Inlet_OS_mFE2(i), _
        Inlet_OS_mFEOH(i), Inlet_OS_mFEOH2(i), Inlet_OS_mFEOH3(i),
Inlet_OS_mH2(i), _
        Inlet_OS_mH(i), Inlet_OS_mOH(i), Inlet_OS_mLi(i), Inlet_OS_gamma1(i), _
        Inlet_OS_gamma2(i), Inlet_kd_chem, Inlet_kd_elect(i), Inlet_kp_elect(i), _
        Inlet_Area_factor, Inlet_InnerOx(i), Inlet_OuterOx(i), Inlet_porosity_in, _
        Inlet_porosity_out, Inlet_tortuosity, Inlet_DFe, Inlet_DH2, _
        Inlet_mt_coeff(i), Inlet_CR(i))
'Adding Adjustment of Bulk Concentration along Feeder
'       Call bulk(j, Inlet_Dia(j), Inlet_Leng(j), Inlet_velocity(j), Inlet_mt_coeff(j),
Inlet_OS_FeTotal(j), Inlet_Bulk_FeTotal)
Next i
```

```
""Outlet
For i = 1 To Outlet_Node
'Outlet_Bulk_FeTotal(1) = Inlet_Bulk_FeTotal(Inlet_Node)
  Outlet_Bulk_FeTotal(i) = Outlet_Bulk_Fesat(i)


'CALCULATE POTENTIALS
  section = "outlet"
  Call Potential(section, Outlet_TKinput, Outlet_Den, Outlet_rxnConstantFe,
Outlet_rxnConstantHonMetal, Outlet_rxnConstantMag, _
        Outlet_rxnConstantH2onMag, Outlet_MO_mFE2(i), Outlet_MO_mH(i),
Outlet_MO_mH2(i), Outlet_MO_gamma1(i), _
        Outlet_MO_gamma2(i), Outlet_OS_mFEOH2(i), Outlet_OS_mH(i),
Outlet_OS_mH2(i), Outlet_OS_gamma1(i), _
        Outlet_OS_gamma2(i), Outlet_MOPot(i), Outlet_OSPot(i), Outlet_CorrCur(i),
Outlet_Eeq1(i), Outlet_Eeq2(i), _
        Outlet_Eeq3(i), Outlet_Eeq4(i), Outlet_Io1(i), Outlet_Io2(i), Outlet_Io3(i),
Outlet_Io4(i))

'CALCULATE CORROSION RATE
  Call CorrosionRate(Outlet_CorrCur(i), Outlet_CR(i))

'CALCULATE OXIDE THICKNESS
  Call Oxide(Outlet_InnerOx(i), Outlet_OuterOx(i), Outlet_TCinput, Outlet_TKinput,
Outlet_Den, Outlet_CR(i), _
        Outlet_Bulk_FeTotal(i), Outlet_MO_FeTotal(i), Outlet_MO_mFE2(i),
Outlet_MO_mFEOH(i), Outlet_MO_mFEOH2(i), _
        Outlet_MO_mFEOH3(i), Outlet_MO_mH2(i), Outlet_MO_mH(i),
Outlet_MO_mOH(i), Outlet_MO_mLi(i), Outlet_MO_gamma1(i), _
        Outlet_MO_gamma2(i), Outlet_OS_Fesat(i), Outlet_OS_FeTotal(i),
Outlet_OS_mFE2(i), Outlet_OS_mFEOH(i), _
        Outlet_OS_mFEOH2(i), Outlet_OS_mFEOH3(i), Outlet_OS_mH2(i),
Outlet_OS_mH(i), Outlet_OS_mOH(i), Outlet_OS_mLi(i), _
        Outlet_OS_gamma1(i), Outlet_OS_gamma2(i), Outlet_kd_chem, Outlet_kd_elect(i),
Outlet_kp_chem, Outlet_kp_elect(i), _
        Outlet_Area_factor, Outlet_porosity_in, Outlet_porosity_out, Outlet_tortuosity,
Outlet_DFe, Outlet_DH2, _
        Outlet_mt_coeff(i), section, Outlet_rxnConstantFe, Outlet_rxnConstantHonMetal,
Outlet_rxnConstantMag, _
        Outlet_rxnConstantH2onMag, Outlet_MOPot(i), Outlet_OSPot(i), Outlet_CorrCur(i))

'CALCULATE OXIDE THICKNESS (SPALLING EFFECT)
  Call Spall(i, section, Outlet_Den, Outlet_velocity(i), Outlet_Inner_SpallingFrequency,
Outlet_InnerSize, _
        Outlet_Outer_SpallingFrequency, Outlet_OuterSize, Outlet_OS_Fesat(i),
Outlet_OS_FeTotal(i), _
        Outlet_spconst_in, Outlet_spconst_out, Outlet_porosity_in, Outlet_porosity_out,
Outlet_tortuosity, _
        Outlet_kd_elect(i), Outlet_kp_elect(i), Outlet_Area_factor, Outlet_InnerOx(i),
Outlet_OuterOx(i), _
        Outlet_CR(i), Outlet_In_SpallTime(i), Outlet_Out_SpallTime(i))

'ELECTROCHEMICAL EFFECT
  Call PotentialEffect(section, Outlet_TKinput, Outlet_Den, Outlet_MO_mH(i),
Outlet_OS_Fesat(i), Outlet_OS_FeTotal(i), _
```

```
                Outlet_OS_mFEOH2(i),        Outlet_OS_mH(i),        Outlet_OS_gamma1(i),
Outlet_OS_gamma2(i), Outlet_kd_chem, _
                Outlet_kp_chem,   Outlet_kd_elect(i),   Outlet_kp_elect(i),   Outlet_MOPot(i),
Outlet_OSPot(i))
  Call   OSSatConcentration(Outlet_TKinput,   Outlet_OS_Fesat(i),   Outlet_OS_mFE2(i),
Outlet_OS_mFEOH(i), Outlet_OS_mFEOH2(i), _
                  Outlet_OS_mFEOH3(i),        Outlet_OS_mH(i),        Outlet_OS_gamma1(i),
Outlet_OS_gamma2(i))

'ADJUST CONCENTRATION
  Call ConcAdjustment(Outlet_TCinput, Outlet_TKinput, Outlet_Den, Outlet_Bulk_FeTotal(i),
Outlet_MO_FeTotal(i), _
                Outlet_MO_mFE2(i),      Outlet_MO_mFEOH(i),      Outlet_MO_mFEOH2(i),
Outlet_MO_mFEOH3(i), Outlet_MO_mH2(i), _
                Outlet_MO_mH(i),          Outlet_MO_mOH(i),          Outlet_MO_mLi(i),
Outlet_MO_gamma1(i), Outlet_MO_gamma2(i), _
                Outlet_OS_Fesat(i),          Outlet_OS_FeTotal(i),          Outlet_OS_mFE2(i),
Outlet_OS_mFEOH(i), Outlet_OS_mFEOH2(i), _
                Outlet_OS_mFEOH3(i),          Outlet_OS_mH2(i),          Outlet_OS_mH(i),
Outlet_OS_mOH(i), Outlet_OS_mLi(i), _
                Outlet_OS_gamma1(i),          Outlet_OS_gamma2(i),          Outlet_kd_chem,
Outlet_kd_elect(i), Outlet_kp_elect(i), _
                Outlet_Area_factor, Outlet_InnerOx(i), Outlet_OuterOx(i), Outlet_porosity_in,
Outlet_porosity_out, _
                Outlet_tortuosity, Outlet_DFe, Outlet_DH2, Outlet_mt_coeff(i), Outlet_CR(i))
'Adding Adjustment of Bulk Concentration along Feeder
'       Call  bulk(j,  Outlet_Dia(j),  Outlet_Leng(j),  Outlet_velocity(j),  Outlet_mt_coeff(j),
Outlet_OS_FeTotal(j), Outlet_Bulk_FeTotal)
Next i

'"PRINT OUT RESULTS

If (K - 1) Mod (Int(period / 1000) + 1) = 0 And K <> 1 Then
'If (K - 1) Mod (Int(period / 10000) + 1) = 0 And K <> 1 Then
'If (K - 1) Mod 1 = 0 Then
  PrintIter = PrintIter + 1

  'Inlet
    For i = 1 To Inlet_Node
      ii = i
      Call OutputVariables(Results1(ii, PrintIter), K, Inlet_InnerOx(i), Inlet_OuterOx(i), _
              Inlet_CR(i), Inlet_CorrCur(i), Inlet_MOPot(i), _
              Inlet_OSPot(i), Inlet_Bulk_FeTotal(i), Inlet_MO_FeTotal(i), _
              Inlet_OS_FeTotal(i), Inlet_OS_Fesat(i), Inlet_MO_mH(i), Inlet_OS_mH(i),
Inlet_kd_elect(i), _
              Inlet_Eeq1(i),  Inlet_Eeq2(i),  Inlet_Eeq3(i),  Inlet_Eeq4(i),  Inlet_Io1(i),
Inlet_Io2(i), _
              Inlet_Io3(i), Inlet_Io4(i), Inlet_In_SpallTime(i), Inlet_Out_SpallTime(i))
    Next i

    'Outlet
  For i = 1 To Outlet_Node
    ii = i + 7
    Call  OutputVariables(Results1(ii,  PrintIter),  K,  Outlet_InnerOx(i),  Outlet_OuterOx(i),
Outlet_CR(i), Outlet_CorrCur(i), _
              Outlet_MOPot(i),          Outlet_OSPot(i),          Outlet_Bulk_FeTotal(i),
Outlet_MO_FeTotal(i), Outlet_OS_FeTotal(i), _
```

```
                Outlet_OS_Fesat(i),          Outlet_MO_mH(i),          Outlet_OS_mH(i),
Outlet_kd_elect(i), Outlet_Eeq1(i), _
                Outlet_Eeq2(i), Outlet_Eeq3(i), Outlet_Eeq4(i), Outlet_Io1(i), Outlet_Io2(i),
Outlet_Io3(i), _
                Outlet_Io4(i), Outlet_In_SpallTime(i), Outlet_Out_SpallTime(i))
  Next i


End If

Next K

'Close Spalling Data
  wbDISTRIBUTION.Close

' Output data to Template
  Call testupdate

' Show Benchmark time

MsgBox ("Calculation Time: " & Timer- BenchMark & " sec")


End Sub

Public Sub System(ByVal pH25, ByRef mLitotal, ByRef mLi)

'CALCULATE CONCENTRATION OF TOTAL Li
  first_gamma1 = 1#
  first_gamma2 = 1#

Do
'CALCULATE KW, H+, OH-, AT 25 C
  KW = KW_Calculation(25) '(mol/kg)^2  at T=25C or 298K
  mH25 = 10# ^ (-pH25) * 1000 / 1000 'density of coolant~1000kg/m3
  mOH25 = (KW / (mH25 * first_gamma1)) / first_gamma1 '(mol/kg) or (molal)


'CALCULATE KLi, Li Total AT 25 C
  KLi = KLi_Calculation(25)
  mLitotal = ((mOH25 ^ 2 * first_gamma1 ^ 2) / KLi) + mOH25 '(mol/kg) or (molal)
  mLi = mOH25

'CALCULATE IONIC STRENGTH
  IonicStrength = (mH25 + mOH25 + mLi) / 2

'DHC CONSTANT
  DHC = DH_constant1 + DH_constant2 * 25 + DH_constant3 * (25 ^ 2) + _
    DH_constant4 * (25 ^ 3) + DH_constant5 * (25 ^ 4) 'T=25 C

'CALCULATE ACTIVITY COEFFICIENT
  gamma1 = 10 ^ (-(DHC * (IonicStrength ^ 0.5)) / (1 + (IonicStrength ^ 0.5)))
'    DiffGamma1 = Abs(gamma1 - first_gamma1)
'Normailizing Error
    DiffGamma1 = Abs(gamma1 - first_gamma1) / ((gamma1 + first_gamma1) / 2)
    first_gamma1 = gamma1
Loop Until DiffGamma1 < ErrGamma
```

```
End Sub

Public Function KW_Calculation(ByVal temp1)

'Note that temp1 is in Celcius and temp2 is in Kelvin



' CALCULATE THE EQUILIBRIUM CONSTANT FOR WATER (QW) AT A GIVEN IONIC STRENGTH AT THE TEMPERATURE T (CELCIUS)
  KW_Calculation = 10# ^ (MF_constant1 + MF_constant2 * temp1 + MF_constant3 * (temp1 ^ 2) + MF_constant4 * (temp1 ^ 3) + MF_constant5 * (temp1 ^ 4))

End Function

Public Function KLi_Calculation(ByVal temp1)

' CALCULATE EQUILIBRIUM CONSTANT FOR Li IN LiOH (QL) AT TEMPERATURE T (CELCIUS)
  KLi_Calculation = 10# ^ (Li_constant1 + Li_constant2 * temp1 + Li_constant3 * (temp1 ^ 2))

End Function

'Public Sub Fesat(TC_input, TK_input, mLitotal, mH2, Fesat, mLi, mH, mOH)

Public Sub Fesat(ByVal TC_input, ByVal TK_input, ByVal mLitotal, ByVal mH2, ByRef Fesat, ByRef mLi, ByRef mH, ByRef mOH)

  TC = TC_input
  TK = TK_input
  first_gamma1 = 1#
  first_gamma2 = 1#

Do
'CALCULATE KLi AND OH-
  KLi = KLi_Calculation(TC)
  mOH = (-KLi + Sqr(KLi ^ 2 + 4 * first_gamma1 ^ 2 * KLi * mLitotal)) / (2 * first_gamma1 ^ 2)
  If mOH >= 0 Then
    mOH = mOH
  Else
    mOH = (-KLi - Sqr(KLi ^ 2 + 4 * first_gamma1 ^ 2 * KLi * mLitotal)) / (2 * first_gamma1 ^ 2)
  End If
  mLi = mOH 'ASSUME THAT LiOH DISSOCIATE 100% AS A STRONG BASE

'CALCULATE KW, H+, SAT
  KW = KW_Calculation(TC)
  mH = (KW / (mOH * first_gamma1)) / first_gamma1
  Fesat = TL_solubility(mH, mH2, TC)

  Call composition(TK_input, Fesat, fe2_sat, feoh_sat, feoh2_sat, feoh3_sat, mH, mOH, first_gamma1, first_gamma2)
  Call DebyeHuckel(fe2_sat, feoh_sat, feoh3_sat, mH, mOH, mLi, gamma1, gamma2, TC)
```

```
'     DiffGamma1 = Abs(gamma1 - first_gamma1)
'     DiffGamma2 = Abs(gamma2 - first_gamma2)
'Normalizing Error
      DiffGamma1 = Abs(gamma1 - first_gamma1) / ((gamma1 + first_gamma1) / 2)
      DiffGamma2 = Abs(gamma2 - first_gamma2) / ((gamma2 + first_gamma2) / 2)
      first_gamma1 = gamma1
      first_gamma2 = gamma2
Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)

End Sub

Sub composition(ByVal TK, ByVal Total, ByRef Fe2, ByRef FeOH, ByRef FeOH2, ByRef
FeOH3, ByVal h, ByVal oh, ByVal g1, ByVal g2)

'CALCULATE HYDROLYSIS CONSTANTS
   KFEOH = 10 ^ (FeOH_Constant1 * TK ^ 4 + FeOH_Constant2 * TK ^ 3 + FeOH_Constant3
* TK ^ 2 + FeOH_Constant4 * TK + FeOH_Constant5)
   KFEOH2 = 10 ^ (FeOH2_Constant1 * TK ^ 4 + FeOH2_Constant2 * TK ^ 3 +
FeOH2_Constant3 * TK ^ 2 + FeOH2_Constant4 * TK + FeOH2_Constant5)
   KFEOH3_ = 10 ^ (FeOH3_Constant1 * TK ^ 4 + FeOH3_Constant2 * TK ^ 3 +
FeOH3_Constant3 * TK ^ 2 + FeOH3_Constant4 * TK + FeOH3_Constant5)

'CALCULATE CONCENTRATION OF Fe SPECIES
   Fe2 = Total / (1 + (KFEOH * g2 / (h * g1 * g1)) + (KFEOH2 * g2 / (h * g1) ^ 2) + _
      (KFEOH3_ * g2 / ((h * g1) ^ 3 * g1)))
   FeOH = (KFEOH * Fe2 * g2) / (h * g1) / g1
   FeOH2 = (KFEOH2 * Fe2 * g2) / (h * g1) ^ 2
   FeOH3 = (KFEOH3_ * Fe2 * g2) / (h * g1) ^ 3 / g1

End Sub

'Sub DebyeHuckel(Fe2, FeOH, FeOH3, h, oh, Li, g1, g2, temp1)
Sub DebyeHuckel(ByVal Fe2, ByVal FeOH, ByVal FeOH3, ByVal h, ByVal oh, ByVal Li,
ByRef g1, ByRef g2, ByVal temp1)

'CALCULATE IONICE STRENGTH
   IonicStrength = (h + oh + 4 * Fe2 + FeOH + FeOH3 + Li) / 2#

'DHC CONSTANT
   DHC = DH_constant1 + DH_constant2 * temp1 + DH_constant3 * (temp1 ^ 2) + _
      DH_constant4 * (temp1 ^ 3) + DH_constant5 * (temp1 ^ 4)


'CALCULATE ACTIVITY COEFFICIENT
   g1 = 10 ^ (-(DHC * (IonicStrength ^ 0.5)) / (1 + (IonicStrength ^ 0.5)))
   g2 = 10 ^ (-4 * (DHC * (IonicStrength ^ 0.5)) / (1 + (IonicStrength ^ 0.5)))

End Sub

Public Sub BulkSystem(ByVal TC_input, ByVal TK_input, ByVal FeTotal, ByRef mFE2,
ByRef mFEOH, ByRef mFEOH2, ByRef mFEOH3, _
            ByVal mLi, ByVal mH, ByVal mOH, ByRef gamma1, ByRef gamma2)

'CALCULATE ACTIVITY COEFF. FOR BULK SYSTEM AT 310 C
   TC = TC_input
   TK = TK_input
   first_gamma1 = 1#
   first_gamma2 = 1#
```

```
Do
  Call composition(TK_input, FeTotal, mFE2, mFEOH, mFEOH2, mFEOH3, mH, mOH,
first_gamma1, first_gamma2)
  Call DebyeHuckel(mFE2, mFEOH, mFEOH3, mH, mOH, mLi, gamma1, gamma2, TC)
'    DiffGamma1 = Abs(gamma1 - first_gamma1)
'    DiffGamma2 = Abs(gamma2 - first_gamma2)
'Normalizing Error
    DiffGamma1 = Abs(gamma1 - first_gamma1) / ((gamma1 + first_gamma1) / 2)
    DiffGamma2 = Abs(gamma2 - first_gamma2) / ((gamma2 + first_gamma2) / 2)
    first_gamma1 = gamma1
    first_gamma2 = gamma2
Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)

End Sub

Public Sub Potential(ByVal section, ByVal TK_input, ByVal Den, ByVal rxnConstantFe,
ByVal rxnConstantHonMetal, _
        ByVal rxnConstantMag, ByVal rxnConstantH2onMag, ByVal MO_mFE2, ByVal
MO_mH, ByVal MO_mH2, _
        ByVal MO_gamma1, ByVal MO_gamma2, ByVal OS_mFEOH2, ByVal OS_mH,
ByVal OS_mH2, ByVal OS_gamma1, _
        ByVal OS_gamma2, ByRef MO_Pot, ByRef OS_Pot, ByRef Corr_Cur, ByRef
equilPotentialFe, _
        ByRef equilPotentialH2_MO, ByRef equilPotentialMag, ByRef
equilPotentialH2_OS, _
        ByRef exchangecurrentFe, ByRef exchangecurrentHonFe, ByRef
exchangecurrentMag, _
        exchangecurrentHonMag)
Dim Er As Double

'AT METAL SURFACE AND METAL-OXIDE INTERFACE; Rxns: Fe to Fe2+, Hydrogen
evolution

'Oxidation reaction Fe/Fe2+
  If (section = "inlet") Then 'Eo =-0.44 V
    equilPotentialFe = -0.44 + R * TK_input / (2 * F) * Log(MO_mFE2 * MO_gamma2 *
Den) 'conc is in (mol/L)
  ElseIf (section = "outlet" Or section = "header") Then 'Eo =-0.42 V
    equilPotentialFe = -0.42 + R * TK_input / (2 * F) * Log(MO_mFE2 * MO_gamma2 *
Den) 'conc is in (mol/L)
  End If

    exchangecurrentFe = rxnConstantFe * (MO_mFE2 * Den / 1000) * 2 * F _
            * Exp(-(1 - 0.5) * 2 * F * equilPotentialFe / (R * TK_input)) 'conc is in
(mol/cm3)

'Reduction reaction H+/H2
  equilPotentialH2_MO = -R * TK_input / (2 * F) * Log((MO_mH2 * Den) / (MO_mH *
MO_gamma1 * Den) ^ 2) 'conc is in (mol/L)
  'beta of H+ to H2 is 0.5
  exchangecurrentHonFe = rxnConstantHonMetal * (MO_mH * Den / 1000) * 2 * F * Exp(-(1
- 0.5) * 2 * F * equilPotentialH2_MO _
            / (R * TK_input))
```

```
''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''ESTIMATE POTENTIAL FROM EQUATION (ONLY
WHEN Beta = 0.5), NOT NUMERICAL METHOD''''''''''''''''''''''''''''''''''''''''''
'   MO_Pot = 0.00004309 * TK_input * Log((exchangecurrentFe * Exp((11605 / TK_input) *
equilPotentialFe) _
        + exchangecurrentHonFe * Exp((11605 / TK_input) * equilPotentialH2_MO)) _
        / (exchangecurrentFe * Exp((-11605 / TK_input) * equilPotentialFe) _
        + exchangecurrentHonFe * Exp((-11605 / TK_input) * equilPotentialH2_MO)))
   MO_Pot = R / (2 * F) * TK_input * _
        Log((exchangecurrentFe * Exp((2 * F * 0.5 / R / TK_input) * equilPotentialFe) _
        + exchangecurrentHonFe * Exp((2 * F * 0.5 / R / TK_input) * equilPotentialH2_MO)) _
        / (exchangecurrentFe * Exp((-2 * F * 0.5 / R / TK_input) * equilPotentialFe) _
        + exchangecurrentHonFe * Exp((-2 * F * 0.5 / R / TK_input) * equilPotentialH2_MO)))



   Corr_Cur = exchangecurrentFe * Exp(0.5 * 2 * F * (MO_Pot - equilPotentialFe) / (R *
TK_input)) _
        - exchangecurrentFe * Exp(-(1 - 0.5) * 2 * F * (MO_Pot - equilPotentialFe) / (R *
TK_input)) '(Amp/cm2 s)

   Corr_Cur = Round(Corr_Cur, 8)
'   Corr_Cur = Round(Corr_Cur, 7)

'AT OXIDE-SOLUTION INTERFACE; Rxns: Fe3O4 to Fe(OH)2, Hydrogen

'Reductive Dissolution of Magnetite
   If (section = "inlet") Then 'Eo =-1.1486 V
      equilPotentialMag = -1.1486 - (R * TK_input * Log(OS_mFEOH2 * Den) / (2 / 3 * F)) _
                    + (R * TK_input * Log((OS_mH * OS_gammal * Den) ^ (2 / 3)) / (2 / 3 *
F)) 'n=2/3
```

```
   ElseIf (section = "outlet" Or section = "header") Then 'Eo =-1.1958 V
      equilPotentialMag = -1.1958 - (R * TK_input * Log(OS_mFEOH2 * Den) / (2 / 3 * F)) _
                    + (R * TK_input * Log((OS_mH * OS_gammal * Den) ^ (2 / 3)) / (2 / 3 *
F)) 'n=2/3
   End If
   'beta of magnetite dissolution = 0.5
   exchangecurrentMag = rxnConstantMag * (OS_mFEOH2 * Den / 1000) * (2 / 3) * F _
            * Exp(0.5 * 2 / 3 * F * equilPotentialMag / (R * TK_input)) 'n=2/3

'Oxidation reaction H2 to H+
   equilPotentialH2_OS = -R * TK_input / (2 / 3 * F) * Log(((OS_mH2 * Den) ^ (1 / 3)) / _
                ((OS_mH * OS_gammal * Den) ^ (2 / 3))) 'n=2/3
   'beta of H+ to H2 at O/S = 0.5
   exchangecurrentHonMag = rxnConstantH2onMag * ((OS_mH * Den / 1000)) * 2 / 3 * F _
                * Exp(-(1 - 0.5) * 2 / 3 * F * equilPotentialH2_OS / (R * TK_input)) 'n=2/3

''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''''ESTIMATE POTENTIAL FROM EQUATION (ONLY
WHEN Beta = 0.5), NOT NUMERICAL METHOD''''''''''''''''''''''''''''''''''''''''''

   OS_Pot = (R * TK_input / (2 / 3 * F)) * Log((exchangecurrentMag * Exp((2 / 3 * F / (2 * R *
TK_input)) * equilPotentialMag) _
        + exchangecurrentHonMag * Exp((2 / 3 * F / (2 * R * TK_input)) *
equilPotentialH2_OS)) _
        / (exchangecurrentMag * Exp((-2 / 3 * F / (2 * R * TK_input)) * equilPotentialMag) _
        + exchangecurrentHonMag * Exp((-2 / 3 * F / (2 * R * TK_input)) *
equilPotentialH2_OS)))

End Sub
```

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```
Public Sub CorrosionRate(ByVal Corr_Cur, ByRef CR)

  CR = Corr_Cur / (2 * F) 'mol/cm2 s

  If CR <= 0 Then
    CR = 0
  End If

End Sub

Public Sub Oxide(INNER, OUTER, ByVal RK_TC, ByVal RK_TK, ByVal RK_Den, ByVal
RK_Corr, ByVal RK_Bulk_Fetotal, _
        ByVal RK_MO_Fetotal, ByVal RK_MO_mFE2, ByVal RK_MO_mFEOH, ByVal
RK_MO_mFEOH2, ByVal RK_MO_mFEOH3, _
        ByVal RK_MO_mH2, ByVal RK_MO_mH, RK_MO_mOH, ByVal RK_MO_mLi,
ByVal RK_MO_gamma1, ByVal RK_MO_gamma2, _
        ByVal RK_OS_Fesat, ByVal RK_OS_Fetotal, ByVal RK_OS_mFE2, ByVal
RK_OS_mFEOH, ByVal RK_OS_mFEOH2, _
        ByVal RK_OS_mFEOH3, ByVal RK_OS_mH2, ByVal RK_OS_mH, ByVal
RK_OS_mOH, ByVal RK_OS_mLi, ByVal RK_OS_gamma1, _
        ByVal RK_OS_gamma2, ByVal RK_kd_chem, ByVal RK_kd_elect, ByVal
RK_kp_chem, ByVal RK_kp_elect, _
        ByVal RK_Area_Factor, ByVal RK_porosity_in, ByVal RK_porosity_out, ByVal
RK_tortuosity, ByVal RK_DFe, _
        ByVal RK_DH2, ByVal RK_mt_coeff, ByVal RK_section, ByVal
RK_rxnConstantFe, ByVal RK_rxnConstantHonMetal, _
        ByVal RK_rxnConstantMag, ByVal RK_rxnConstantH2onMag, ByVal RK_MO_Pot,
ByVal RK_OS_Pot, ByVal RK_Corr_Cur)

Dim RK_ITER As Long 'Runge-Kutta4
Dim RK_INNER As Double, RK_OUTER As Double
Dim Sat As Double, Total As Double
Dim RK1_MO_Fetotal As Double, RK1_OS_Fetotal As Double
Dim DiffConcMO As Double, DiffConcOS As Double
Dim ErrConcMO As Double, ErrConcOS As Double
Dim TopGrowthIn As Double, TopGrowthOut As Double
Dim RK_K(4) As Double, RK_KK(4) As Double

  Sat = RK_OS_Fesat * RK_Den / 1000 'mol/cm3
  Total = RK_OS_Fetotal * RK_Den / 1000 'mol/cm3
  ErrConcMO = 0.000000001 '1E-15
  ErrConcOS = 0.000000001 '1E-15

  RK_INNER = INNER
  RK_OUTER = OUTER

For RK_ITER = 1 To 4

'CALCULATE CONCENTRATIONS (WHICH ARE FUNCTIONS OF OXIDE THICKNESS)
    Call ConcAdjustment(RK_TC, RK_TK, RK_Den, RK_Bulk_Fetotal, RK_MO_Fetotal,
RK_MO_mFE2, RK_MO_mFEOH, RK_MO_mFEOH2, _
            RK_MO_mFEOH3, RK_MO_mH2, RK_MO_mH, RK_MO_mOH,
RK_MO_mLi, RK_MO_gamma1, RK_MO_gamma2, RK_OS_Fesat, _
            RK_OS_Fetotal, RK_OS_mFE2, RK_OS_mFEOH, RK_OS_mFEOH2,
RK_OS_mFEOH3, RK_OS_mH2, RK_OS_mH, RK_OS_mOH, _
            RK_OS_mLi, RK_OS_gamma1, RK_OS_gamma2, RK_kd_chem,
RK_kd_elect, RK_kp_elect, RK_Area_Factor, RK_INNER, _
```

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```
            RK_OUTER, RK_porosity_in, RK_porosity_out, RK_tortuosity, RK_DFe,
RK_DH2, RK_mt_coeff, RK_Corr)
"'NO Do Loop""
'  Do
    RK1_MO_Fetotal = RK_MO_Fetotal
    RK1_OS_Fetotal = RK_OS_Fetotal

'CALCULATE POTENTIAL
    Call Potential(RK_section, RK_TK, RK_Den, RK_rxnConstantFe,
RK_rxnConstantHonMetal, RK_rxnConstantMag, _
            RK_rxnConstantH2onMag, RK_MO_mFE2, RK_MO_mH, RK_MO_mH2,
RK_MO_gamma1, RK_MO_gamma2, RK_OS_mFEOH2, _
            RK_OS_mH, RK_OS_mH2, RK_OS_gamma1, RK_OS_gamma2, RK_MO_Pot,
RK_OS_Pot, RK_Corr_Cur, RK_Eeq1, RK_Eeq2, _
            RK_Eeq3, RK_Eeq4, RK_Io1, RK_Io2, RK_Io3, RK_Io4)

'Public Sub Potential(ByVal section, ByVal TK_input, ByVal Den, ByVal rxnConstantFe,
ByVal rxnConstantHonMetal, _
            ByVal rxnConstantMag, ByVal rxnConstantH2onMag, ByVal MO_mFE2, ByVal
MO_mH, ByVal MO_mH2, _
            ByVal MO_gamma1, ByVal MO_gamma2, ByVal OS_mFEOH2, ByVal OS_mH,
ByVal OS_mH2, ByVal OS_gamma1, _
            ByVal OS_gamma2, ByRef MO_Pot, ByRef OS_Pot, ByRef Corr_Cur, ByRef
equilPotentialFe, _
            ByRef equilPotentialH2_MO, ByRef equilPotentialMag, ByRef
equilPotentialH2_OS, _
            ByRef exchangecurrentFe, ByRef exchangecurrentHonFe)

'CALCULATE CORROSION RATE
    Call CorrosionRate(RK_Corr_Cur, RK_Corr)

'CALCULATE POTENTIAL EFFECT
    Call PotentialEffect(RK_section, RK_TK, RK_Den, RK_MO_mH, RK_OS_Fesat,
RK_OS_Fetotal, RK_OS_mFEOH2, RK_OS_mH, RK_OS_gamma1, _
            RK_OS_gamma1, RK_kd_chem, RK_kp_chem, RK_kd_elect, RK_kp_elect,
RK_MO_Pot, RK_OS_Pot)

'CALCULATE FESAT AT O/S INTERFACE
    Call OSSatConcentration(RK_TK, RK_OS_Fesat, RK_OS_mFE2, RK_OS_mFEOH,
RK_OS_mFEOH2, RK_OS_mFEOH3, RK_OS_mH, _
            RK_OS_gamma1, RK_OS_gamma2)
'CALCULATE CONCENTRATIONS
    Call ConcAdjustment(RK_TC, RK_TK, RK_Den, RK_Bulk_Fetotal, RK_MO_Fetotal,
RK_MO_mFE2, RK_MO_mFEOH, RK_MO_mFEOH2, _
            RK_MO_mFEOH3, RK_MO_mH2, RK_MO_mH, RK_MO_mOH,
RK_MO_mLi, RK_MO_gamma1, RK_MO_gamma2, RK_OS_Fesat, _
            RK_OS_Fetotal, RK_OS_mFE2, RK_OS_mFEOH, RK_OS_mFEOH2,
RK_OS_mFEOH3, RK_OS_mH2, RK_OS_mH, RK_OS_mOH, _
            RK_OS_mLi, RK_OS_gamma1, RK_OS_gamma2, RK_kd_chem,
RK_kd_elect, RK_kp_elect, RK_Area_Factor, RK_INNER, _
            RK_OUTER, RK_porosity_in, RK_porosity_out, RK_tortuosity, RK_DFe,
RK_DH2, RK_mt_coeff, RK_Corr)

'    DiffConcMO = Abs(RK1_MO_Fetotal - RK_MO_Fetotal) / RK1_MO_Fetotal
'    DiffConcOS = Abs(RK1_OS_Fetotal - RK_OS_Fetotal) / RK1_OS_Fetotal

'  Loop Until ((DiffConcMO <= 0.01) And (DiffConcOS <= 0.01))
```

```
If Total < (Sat * 1.1) Then 'Dissolution
  If RK_OUTER > 0 Then
    TopGrowthOut = RK_kd_elect * RK_Area_Factor * (Total- (Sat * 1.1)) * (1 / 3) _
        * MW_mag / Den_mag / (1 - RK_porosity_out) * 10000 '(micron/s)
    TopGrowthIn = 0
  Else 'RK_Outer <= 0 Then 'inner dissolves
    TopGrowthIn = RK_kd_elect * RK_Area_Factor * (Total- (Sat * 1.1)) * (1 / 3) _
        * MW_mag / Den_mag / (1 - RK_porosity_in) * 10000 '(micron/s)
    TopGrowthOut = 0
  End If

  ElseIf Total >= (Sat * 1.1) Then 'precipitation ...Only outer oxide occur as precipitation at
oxide-solution interface.

'"Assume no particle size effect on solubility
    TopGrowthOut = RK_kd_elect * RK_Area_Factor * (Total- Sat) * (1 / 3) _
        * MW_mag / Den_mag / (1 - RK_porosity_out) * 10000 '(micron/s)
  End If

  BottomGrowth = RK_Corr * MW_metal / Den_metal * 10000 '(micron/s)

  RK_K(RK_ITER) = Incr * (BottomGrowth + TopGrowthIn)

'  If TopGrowthOut > 0 Then
'    RK_KK(RK_ITER) = Incr * TopGrowthOut
'  Else 'TopGrowthOut <= 0
'    RK_KK(RK_ITER) = 0
'  End If
  RK_KK(RK_ITER) = Incr * TopGrowthOut

  If RK_ITER < 3 Then
    RK_INNER = INNER + RK_K(RK_ITER) / 2#
    RK_OUTER = OUTER + RK_KK(RK_ITER) / 2#
  ElseIf RK_ITER = 3 Then
    RK_INNER = INNER + RK_K(RK_ITER)
    RK_OUTER = OUTER + RK_KK(RK_ITER)
  End If

Next RK_ITER

  INNER = INNER + (RK_K(1) + 2 * RK_K(2) + 2 * RK_K(3) + RK_K(4)) / 6#
  OUTER = OUTER + (RK_KK(1) + 2 * RK_KK(2) + 2 * RK_KK(3) + RK_KK(4)) / 6#

End Sub

Public Sub Spall(ByVal jj, ByVal section, ByVal Den, ByVal velocity, ByVal
Inner_SpallingFrequency,ByVal InnerSize, _
        ByVal Outer_SpallingFrequency, ByVal OuterSize, ByVal OS_Fesat, ByVal
OS_Fetotal, ByVal spconst_in, _
        ByVal spconst_out, ByVal porosity_in, ByVal porosity_out, ByVal tortuosity,
ByVal kd_elect, _
        ByVal kp_elect, ByVal Area_factor, ByRef INNER, ByRef OUTER, ByVal
Corr, ByRef InSPTime, ByRef OutSPTime)
Dim Inner_Oxide As Double, Outer_Oxide As Double
'dim InSPTime As Double, OutSPTime As Double,
Dim InSPSize As Double,OutSPSize As Double
Dim StuckParticle As Double
Dim VelocityFunction As Long
```

```
Dim OxLimit As Double
Dim LgstRow As Long
Dim SpallIn As Double, SpallOut As Double

Dim OuterNum As Double, InnerNum As Double, UpperOuterNum As Double,
UpperInnerNum As Double
Dim ssenh As Double
Dim MaxRow_outer As Long, MaxRow_inner As Long
Dim Time_Step As Double

'Assign Shear Stress Enhancement (ssenh)
If (section = "inlet") Then
   ssenh = 1
ElseIf (section = "outlet") Then
'      ssenh = 1.7
       ssenh = 2.3
ElseIf (section = "header") Then
   ssenh = 1
End If


   CSat = OS_Fesat * 56 * Den / 1000 '(g/cm3), and 56 is molecular wt. of Fe
   CFe = OS_Fetotal * 56 * Den / 1000 '(g/cm3)

   OxLimit = (INNER + OUTER) / 2
'  OxLimit = (INNER + OUTER) / 2

'SPALLING FOR THE OUTER OXIDE

'Assign MaxRow for Outer Oxide
If (section = "inlet") Then
   MaxRow_outer = 51
ElseIf (section = "outlet") Then
   MaxRow_outer = 10
ElseIf (section = "header") Then
   MaxRow_outer = 10
End If

   If (OUTER > 0#) Then
      If OuterTimeCou > 0 Then
         GoTo 77
      Else 'OuterTimeCou <= 0 then
         LgstRow = 0

         For ii = 1 To MaxRow_outer
            If OuterSize(ii) < OxLimit Then
               LgstRow = LgstRow + 1
            Else
               Exit For
            End If
         Next ii

         If LgstRow > 0 Then
            UpperOuterNum = Outer_SpallingFrequency(LgstRow, 1)
         Else
            UpperOuterNum = Outer_SpallingFrequency(1, 1) 'zero
         End If
```

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```
        Randomize '??? Verify randomness
        OuterNum = (UpperOuterNum - 0) * Rnd()
'       OuterNum = (UpperOuterNum - 0) * 0.5

'''Try setting OuterNum
'       OuterNum = 0.3


        If LgstRow <> 0 Then
          For A = 2 To LgstRow
'         For A = 2 To (LgstRow + 1)
            If (OuterNum < Outer_SpallingFrequency(A, 1) And OuterNum >=
Outer_SpallingFrequency((A - 1), 1)) Then
              OutSPSize = OuterSize(A - 1) 'micron
              Exit For
            ElseIf (OuterNum = Outer_SpallingFrequency(LgstRow, 1)) Then
              OutSPSize = OuterSize(LgstRow)
              Exit For
            End If
          Next A
'Exception case: Lgst=0
        ElseIf LgstRow = 0 Then
          OutSPSize = OuterSize(1)
        End If

        If (OS_Fesat * 1.1) > OS_Fetotal Then 'undersaturated
          OutSPTime = spconst_out * (OutSPSize ^ 2) / _
                 (ssenh * velocity ^ 2 * porosity_out * kd_elect * Area_factor _
                 * Abs((CSat * 1.1) - CFe))   'Spallingtime is in second unit
        Else 'saturated
          OutSPTime = spconst_out * (OutSPSize ^ 2) / (ssenh * velocity ^ 2)
        End If

      End If

77    Time_Step = Incr
      OuterTimeCou = OuterTimeCou + Time_Step

'     If (OuterTimeCou + (Time_Step / 2)) >= OutSPTime Then
'       SpallOut = OutSPSize
'       OuterTimeCou = 0
'     ElseIf (OuterTimeCou + (Time_Step / 2)) < OutSPTime Then 'NO Spalling
'       SpallOut = 0#
'     End If

';;;;;;;;No carry on the OuterTimeCou to the next iteration;;;;;;;
'     If (Time_Step + (Time_Step / 2)) >= OutSPTime Then
'       SpallOut = OutSPSize
'     ElseIf (Time_Step + (Time_Step / 2)) < OutSPTime Then 'NO Spalling
'       SpallOut = 0#
'     End If
      If Time_Step >= OutSPTime Then
        SpallOut = OutSPSize
      ElseIf Time_Step < OutSPTime Then  'NO Spalling
        SpallOut = 0#
      End If
';;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;
    Else 'Outer<=0
      SpallOut = 0#
```

```
  End If


' SPALLING FOR THE INNER OXIDE
'DEFINE VelocityFunction for INNER OXIDE
If (section = "inlet") Then
  VelocityFunction = 1
ElseIf (section = "outlet" Or section = "header") Then
  If (velocity < 1100) Then
    VelocityFunction = 1
  ElseIf (velocity >= 1100 And velocity < 1200) Then
    VelocityFunction = 2
  ElseIf (velocity >= 1200 And velocity < 1300) Then
    VelocityFunction = 3
  ElseIf (velocity >= 1300 And velocity < 1400) Then
    VelocityFunction = 4
  ElseIf (velocity >= 1400 And velocity < 1500) Then
    VelocityFunction = 5
  ElseIf (velocity >= 1500 And velocity < 1600) Then
    VelocityFunction = 6
  ElseIf (velocity >= 1600) Then
    VelocityFunction = 7
  End If
End If

'Assign MaxRow for Inner Oxide
If (section = "inlet") Then
    MaxRow_inner = 51
ElseIf (section = "outlet" Or section = "header") Then
  If (velocity < 1100) Then
    MaxRow_inner = 117
  ElseIf (velocity >= 1100 And velocity < 1200) Then
    MaxRow_inner = 110
  ElseIf (velocity >= 1200 And velocity < 1300) Then
    MaxRow_inner = 105
  ElseIf (velocity >= 1300 And velocity < 1400) Then
    MaxRow_inner = 102
  ElseIf (velocity >= 1400 And velocity < 1500) Then
    MaxRow_inner = 99
  ElseIf (velocity >= 1500 And velocity < 1600) Then
    MaxRow_inner = 86
  ElseIf (velocity >= 1600) Then
    MaxRow_inner = 76
  End If
End If


  If (INNER > 0#) And (OUTER = 0) Then
    If InnerTimeCou > 0 Then
      GoTo 87
    Else 'InnerTimeCou <= 0 then
      LgstRow = 0

      For ii = 1 To MaxRow_inner 'Maximum row of inner size = 117 (see Spalling
Reciprocal Distribution.xls file)
        If InnerSize(ii) < OxLimit Then
          LgstRow = LgstRow + 1
        Else
          Exit For
```

```
        End If
      Next ii

      If LgstRow > 0 Then
        UpperInnerNum = Inner_SpallingFrequency(LgstRow, VelocityFunction)
      Else
        UpperInnerNum = Inner_SpallingFrequency(1, VelocityFunction)
      End If

      Randomize
      InnerNum = (UpperInnerNum - 0) * Rnd()
'     InnerNum = (UpperInnerNum - 0) * 0.5

'"Try setting InnerNum
'     InnerNum = 0.3

     If LgstRow <> 0 Then
       For A = 2 To LgstRow
'      For A = 2 To (LgstRow + 1)
         If (InnerNum < Inner_SpallingFrequency(A, VelocityFunction) And _
           InnerNum >= Inner_SpallingFrequency((A - 1), VelocityFunction)) Then
           InSPSize = InnerSize(A - 1) 'micron
           Exit For
         ElseIf (InnerNum = Inner_SpallingFrequency(LgstRow, VelocityFunction)) Then
           InSPSize = InnerSize(LgstRow)
           Exit For
         End If
       Next A
'Exception case: Lgst=0
     ElseIf LgstRow = 0 Then
       InSPSize = InnerSize(1)
     End If

     If (OS_Fesat * 1.1) > OS_Fetotal Then 'undersaturated condition
       InSPTime = spconst_in * (InSPSize ^ 2) / _
           (ssenh * velocity ^ 2 * porosity_in * kd_elect * Area_factor * _
           ((CSat * 1.1) - CFe))
     Else 'saturated
       InSPTime = spconst_in * (InSPSize ^ 2) / (ssenh * velocity ^ 2)
     End If

   End If

87   Time_Step = Incr
   InnerTimeCou = InnerTimeCou + Time_Step
'    If (InnerTimeCou + (Time_Step / 2)) >= InSPTime Then 'Spalling occurs
'      Spallin = InSPSize
'      InnerTimeCou = 0
'    ElseIf (InnerTimeCou + (Time_Step / 2)) < InSPTime Then 'NO Spalling
'      Spallin = 0#
'    End If

';;;;;;;;No carry on the OuterTimeCou to the next iteration;;;;;;;
'    If (Time_Step + (Time_Step / 2)) >= InSPTime Then
'      SpallIn = InSPSize
'    ElseIf (Time_Step + (Time_Step / 2)) < InSPTime Then 'NOSpalling
'      SpallIn = 0#
'    End If
```

```
    If Time_Step >= InSPTime Then
      SpallIn = InSPSize
    ElseIf Time_Step < InSPTime Then 'NO Spalling
      SpallIn = 0#
    End If ';;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;

'''If there is no spalling, re-calculate for next iteration
'87    Time_Step = Incr
'        If (Time_Step + Time_Step / 2) >= InSPTime Then
'          Spallin = InSPSize
'        Else 'NO Spalling
'          Spallin = 0#
'        End If

  Else 'Inner<=0 or Outer>0
    SpallIn = 0#

  End If

''''''''''''''''''''''''''''''''''''''''''MOVE THIS SECTION TO SUB OXIDE''''''''''''''''''''''''''''''''''''''''''
''DISSOLUTION/PRECIPITATION OF MAGNETITE
'
'  Sat = OS_Fesat * Den / 1000 'mol/cm3
'  Total = OS_Fetotal * Den / 1000 'mol/cm3
'
'  If Total < (Sat * 1.1) Then 'dissolution
'
'    If OUTER > 0 Then
'
''''Sat*1.1 ;particle size factor
'       TopGrowth = kd_elect * Area_factor * (Total - (Sat * 1.1)) * (1 / 3) _
'               * MW_mag / Den_mag / (1 - porosity_out) * 10000 '(micron/s)
'
'    Else 'Outer <= 0 Then 'inner dissolves
'
'       TopGrowth = kd_elect * Area_factor * (Total - (Sat * 1.1)) * (1 / 3) _
'               * MW_mag / Den_mag / (1 - porosity_in) * 10000 '(micron/s)
'    End If
'
'  ElseIf Total >= (Sat * 1.1) Then 'precipitation ...Only outer oxide occur as precipitation at
oxide-solution interface.
'
''''Assume no particle size effect on solubility
'    TopGrowth = kd_elect * Area_factor * (Total - Sat) * (1 / 3) _
'            * MW_mag / Den_mag / (1 - porosity_out) * 10000 '(micron/s)
'  End If
'
'  BottomGrowth = Corr * MW_metal / Den_metal * 10000 '(micron/s)
'
''''''''''''''''''''''''''''''''''''''''
'  OUTER = 0
  If OUTER <= 0 Then
    OUTER = 0
'    INNER = INNER + TopGrowth * Incr + BottomGrowth * Incr - Spallin 'micron
    INNER = INNER - SpallIn  'micron
  Else 'If Outer > 0 Then
'    OUTER = OUTER + TopGrowth * Incr - SpallOut 'micron
'    INNER = INNER + BottomGrowth * Incr 'micron
```

```
    OUTER = OUTER - SpallOut 'micron
  End If

  If INNER <= 0 Then
  INNER = 0.0000000001 'micron
  End If

  If OUTER <= 0 Then
  OUTER = 0
  End If

End Sub

Public Sub PotentialEffect(ByVal section, ByVal TK_input, ByVal Den, ByRef MO_mH,
ByVal OS_Fesat, ByVal OS_Fetotal, _
                ByRef OS_mFEOH2, ByVal OS_mH, ByVal OS_gamma1, ByVal
OS_gamma2, ByVal kd_chem, _
                ByVal kp_chem, ByRef kd_elect, ByRef kp_elect, ByVal MO_Pot, ByVal
OS_Pot)


'ON H+ CONCENTRATION

  z = 1 'charge of H+ = 1
  MO_mH = OS_mH * (1 - (z * F * (MO_Pot - OS_Pot)) / (R * TK_input))


'ON DISSOLUTION RATE CONSTANT
  If OS_Fetotal < (OS_Fesat * 1.1) Then 'dissolution
    kd_elect = kd_chem * Exp(-(1 - beta) * (2 / 3) * F * OS_Pot / (R * TK_input))
'    kd_elect = kd_chem * Exp((1 - beta) * (2 / 3) * F * OS_Pot / (R * TK_input)) "Vermilyea
  ElseIf OS_Fetotal >= (OS_Fesat * 1.1) Then 'precititation
    kd_elect = kd_chem * Exp(beta * (2 / 3) * F * OS_Pot / (R * TK_input))
'    kp_elect = kp_chem * Exp(-beta * (2 / 3) * F * OS_Pot / (R * TK_input)) "Vermilyea
  End If

'ON SOLUBILITY AT O/S INTERFACE
  If (section = "inlet") Then 'Eo=-1.1486 V
    OS_mFEOH2 = (Exp((-1.1486 - OS_Pot) * 2 / 3 * F / (R * TK_input)) * ((OS_mH *
OS_gamma1 * Den) ^ (2 / 3))) _
          / Den    'Eo=-1.1486 V, n=2/3, and conc in mol/kg 'n=2/3
  ElseIf (section = "outlet" Or section = "header") Then 'Eo=1.1958 V
    OS_mFEOH2 = (Exp((-1.1958 - OS_Pot) * 2 / 3 * F / (R * TK_input)) * ((OS_mH *
OS_gamma1 * Den) ^ (2 / 3))) _
          / Den    'Eo=-1.1958 V, n=2/3, and conc in mol/kg 'n=2/3
  End If

End Sub

Sub OSSatConcentration(ByVal TK, ByRef Sat, ByRef Fe2, ByRef FeOH, ByVal FeOH2,
ByRef FeOH3, ByVal h, ByVal g1, ByVal g2)


'CALCULATE HYDROLYSIS CONSTANTS
  KFEOH = 10 ^ (FeOH_Constant1 * TK ^ 4 + FeOH_Constant2 * TK ^ 3 + FeOH_Constant3
* TK ^ 2 + FeOH_Constant4 * TK + FeOH_Constant5)
  KFEOH2 = 10 ^ (FeOH2_Constant1 * TK ^ 4 + FeOH2_Constant2 * TK ^ 3 +
FeOH2_Constant3 * TK ^ 2 + FeOH2_Constant4 * TK + FeOH2_Constant5)
```

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  KFEOH3_ = 10 ^ (FeOH3_Constant1 * TK ^ 4 + FeOH3_Constant2 * TK ^ 3 +
FeOH3_Constant3 * TK ^ 2 + FeOH3_Constant4 * TK + FeOH3_Constant5)

"CALCULATE Fe2+
  Fe2 = ((FeOH2 * (h * g1) ^ 2) / KFEOH2) / g2

"CALCULATE Fe(OH)+
  FeOH = ((KFEOH * Fe2 * g2) / (h * g1)) / g1

"CALCULATE Fe(OH)3-
  FeOH3 = ((KFEOH3_ * Fe2 * g2) / (h * g1) ^ 3) / g1

"CALCULATE Fe(II)
  Sat = Fe2 + FeOH + FeOH2 + FeOH3

End Sub

Public Sub ConcAdjustment(ByVal TC_input, ByVal TK_input, ByVal Den, ByVal
Bulk_Fetotal, ByRef MO_Fetotal, ByRef MO_mFE2, _
            ByRef MO_mFEOH, ByRef MO_mFEOH2, ByRef MO_mFEOH3, ByRef
MO_mH2, ByVal MO_mH, ByVal MO_mOH, _
            ByVal MO_mLi, ByRef MO_gamma1, ByRef MO_gamma2, ByVal
OS_Fesat, ByRef OS_Fetotal, ByRef OS_mFE2, _
            ByRef OS_mFEOH, ByRef OS_mFEOH2, ByRef OS_mFEOH3, ByVal
OS_mH2, ByVal OS_mH, ByVal OS_mOH, _
            ByVal OS_mLi, ByRef OS_gamma1, ByRef OS_gamma2, ByVal kd_chem,
ByVal kd_elect, ByVal kp_elect, _
            ByVal Area_factor, ByVal Inner_Ox, ByVal Outer_Ox, ByVal porosity_in,
ByVal porosity_out, _
            ByVal tortuosity, ByVal DFe, ByVal DH2, ByVal mt_coeff, ByVal Cor)
'"ADJUST CONCENTRATION
'CONCENTRATION OF Fe SPECIES AT OXIDE-SOLUTION INTERFACE

'"Particle size factor = 1.1 ,times to Fesat
  OS_Fetotal = ((Corr * (1 - fraction * (1 - porosity_in))) + _
          (mt_coeff * Bulk_Fetotal * Den / 1000)+ _
          (kd_elect * Area_factor * OS_Fesat * 1.1 * Den / 1000)) / _
          (mt_coeff + kd_elect * Area_factor) * 1000 / Den 'mol/kg
  Do
    Call composition(TK_input, OS_Fetotal, OS_mFE2, OS_mFEOH, OS_mFEOH2,
OS_mFEOH3, OS_mH, OS_mOH, OS_gamma1, OS_gamma2)
      old_gamma1 = OS_gamma1
      old_gamma2 = OS_gamma2
    Call DebyeHuckel(OS_mFE2, OS_mFEOH, OS_mFEOH3, OS_mH, OS_mOH, OS_mLi,
OS_gamma1, OS_gamma2, TC_input)
      DiffGamma1 = Abs(OS_gamma1 - old_gamma1) / ((OS_gamma1 + old_gamma1) / 2)
      DiffGamma2 = Abs(OS_gamma2 - old_gamma2) / ((OS_gamma2 + old_gamma2) / 2)
  Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)

'CONCENTRATION OF Fe SPECIES AT METAL SURFACE
  MO_Fetotal = Corr * (1 - fraction * (1 - porosity_in)) _
        * ((Inner_Ox / 10000 * tortuosity / DFe / porosity_in) _
        + (Outer_Ox / 10000 * tortuosity / DFe / porosity_out)) * 1000 / Den _
        + OS_Fetotal 'mol/kg
  Do
    Call composition(TK_input, MO_Fetotal, MO_mFE2, MO_mFEOH, MO_mFEOH2,
MO_mFEOH3, MO_mH, MO_mOH, MO_gamma1, MO_gamma2)
      old_gamma1 = MO_gamma1
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        old_gamma2 = MO_gamma2
    Call DebyeHuckel(MO_mFE2, MO_mFEOH, MO_mFEOH3, MO_mH, MO_mOH,
MO_mLi, MO_gamma1, MO_gamma2, TC_input)
    DiffGamma1 = Abs(MO_gamma1 - old_gamma1) / ((MO_gamma1 + old_gamma1) / 2)
    DiffGamma2 = Abs(MO_gamma2 - old_gamma2) / ((MO_gamma2 + old_gamma2) / 2)
  Loop Until (DiffGamma1 < ErrGamma And DiffGamma2 < ErrGamma)

'CONCENTRATION OF H2 AT METAL SURFACE
      MO_mH2 = (OS_mH2 * Den / 1000 + (1 - porosity_in) * Corr * (MW_metal /
Den_metal) _
            * (Den_mag / MW_mag) * (Inner_Ox / 10000 + Outer_Ox / 10000) _
            * tortuosity / DH2 / porosity_in) * 1000 / Den 'mol/kg
End Sub

Public Sub bulk(ByVal jj, ByVal Dia, ByVal Leng, ByVal Vel, ByVal mt_coeff, ByVal Cos,
ByRef Cbulk)

A = 4 * mt_coeff / (Vel * Dia) * (Cos - Cbulk(jj))
Cbulk(jj + 1) = Cbulk(jj) + A * Leng

End Sub

Public Sub OutputVariables(Results1 As Output, K, InnerOx, OuterOx, CR, CorrCur, MOPot,
OSPot, _
            Bulk_Fetotal, MO_Fetotal, OS_Fetotal, OS_Fesat, MO_mH, OS_mH,
kd_elect, Eeq1, Eeq2, Eeq3, Eeq4, _
            Io1, Io2, Io3, Io4, In_SpallTime, Out_SpallTime)

'       Call OutputVariables(Results1(ii, PrintIter), K, Outlet_InnerOx(i), Outlet_OuterOx(i),
Outlet_CR(i), Outlet_CorrCur(i), _
            Outlet_MOPot(i),    Outlet_OSPot(i),    Outlet_Bulk_FeTotal(i),
Outlet_MO_FeTotal(i), Outlet_OS_FeTotal(i), _
            Outlet_OS_Fesat(i),    Outlet_MO_mH(i),    Outlet_OS_mH(i),
Outlet_kd_elect(i), Outlet_Eeq1(i), _
            outlet_eeq2(i), Outlet_Eeq3(i), Outlet_Eeq4(i), Outlet_Io1(i), Outlet_Io2(i),
Outlet_Io3(i), _
            Outlet_Io4(i), Outlet_In_SpallTime(i), Outlet_Out_SpallTime(i))
  With Results1
    .K = K
    .InnerOx = InnerOx
    .OuterOx = OuterOx
    .CR = CR
    .CorrCur = CorrCur
    .MOPot = MOPot
    .OSPot = OSPot
    .CB = Bulk_Fetotal
    .CW = MO_Fetotal
    .CS = OS_Fetotal
    .Sat = OS_Fesat
    .Hmo = MO_mH
    .Hos = OS_mH
    .kd = kd_elect
    .Eeq1 = Eeq1
    .Eeq2 = Eeq2
    .Eeq3 = Eeq3
    .Eeq4 = Eeq4
    .Io1 = Io1
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    .Io2 = Io2
    .Io3 = Io3
    .Io4 = Io4
    .In_SPTime = In_SpallTime
    .Out_SPTime = Out_SpallTime
  End With

End Sub

Public Sub testupdate()

'  Workbooks.Open Filename:=FILEPATH & "\OutTemplate1.xlt"
  Workbooks.Open Filename:=FILEPATH & "\Results1.xlt"

  Application.ScreenUpdating = False


  OutputWorkbook = ActiveWorkbook.Name


  'Inlet
  IFeedSheet(1) = "Inlet(1)"
  IFeedSheet(2) = "Inlet(2)"
  IFeedSheet(3) = "Inlet(3)"
  IFeedSheet(4) = "Inlet(4)"
  IFeedSheet(5) = "Inlet(5)"
  IFeedSheet(6) = "Inlet(6)"
  IFeedSheet(7) = "Inlet(7)"

  For i = 1 To Inlet_Node
    iii = i
    Call UpdateSheets(IFeedSheet(i), iii, PrintIter)
  Next i


  'Outlet
  OFeedSheet(1) = "Outlet(1)"
  OFeedSheet(2) = "Outlet(2)"
  OFeedSheet(3) = "Outlet(3)"
  OFeedSheet(4) = "Outlet(4)"
  OFeedSheet(5) = "Outlet(5)"
  OFeedSheet(6) = "Outlet(6)"
  OFeedSheet(7) = "Outlet(7)"

  For i = 1 To Outlet_Node
   iii = i + 7
   Call UpdateSheets(OFeedSheet(i), iii, PrintIter)
  Next i

  Application.ScreenUpdating = True

End Sub

Public Sub UpdateSheets(SheetName, FeederNumber, Total)

  roff = 4 'SET ROW OFFSET
  coff = 0 'SET COLUMN OFFSET
  TotalIter = Total
```

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```
Sheets(SheetName).Activate

For Iter = 1 To TotalIter
        With Results1(FeederNumber, Iter)
    Range(Cells(roff + Iter, coff + 1), Cells(roff + Iter, coff + 1)).Select 'Column A
    ActiveCell.Value = .K
    Range(Cells(roff + Iter, coff + 2), Cells(roff + Iter, coff + 2)).Select 'Column B
    ActiveCell.Value = .InnerOx
    Range(Cells(roff + Iter, coff + 3), Cells(roff + Iter, coff + 3)).Select 'Column C
    ActiveCell.Value = .OuterOx
    Range(Cells(roff + Iter, coff + 4), Cells(roff + Iter, coff + 4)).Select 'Column D
    ActiveCell.Value = .CR * MW_metal / Den_metal * 10000 * 3600 * 24 * 365
'(microns/yr)
    Range(Cells(roff + Iter, coff + 5), Cells(roff + Iter, coff + 5)).Select 'Column E
    ActiveCell.Value = .CorrCur
    Range(Cells(roff + Iter, coff + 6), Cells(roff + Iter, coff + 6)).Select 'Column F
    ActiveCell.Value = .MOPot
    Range(Cells(roff + Iter, coff + 7), Cells(roff + Iter, coff + 7)).Select 'Column G
    ActiveCell.Value = .OSPot
    Range(Cells(roff + Iter, coff + 8), Cells(roff + Iter, coff + 8)).Select 'Column H
    ActiveCell.Value = .CB
    Range(Cells(roff + Iter, coff + 9), Cells(roff + Iter, coff + 9)).Select 'Column I
    ActiveCell.Value = .CW
    Range(Cells(roff + Iter, coff + 10), Cells(roff + Iter, coff + 10)).Select 'Column J
    ActiveCell.Value = .CS
    Range(Cells(roff + Iter, coff + 11), Cells(roff + Iter, coff + 11)).Select 'Column K
    ActiveCell.Value = .Sat * 1.1
    Range(Cells(roff + Iter, coff + 12), Cells(roff + Iter, coff + 12)).Select 'Column L
    ActiveCell.Value = .Hmo
    Range(Cells(roff + Iter, coff + 13), Cells(roff + Iter, coff + 13)).Select 'Column M
    ActiveCell.Value = .Hos
    Range(Cells(roff + Iter, coff + 14), Cells(roff + Iter, coff + 14)).Select 'Column N
    ActiveCell.Value = .kd
    Range(Cells(roff + Iter, coff + 15), Cells(roff + Iter, coff + 15)).Select 'Column O
    ActiveCell.Value = .Eeq1
    Range(Cells(roff + Iter, coff + 16), Cells(roff + Iter, coff + 16)).Select 'Column P
    ActiveCell.Value = .Eeq2
    Range(Cells(roff + Iter, coff + 17), Cells(roff + Iter, coff + 17)).Select 'Column Q
    ActiveCell.Value = .Eeq3
    Range(Cells(roff + Iter, coff + 18), Cells(roff + Iter, coff + 18)).Select 'Column R
    ActiveCell.Value = .Eeq4
    Range(Cells(roff + Iter, coff + 19), Cells(roff + Iter, coff + 19)).Select 'Column S
    ActiveCell.Value = .Io1
    Range(Cells(roff + Iter, coff + 20), Cells(roff + Iter, coff + 20)).Select 'Column T
    ActiveCell.Value = .Io2
    Range(Cells(roff + Iter, coff + 21), Cells(roff + Iter, coff + 21)).Select 'Column U
    ActiveCell.Value = .Io3
    Range(Cells(roff + Iter, coff + 22), Cells(roff + Iter, coff + 22)).Select 'Column V
    ActiveCell.Value = .Io4
    Range(Cells(roff + Iter, coff + 23), Cells(roff + Iter, coff + 23)).Select 'Column W
    ActiveCell.Value = .In_SPTime
    Range(Cells(roff + Iter, coff + 24), Cells(roff + Iter, coff + 24)).Select 'Column X
    ActiveCell.Value = .Out_SPTime
    End With
     Next Iter

End Sub
```

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CURRICULUM VITAE

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2001-2005 Bachelor Degree of Science in Chemical Engineering, Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

Working Experience:

2004	Position:	Process Engineer Intern Student
	Company name:	The Aromatics (Thailand) Public Company Limited (ATC), Rayong, Thailand
2006-2007	Position:	Research Assistant
	Company name:	Centre for Nuclear Energy Research, Fredericton, New Brunswick, Canada