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APPENDICES

Appendix A Input for the program

A.1 Sheet "pipe"

Inlet Section

Number of Nodes	7						
Diameter of Piping (cm)	44.3	50	106	5.68	5.68	5.68	5.68
Velocity of Coolant (cm/s)	1530	1200	270	985	985	985	985
Length of Piping (cm)	477.6	281.8	78.6	350	350	350	350
Surface Area (cm^2)	6.65E+04	4.43E+04	2.62E+04	5.93E+05	5.93E+05	5.93E+05	5.93E+05
Temperature (°C)	265	265	265	265	265	265	265
Solubility (g/cm^3)	7.48E-10	7.48E-10	7.48E-10	7.48E-10	7.48E-10	7.48E-10	7.48E-10

Outlet Section-Feeders

Number of Nodes	7						
Temperature (°C)	312	311	311	310	310	310	310
Solubility (g/cm^3)	1.32E-09	1.32E-09	1.32E-09	1.32E-09	1.32E-09	1.32E-09	1.32E-09

Steam Generator Section

Number of Nodes	18					
Surface Area	5.30E+04	3.20E+04	6.00E+05	2.30E+06	2.30E+06	3.20E+06
	3.20E+06	3.20E+06	3.20E+06	3.20E+06	3.20E+06	9.00E+05
	9.00E+05	9.00E+05	9.00E+05	9.00E+05	6.00E+05	3.20E+04

Constants

Outer Oxide Porosity	0.3
Tortuosity	1.15
Fraction of Fe in Fe_3O_4	0.724
Surface Area Factor	1.732
Density of Metal (g/cm^3)	7.86
Density of Oxide (g/cm^3)	5.2
Period (hours)	100
Time Increment (seconds)	3600
Symmetry Coefficient	0.5
Iron Molecular Weight (g/mol)	55.9
Magnetite Molecular Weight (g/mol)	231.7
Activation Energy for $Fe = Fe^{2+} + 2e$	140800
Activation Energy for $FeOH = Fe_3O_4$	120000
Activation Energy for $Fe^{2+} = Fe_3O_4$	125000
Activation Energy for $H^+ = H_2$	90000

Inlet Section	
Inlet Iron Diffusivity (cm^2/s)	3.20E-04
Inlet Iron Transport Coefficient (cm^2/s)	1.71E-04
Inlet Inner Oxide Porosity	0.1
Inlet Inner Oxide Spalling Constant	2.5E+14
Inlet Outer Spalling Constant	6.0E+13
Inlet Density of Water (g/cm^3)	0.783
Inlet Viscosity of Water (g/cm s)	1.01E-03
Inlet Hydrogen Concentration (g/cm^3)	2.00E-11
Inlet Hydrogen Diffusivity (cm^2/s)	7.45E-04
Inlet Supersaturation Factor	1.1
Outlet Section	
Outlet Iron Diffusivity (cm^2/s)	4.10E-04
Outlet Iron Transport Coefficient (cm^2/s)	1.65E-04
Outlet Inner Oxide Porosity	0.1
Outlet Inner Oxide Spalling Constant	0.224
Outlet Outer Spalling Constant	0.01
Outlet Density of Water (g/cm^3)	0.691
Outlet Viscosity of Water (g/cm s)	8.22E-04
Outlet Hydrogen Concentration (g/cm^3)	8.00E-10
Outlet Hydrogen Diffusivity (cm^2/s)	9.93E-04
Outlet Supersaturation Factor	1.1
Favourite outlet feeder 1	84
Favourite outlet feeder 2	40
Favourite outlet feeder 3	21
Favourite outlet feeder 4	86
Favourite outlet feeder 5	64
Print Frequency ratio	5
pH at room temperature	10.2
pH at high temperature	7.71

A.2 Velocity of outlet feeders

Feeder	Node 1 V (cm/s)	Feeder	Node 1 V (cm/s)	Feeder	Node 1 V (cm/s)
A09	1229	J01	1302	O10	1678
A11	1378	J03	1425	P03	1352
B06	1187	J05	1617	P05	1625
B08	1578	J07	1667	P07	1725
B10	1199	J09	1657	P09	1682
C05	1305	J11	1663	P11	1708
C07	1180	K02	1228	Q02	1410
C09	1412	K04	1636	Q04	1399
C11	1441	K06	1653	Q06	1623
D04	1333	K08	1647	Q08	1688
D06	1244	K10	1641	Q10	1662
D08	1533	L01	1393	R03	1054
D10	1603	L03	1535	R05	1377
E03	1307	L05	1664	R07	1619
E05	1569	L07	1682	R09	1662
E07	1299	L09	1652	R11	1680
E09	1569	L11	1619	S04	1052
E11	1621	M02	1290	S06	1388
F04	1281	M04	1686	S08	1619
F06	1563	M06	1715	S10	1669
F08	1651	M08	1670	T05	1035
F10	1618	M10	1639	T07	1369
G03	1213	N01	1367	T09	1548
G05	1519	N03	1516	T11	1552
G07	1666	N05	1705	U06	1384
G09	1642	N07	1714	U08	1249
G11	1654	N09	1667	U10	1379
H02	1584	N11	1650	V07	1212
H04	1512	O02	1194	V09	987
H06	1653	O04	1634	V11	1149
H08	1659	O06	1749	W10	1178
H10	1645	O08	1710		

A.3 Diameter of outlet feeders

Feeder	Node 1 D (cm)	Node 2 D (cm)	Node 3 D (cm)	Node 4 D (cm)	Node 5 D (cm)	Node 6 D (cm)	Node 7 D (cm)
F11	**6.4**	**6.4**	**6.4**	**6.4**	**6.4**	**6.4**	**6.4**
A09	5.1	5.1	5.1	5.1	5.1	5.1	5.1
A11	5.1	5.1	5.1	5.1	5.1	5.1	5.1
B06	5.1	5.1	5.1	5.1	5.1	5.1	5.1
B08	5.1	5.1	5.1	6.4	6.4	6.4	6.4
B10	6.4	6.4	6.4	6.4	6.4	6.4	6.4
C05	5.1	5.1	5.1	5.1	5.1	5.1	5.1
C07	6.4	6.4	6.4	6.4	6.4	6.4	6.4
C09	6.4	6.4	6.4	6.4	6.4	6.4	6.4
C11	6.4	6.4	6.4	6.4	6.4	7.6	7.6
D04	5.1	5.1	5.1	5.1	5.1	5.1	5.1
D06	6.4	6.4	6.4	6.4	6.4	6.4	6.4
D08	6.4	6.4	6.4	6.4	6.4	7.6	7.6
D10	6.4	6.4	6.4	6.4	7.6	7.6	7.6
E03	5.1	5.1	5.1	5.1	6.4	6.4	6.4
E05	6.4	6.4	6.4	6.4	6.4	6.4	6.4
E07	6.4	6.4	6.4	6.4	6.4	7.6	7.6
E09	6.4	6.4	6.4	6.4	6.4	8.9	8.9
E11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
F04	6.4	6.4	6.4	6.4	6.4	6.4	6.4
F06	6.4	6.4	6.4	6.4	6.4	7.6	7.6
F08	6.4	6.4	6.4	6.4	6.4	8.9	8.9
F10	6.4	6.4	6.4	6.4	6.4	8.9	8.9
G03	6.4	6.4	6.4	6.4	6.4	6.4	6.4
G05	6.4	6.4	6.4	6.4	6.4	8.9	8.9
G07	6.4	6.4	6.4	6.4	6.4	8.9	8.9
G09	6.4	6.4	6.4	6.4	6.4	8.9	8.9
G11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
H02	6.4	6.4	6.4	6.4	6.4	6.4	6.4
H04	6.4	6.4	6.4	6.4	7.6	7.6	7.6
H06	6.4	6.4	6.4	6.4	6.4	8.9	8.9
H08	6.4	6.4	6.4	6.4	6.4	8.9	8.9
H10	6.4	6.4	6.4	6.4	6.4	8.9	8.9
J01	5.1	5.1	5.1	5.1	5.1	6.4	8.9
J03	6.4	6.4	6.4	6.4	8.9	8.9	8.9
J05	6.4	6.4	6.4	6.4	8.9	8.9	8.9
J07	6.4	6.4	6.4	6.4	8.9	8.9	8.9
J09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
J11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
K02	6.4	6.4	6.4	6.4	6.4	6.4	6.4
K04	6.4	6.4	6.4	6.4	8.9	8.9	8.9
K06	6.4	6.4	6.4	6.4	8.9	8.9	8.9
K08	6.4	6.4	6.4	6.4	8.9	8.9	8.9
K10	6.4	6.4	6.4	6.4	8.9	8.9	8.9
L01	5.1	5.1	5.1	5.1	6.4	6.4	6.4
L03	6.4	6.4	6.4	6.4	7.6	7.6	7.6
L05	6.4	6.4	6.4	8.9	8.9	8.9	8.9

Diameter of outlet feeders (continued)

L07	6.4	6.4	6.4	6.4	8.9	8.9	8.9
L09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
L11	6.4	6.4	6.4	6.4	6.4	8.9	8.9
M02	6.4	6.4	6.4	6.4	6.4	6.4	6.4
M04	6.4	6.4	6.4	6.4	8.9	8.9	8.9
M06	6.4	6.4	6.4	6.4	8.9	8.9	8.9
M08	6.4	6.4	6.4	6.4	8.9	8.9	8.9
M10	6.4	6.4	6.4	6.4	8.9	8.9	8.9
N01	5.1	5.1	5.1	5.1	6.4	6.4	6.4
N03	6.4	6.4	6.4	6.4	7.6	7.6	7.6
N05	6.4	6.4	6.4	6.4	8.9	8.9	8.9
N07	6.4	6.4	6.4	6.4	8.9	8.9	8.9
N09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
N11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
O02	6.4	6.4	6.4	6.4	6.4	6.4	6.4
O04	6.4	6.4	6.4	6.4	8.9	8.9	8.9
O06	6.4	6.4	6.4	6.4	8.9	8.9	8.9
O08	6.4	6.4	6.4	6.4	8.9	8.9	8.9
O10	6.4	6.4	6.4	6.4	8.9	8.9	8.9
P03	6.4	6.4	6.4	7.6	7.6	7.6	7.6
P05	6.4	6.4	6.4	6.4	8.9	8.9	8.9
P07	6.4	6.4	6.4	6.4	8.9	8.9	8.9
P09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
P11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
Q02	5.1	5.1	5.1	6.4	6.4	6.4	6.4
Q04	6.4	6.4	6.4	6.4	7.6	7.6	7.6
Q06	6.4	6.4	6.4	6.4	8.9	8.9	8.9
Q08	6.4	6.4	6.4	6.4	8.9	8.9	8.9
Q10	6.4	6.4	6.4	6.4	8.9	8.9	8.9
R03	6.4	6.4	6.4	6.4	6.4	6.4	6.4
R05	6.4	6.4	6.4	6.4	7.6	7.6	7.6
R07	6.4	6.4	6.4	6.4	8.9	8.9	8.9
R09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
R11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
S04	6.4	6.4	6.4	6.4	6.4	6.4	6.4
S06	6.4	6.4	6.4	6.4	7.6	7.6	7.6
S08	6.4	6.4	6.4	6.4	8.9	8.9	8.9
S10	6.4	6.4	6.4	8.9	8.9	8.9	8.9
T05	6.4	6.4	6.4	6.4	6.4	6.4	6.4
T07	6.4	6.4	6.4	6.4	7.6	7.6	7.6
T09	6.4	6.4	6.4	6.4	8.9	8.9	8.9
T11	6.4	6.4	6.4	6.4	8.9	8.9	8.9
U06	5.1	5.1	5.1	5.1	6.4	6.4	6.4
U08	6.4	6.4	6.4	6.4	7.6	7.6	7.6
U10	6.4	6.4	6.4	6.4	7.6	7.6	7.6
V07	5.1	5.1	5.1	5.1	6.4	6.4	6.4
V09	6.4	6.4	6.4	6.4	6.4	6.4	6.4
V11	6.4	6.4	6.4	6.4	6.4	6.4	6.4
W10	5.1	5.1	5.1	5.1	6.4	6.4	6.4

A.4 Length of outlet feeders

Feeder	Node 1 L (cm)	Node 2 L (cm)	Node 3 L (cm)	Node 4 L (cm)	Node 5 L (cm)	Node 6 L (cm)	Node 7 L (cm)
F11	**17**	**3.5**	**1**	**1**	**1**	**1**	**1**
A09	17	3.5	107.0	188.2	188.2	188.2	188.2
A11	17	3.5	107.0	189.4	189.4	189.4	189.4
B06	17	3.5	107.0	189.4	189.4	189.4	189.4
B08	17	3.5	107.0	160.0	225.5	225.5	225.5
B10	17	3.5	139.5	197.5	197.5	197.5	197.5
C05	17	3.5	107.0	206.9	206.9	206.9	206.9
C07	17	3.5	139.5	202.5	202.5	202.5	202.5
C09	17	3.5	139.5	208.8	208.8	208.8	208.8
C11	17	3.5	139.5	229.0	229.0	190.0	176.0
D04	17	3.5	107.0	215.7	215.7	215.7	215.7
D06	17	3.5	139.5	215.0	215.0	215.0	215.0
D08	17	3.5	139.5	176.5	176.5	190.0	326.0
D10	17	3.5	139.5	170.0	190.0	248.5	248.5
E03	17	3.5	107.0	226.5	160.0	271.0	271.0
E05	17	3.5	139.5	212.5	212.5	212.5	212.5
E07	17	3.5	139.5	208.0	208.0	190.0	240.0
E09	17	3.5	139.5	208.0	208.0	222.5	211.5
E11	17	3.5	139.5	210.0	222.5	208.3	208.3
F04	17	3.5	139.5	231.3	231.3	231.3	231.3
F06	17	3.5	139.5	227.5	227.5	190.0	246.0
F08	17	3.5	139.5	227.5	227.5	222.5	213.5
F10	17	3.5	139.5	227.5	227.5	222.5	213.5
G03	17	3.5	139.5	238.8	238.8	238.8	238.8
G05	17	3.5	139.5	263.5	263.5	222.5	141.5
G07	17	3.5	139.5	259.0	259.0	222.5	173.5
G09	17	3.5	139.5	259.0	259.0	222.5	173.5
G11	17	3.5	139.5	274.0	222.5	193.3	193.3
H02	17	3.5	139.5	230.0	230.0	230.0	230.0
H04	17	3.5	139.5	292.0	190.0	223.0	223.0
H06	17	3.5	139.5	284.5	284.5	222.5	171.5
H08	17	3.5	139.5	284.5	284.5	222.5	179.5
H10	17	3.5	139.5	284.5	284.5	222.5	171.5
J01	17	3.5	107.0	497.3	497.3	506.0	637.0
J03	17	3.5	139.5	334.0	222.5	206.8	206.8
J05	17	3.5	139.5	346.0	222.5	206.8	206.8
J07	17	3.5	139.5	346.0	222.5	206.8	206.8
J09	17	3.5	139.5	346.0	222.5	206.8	206.8
J11	17	3.5	139.5	346.0	222.5	206.8	206.8
K02	17	3.5	139.5	247.5	247.5	247.5	247.5
K04	17	3.5	139.5	364.0	222.5	208.3	208.3
K06	17	3.5	139.5	380.0	222.5	209.8	209.8
K08	17	3.5	139.5	380.0	222.5	209.8	209.8
K10	17	3.5	139.5	380.0	222.5	209.8	209.8
L01	17	3.5	107.0	186.5	160.0	360.0	360.0
L03	17	3.5	139.5	221.0	190.0	351.0	351.0

Length of outlet feeders (continued)

L05	17	3.5	139.5	222.5	299.8	299.8	299.8
L07	17	3.5	139.5	230.0	222.5	418.8	418.8
L09	17	3.5	139.5	230.0	222.5	418.8	418.8
L11	17	3.5	139.5	319.0	319.0	222.5	143.5
M02	17	3.5	139.5	296.3	296.3	296.3	296.3
M04	17	3.5	139.5	245.0	222.5	372.8	372.8
M06	17	3.5	139.5	151.0	222.5	440.8	440.8
M08	17	3.5	139.5	221.0	222.5	438.8	438.8
M10	17	3.5	139.5	376.0	222.5	395.8	395.8
N01	17	3.5	107.0	290.5	160.0	368.5	368.5
N03	17	3.5	139.5	236.0	190.0	409.0	409.0
N05	17	3.5	139.5	157.0	222.5	434.8	434.8
N07	17	3.5	139.5	332.0	222.5	365.8	365.8
N09	17	3.5	139.5	303.0	222.5	428.8	428.8
N11	17	3.5	139.5	462.0	222.5	206.8	206.8
O02	17	3.5	139.5	313.8	313.8	313.8	313.8
O04	17	3.5	139.5	352.0	222.5	359.8	359.8
O06	17	3.5	139.5	358.0	222.5	376.3	376.3
O08	17	3.5	139.5	294.0	222.5	442.8	442.8
O10	17	3.5	139.5	356.0	222.5	443.8	443.8
P03	17	3.5	139.5	190.0	380.0	380.0	380.0
P05	17	3.5	139.5	358.0	222.5	395.8	395.8
P07	17	3.5	139.5	358.0	222.5	413.8	413.8
P09	17	3.5	139.5	358.0	222.5	449.8	449.8
P11	17	3.5	139.5	434.0	222.5	446.8	446.8
Q02	17	3.5	107.0	160.0	409.9	409.9	409.9
Q04	17	3.5	139.5	416.0	190.0	410.5	410.5
Q06	17	3.5	139.5	136.0	222.5	522.8	522.8
Q08	17	3.5	139.5	352.0	222.5	452.8	452.8
Q10	17	3.5	139.5	306.0	222.5	506.8	506.8
R03	17	3.5	139.5	353.8	353.8	353.8	353.8
R05	17	3.5	139.5	294.0	190.0	517.0	517.0
R07	17	3.5	139.5	440.0	222.5	413.8	413.8
R09	17	3.5	139.5	349.0	222.5	498.8	498.8
R11	17	3.5	139.5	312.0	222.5	544.8	544.8
S04	17	3.5	139.5	361.3	361.3	361.3	361.3
S06	17	3.5	139.5	380.0	190.0	464.5	464.5
S08	17	3.5	139.5	432.0	222.5	460.3	460.3
S10	17	3.5	139.5	222.5	468.8	468.8	468.8
T05	17	3.5	139.5	388.8	388.8	388.8	388.8
T07	17	3.5	139.5	702.0	190.0	331.0	331.0
T09	17	3.5	139.5	267.0	222.5	568.8	568.8
T11	17	3.5	139.5	410.0	222.5	544.3	544.3
U06	17	3.5	107.0	375.5	160.0	544.0	544.0
U08	17	3.5	139.5	236.0	222.5	596.8	596.8
U10	17	3.5	139.5	306.0	222.5	596.8	596.8
V07	17	3.5	107.0	430.5	160.0	556.0	556.0
V09	17	3.5	139.5	430.0	430.0	430.0	430.0
V11	17	3.5	139.5	448.8	448.8	448.8	448.8
W10	17	3.5	107.0	570.5	160.0	539.5	539.5

Appendix B Program code for feeder pipes

It is similar to the previous program[Lang, 2000], but some parts in the program were added. See more in attached CD.

The solubility computation based on Tremaine and Leblanc's work [1980] was added. The expression for dissolution rate constant was corrected to be more accurate.

Appendix C Program code for test probe

```
" Probe variables
Dim di, Velo, dis, ARE As Single

" To calculate solubility
Dim TC1 As Variant   'Inlet temperature
Dim TC2 As Variant   'Outlet temperature
Dim ph1 As Variant
Dim sol1 As Double   'solubility of magnetite at inlet
Dim sol2 As Double   'solubility of magnetite at outlet
Dim delta As Double   'the difference of solubility between inlet and outlet
Dim Sat As Single

" Variables and constants for T&L model
Dim KW As Double   'Dissociation constant of water
Dim KFE2 As Double   'Solubility constant of Fe2+
Dim KFEOH As Double   'T&L: Hydrolysis constant of FeOH+
Dim KFEOH2 As Double   'T&L: Hydrolyisis constant of Fe(OH)2
Dim KFEOH3_ As Double   'T&L: Hydrolyisis constant of Fe(OH)3-
Dim KFEOH3 As Double   'Solubility constant of Fe(OH)3
Dim KFEOH4 As Double   'Solubility constant of Fe(OH)4-

'*** FOR T&L: The solubility/hydrolysis contants are
'evaluated as the 4th order polynomial fit of the Tremaine and LeBlanc (1980) 'data at 100,
150, 200, 250 and 300 deg C.
Dim MFE2 As Double   'Molal concentration of Fe2+
Dim MFEOH As Double   'Molal concentration of FeOH+
Dim MFEOH2 As Double   'Molal concentration of Fe(OH)2
Dim MFEOH3_ As Double   'Molal concentration of Fe(OH)3-
Dim MFEOH3 As Double   'Molal concentration of Fe(OH)3
Dim MFEOH4 As Double   'Molal concentration of Fe(OH)4-
Dim MFESAT As Double   'Solubility of Magnetite
Dim MH As Double   'Molal concentration of acid at Temp = TC
```

```
Dim mHCL As Double   'Molal concentration of HCl at beginning of rxn
Dim Value As Double   'The answer that appears in the text box
Dim mhtemp As Double   'Variable used in Do Loop (see functions)
Dim TK As Variant   'temperature in Kelvin
Dim MatDen
Dim sf   'scaling factor

Const pi = 22 / 7
Const Tconst = 273.15

' COMMON VARIABLES

  Dim INCR, PERIOD As Long
  Dim OP2, TOR, FE, SA, FDEN, OXDEN, H2, PORCON As Single
  Dim BETA, MW, MWFE3O4
  Dim AEFEFE, AEFEFEO, AEHH, AEFEOH
  Dim CounterParticle(125), Counter(125) As Long
  Dim CorrRate(210000), OxideThick(210000), OSSolubility(210000),
        Solubility(210000)

' Variables for Spalling

  Dim SIZE(125), OuterSize(125), ISize(125), IOuterSize(125) As Long
  Dim LABEL(125, 7), OuterLabel(125, 7), ILabel(125, 7), IOuterLabel(125, 7)
  Dim Num, OuterNum, INum
  Dim InnerCon, OuterCon

' OUTLET SECTION VARIABLES

  Dim OFDIF, OTRANS, OH2DIF, oop1, OVIS, OWDEN, OF, OH2
  Dim HD, HDH, KD, ELEKD
  Dim OSAT, CW, CB, CS, H2W, H2OS
  Dim CP, DC, MET, OAveCorr
  Dim OX1, OX2, OAveOx
  Dim POT, OSPOT, MOEXFE, EeFEFE, MOEeH2H, EeFEOHFEO,
```

```
        MOEXFEOH, MOEXH

Private Sub CommandButton1_Click()

End Sub

Private Sub Area_Click()

End Sub

Private Sub AreaBox_Change()

End Sub

Private Sub cmdstart_Click()
   PERIOD = Val(PERIODBox.Text)
   DriveSpec = "C:"
   DirectorySpec = "C:\Users\Orawee\Input"
   FileSpec = "Microsoft Excel Files (*.xls),*.xls"
   Call fileFind(fileToOpen, DriveSpec, DirectorySpec, FileSpec)
   Call DataLoad(fileToOpen, PERIOD)
   Call ITERATE(PERIOD)
End Sub

Private Sub DelSol_Click()

End Sub

Private Sub DelSolBox_Change()

End Sub

Private Sub Dia_Click()

End Sub
```

```
Private Sub DiaBox_Change()
   di = Val(DiaBox.Text)
   dis = Val(LenBox.Text)
   ARE = pi * di * dis
   AreaBox.Text = Format(ARE, "#####.##")
End Sub

Private Sub Frame1_Click()

End Sub

Private Sub InSol_Click()

End Sub

Private Sub InSolBox_Change()

End Sub

Private Sub lblspall_Click()

End Sub

Private Sub LenBox_Change()
   di = Val(DiaBox.Text)
   dis = Val(LenBox.Text)
   ARE = pi * di * dis
   AreaBox.Text = Format(ARE, "#####.##")
End Sub

Private Sub Length_Click()

End Sub
```

```
Private Sub Note_Click()

End Sub

Private Sub OutSol_Click()

End Sub

Private Sub OutSolBox_Change()

End Sub

Private Sub PERIODBox_Change()

End Sub

Private Sub pH_Click()

End Sub

Private Sub pHBox_Change()
   ph1 = Val(pHBox.Text)
   Call TC1Box_Change
   Call TC2Box_Change
End Sub

Private Sub SFBox_Change()
   sf = Val(SFBox.Text)
End Sub

Private Sub SpallBox_Change()

End Sub
```

```
Private Sub SSENHBox_Change()
   SSENH = Val(SSENHBox.Text)
End Sub

Private Sub TC1Box_Change()
   TC1 = Val(TC1Box.Text)
   Call TL_solubility(TC1, ph1, sol1)
   InSolBox.Text = sol1
End Sub

Private Sub TC2Box_Change()
   TC2 = Val(TC2Box.Text)
   Call TL_solubility(TC2, ph1, sol2)
   OutSolBox.Text = sol2
   delta = Abs(sol2 - sol1)
   DelSolBox.Text = delta
End Sub

Private Sub Temp1_Click()

End Sub

Private Sub Temp2_Click()

End Sub

Sub fileFind(fileToOpen, DriveSpec, DirectorySpec, FileSpec)
   ChDrive DriveSpec
   ChDir DirectorySpec
   fileToOpen = Application.GetOpenFilename(FileSpec)
   If fileToOpen <> False Then

   End If
End Sub
```

```
Private Sub Userform_Activate()

End Sub

Sub DataLoad(fileToOpen, PERIOD)

' OPEN APPROPRIATE WORKBOOK
    Workbooks.Open FileName:=fileToOpen
    DataWorkbook = ActiveWorkbook.Name
    UserForm1.Repaint

'  LOAD MISCELLANEOUS CONSTANTS AND VARIABLES
    Sheets("probe").Select
    OP2 = Range("B2").Value
    TOR = Range("B3").Value
    FE = Range("B4").Value
    SA = Range("B5").Value
    FDEN = Range("B6").Value
    OXDEN = Range("B7").Value
    INCR = Range("B8").Value
    BETA = Range("B9").Value
    MW = Range("B10").Value
    MWFE3O4 = Range("B11").Value
    AEFEFE = Range("B12").Value
    AEFEOH = Range("B13").Value
    AEFEFEO = Range("B14").Value
    AEHH = Range("B15").Value
    IFDIF = Range("B17").Value
    ITRANS = Range("B18").Value
    iop1 = Range("B19").Value
    IInnerCon = Range("B20").Value
    IOuterCon = Range("B21").Value
    iwden = Range("B22").Value
    ivis = Range("B23").Value
```

```
IH2 = Range("B24").Value
IH2DIF = Range("B25").Value
IFactor = Range("B26").Value
OFDIF = Range("B28").Value
OTRANS = Range("B29").Value
oop1 = Range("B30").Value
InnerCon = Range("B31").Value
OuterCon = Range("B32").Value
OWDEN = Range("B33").Value
OVIS = Range("B34").Value
OH2 = Range("B35").Value
OH2DIF = Range("B36").Value
OF = Range("B37").Value
pht = range ("B39").Value

' OPTIONAL LOADING OF SPALLING DATA
Sheets("spall").Select
For a = 1 To 125
   SIZE(a) = Range(Cells(a + 3, 1), Cells(a + 3, 1)).Value
   For B = 1 To 7
      LABEL(a, B) = Range(Cells(a + 3, B + 1), Cells(a + 3, B + 1)).Value
   Next B
   OuterSize(a) = Range(Cells(a + 3, 9), Cells(a + 3, 9)).Value
   OuterLabel(a, 1) = Range(Cells(a + 3, 10), Cells(a + 3, 10)).Value
   ISize(a) = Range(Cells(a + 3, 11), Cells(a + 3, 11)).Value
   ILabel(a, 1) = Range(Cells(a + 3, 12), Cells(a + 3, 12)).Value
   IOuterSize(a) = Range(Cells(a + 3, 13), Cells(a + 3, 13)).Value
   IOuterLabel(a, 1) = Range(Cells(a + 3, 14), Cells(a + 3, 14)).Value
   CounterParticle(a) = Range(Cells(a + 3, 15), Cells(a + 3, 15)).Value
Next a
PORCON = 1#
Call DataInitialize(PERIOD)
End Sub
Sub DataInitialize(PERIOD)
Call COEFF(di, Velo, OH2DIF, OWDEN, OVIS, HD, KD, HDH, TC2)
```

```
    Call initials(OH2, sol2, OF, KD, Num, OuterNum, Sat, H2W, CW, CB, CS, CP, OX1,
                OX2, MET, ELEKD)
End Sub

Sub COEFF(di, Velo, H2DIF, WDEN, VIS, HD, KD, HDH, TC)
    V = Velo * 0.01
    B = di * 0.01
    MTENH = 1.3 * 31.2 * VIS ^ 0.24 / (WDEN ^ 0.24 * di ^ 0.24 * Velo ^ 0.24)
    HD = MTENH * 100 * 0.000637 * V ^ (0.82) / B ^ (0.18)
    KD = sf * Exp(0.0879 - 3569 / (TC + 273))
    HDH = 0.02 * H2DIF ^ 0.667 * Velo ^ 0.83 * WDEN ^ 0.5 / (di ^ 0.17 * VIS ^ 0.5)
End Sub

Sub initials(H2, Sol, Factor, KD, Num, OuterNum, Sat, H2W, CW, CB, CS, CP, OX1,
            OX2, MET, ELEKD)

    Randomize
    Num = Rnd()
    OuterNum = Rnd()
    Sat = (10 / 18) ^ (1# / 3#) * Sol
    H2W = H2
    CW = Factor * Sat
    CB = Sat
    CS = Sat
    CP = 0#
    OX1 = 0.00025
    OX2 = 0.00025
    MET = 0#
    ELEKD = KD

End Sub

Sub ITERATE(PERIOD)
    Dim K As Long
    PrintIter = 0
```

```
For K = 1 To PERIOD + 1
   UserForm1.lblIterate.Caption = K
   UserForm1.Repaint
   CorrosionTime = (K - 1)
   CBtot = 0
   CPtot = 0
   Flowtot = 0
   Isat = (10 / 18) ^ (1# / 3#) * sol1
   ICB = Isat
   CB = ICB

   InnerCon = Val(SpallBox.Text)
   If (K - 1) <> 0# Then
      Call SPALL(LABEL, OuterLabel, SIZE, OuterSize, Num, OuterNum,
                  TIMECOU, OUTERTIMECOU, di, dis, Velo, Sat, CS, CP,
                  OX1, OX2, ELEKD, InnerCon, OuterCon, CounterParticle,
                  Counter, oop1)
   End If
   Call corrode(PERIOD, TC2, HD, KD, ELEKD, HDH, di, Velo, dis, Sat, OF, DC,
               CW, CB, CS, OX1, OX2, MET, OFDIF, OTRANS, OH2DIF, oop1,
               OH2W, OH2OS, OAveOx, OAveCorr, OH2, POT, OSPOT, MOEXFE,
               EeFEFE, MOEeH2H, EeFEOHFEO, MOEXFEOH, MOEXH)
   If (CorrosionTime = PERIOD) Then
      OAveOx = OAveOx / 2000
      OAveCorr = OAveCorr / 2000
   End If

   If (K <> 1 And K < PERIOD) Then
      CorrRate(K) = DC * 8640000000#
      OxideThick(K) = OX1 * 10000# / (OXDEN * (1 - (oop1 + OOX1 * PORCON)))
      OSSolubility(K) = Sat
      Solubility(K) = CW
   End If
```

```
      If (K = PERIOD) Then
        Results3 = MET * 10000# / (FDEN * (K - 1) / 24# / 365#)
      End If

' ASSIGN DATA TO BE SAVED TO RESULTS ARRAY

      If (K - 1) Mod (Int(PERIOD / 100) + 1) = 0 And K <> 1 Then
        PrintIter = PrintIter + 1

        Call OutputDataVariables(DC, CS, OX1, OX2, POT, OSPOT)
      End If
    Next K

End Sub

Sub SPALL(ILabel, OLABEL, ISize, OSIZE, INum, ONUM, ITimeCou, OTIMECOU,
          di, dis, Velo, Sat, CS, CP, IOX, OOX, KD, ISPALLCON, OSPALLCON,
          CounterParticle, Counter, op1)

' SPALLING PORTION OF THE PROGRAM

    Dim OXIDE, OOXIDE, IPARSIZE, OPARSIZE, ISPALLT, OSPALLT
    Dim StuckParticle, IPAR, OPAR, PAR, SSENH

' ASSIGNING THE APPROPRIATE PARTICLE SIZE DISTRIBUTION TO
' THE APPROPRIATE VELOCITY PROBE

    E = 1
    F = 125
    C = 125

    SSENH = Val(SSENHBox.Text)
      If (Velo <= 1099) Then
        B = 1
      ElseIf (Velo > 1100 And Velo <= 1199) Then
```

```
      B = 2
    ElseIf (Velo >= 1200 And Velo <= 1299) Then
      B = 3
    ElseIf (Velo >= 1300 And Velo <= 1399) Then
      B = 4
    ElseIf (Velo >= 1400 And Velo <= 1499) Then
      B = 5
    ElseIf (Velo >= 1500 And Velo <= 1599) Then
      B = 6
    ElseIf (Velo >= 1600) Then
      B = 7
    End If

' SPALLING FOR THE OUTER OXIDE

  If (OOX > 0#) Then
22    For D = 1 To F
      If (ONUM < OLABEL(D, E) And ONUM >= OLABEL((D - 1), E)) Then
        OPARSIZE = OSIZE(D - 1)
      End If
    Next D
      OOXIDE = OOX * 10000 / OXDEN - OPARSIZE
      If (OOXIDE < 0.1 And OOXIDE > 0#) Then
        Randomize
        ONUM = Rnd()
        GoTo 22
      Else
        GoTo 23
      End If
23        OSPALLT = OSPALLCON * OPARSIZE / (SSENH * Velo ^ 2 * KD * (Sat –
                CS))
    OTIMECOU = OTIMECOU + 3600
    If (OTIMECOU + 1800 >= OSPALLT And OSPALLT > 0) Then
      OOXIDE = OOX * 10000 / OXDEN - OPARSIZE
      StuckParticle = OPARSIZE - OOX * 10000 / OXDEN
```

```
        OOX = OOXIDE * 0.0001 * OXDEN
        If (OOX < 0# And StuckParticle > 0#) Then
          OOX = 0#
          IOXIDE = IOX * 10000 / OXDEN - StuckParticle
          IOX = IOXIDE * 0.0001 * OXDEN
        End If
        If (OPARSIZE > 0.2) Then
          OPAR = 0.000000111 * OPARSIZE * OXDEN * dis / (di * Velo)
        Else
          OPAR = 0#
        End If
        For Y = 1 To 125
          If (CounterParticle(Y) = OPARSIZE) Then
            Counter(Y) = Counter(Y) + 1
          End If
        Next Y
        Randomize
        ONUM = Rnd()
        OTIMECOU = 0#
        End If
      Else
        OPAR = 0#
      End If

' SPALLING FOR THE INNER OXIDE

    For a = 1 To C
      If (INum < ILabel(a, B) And INum >= ILabel((a - 1), B)) Then
        IPARSIZE = ISize(a - 1)
      End If
    Next a
      ISPALLT = ISPALLCON * IPARSIZE / (SSENH * Velo ^ 2 * KD * (Sat – CS) * (op1
                  + IOX * PORCON))
    ITimeCou = ITimeCou + 3600
    If (ITimeCou + 1800 >= ISPALLT And OOX = 0# And ISPALLT > 0) Then
```

```
        IOXIDE = IOX * 10000 / OXDEN - IPARSIZE
        IOX = IOXIDE * 0.0001 * OXDEN
        If (IOX < 0#) Then
          IOX = 0#
        End If
        If (IPARSIZE > 0.2) Then
          IPAR = 0.0000001111 * IPARSIZE * OXDEN * dis / (di * Velo)
        Else
          IPAR = 0#
        End If
        For W = 1 To 125
          If (CounterParticle(W) = IPARSIZE) Then
            Counter(W) = Counter(W) + 1
          End If
        Next W
        Randomize
        INum = Rnd()
        ITimeCou = 0#
    Else
        IPAR = 0#
    End If

    PAR = IPAR + OPAR
    Call Particulate(CP, PAR)

End Sub

Sub Particulate(CP, Particulate)
    CP = CP + Particulate
End Sub

Sub corrode(PERIOD, TC, HD, CKD, ELEKD, HDH, di, Velo, dis, Sat, F, DC, CW, CB,
            OX1, OX2, MET, FDIF, TRANS, H2DIF, op1, H2W, H2OS, AveOx, AveCorr,
            H2, POT, OSPOT, MOEXFE, EeFEFE, MOEeH2H, EeFEOHFEO,
           MOEXFEOH, MOEXH)
```

```
  Dim ITER As Integer
  Dim DD, MM, SOX, DD2, SOX2, SMET, AA(10)
  Dim KK(4), KK2(4), HH(4)

  CBB = CB
  SOX = OX1
  SOX2 = OX2
  SMET = MET
  ' CORROSION RATE
  ITER = 0
49 ITER = ITER + 1
  AA(1) = 0.476 * (1.101 + (op1 + SOX * PORCON)) / (HD + ELEKD * SA)
  AA(2) = 0.476 * (1.101 + (op1 + SOX * PORCON)) * TOR / (FDIF * OXDEN * (op1
        + SOX * PORCON) * (1 - (op1 + SOX * PORCON)))
  AA(3) = ELEKD * SA / (HD + ELEKD * SA)
  AA(4) = 0.476 * (1.101 + (op1 + SOX * PORCON)) * TOR / (FDIF * OXDEN * OP2
        * (1  - OP2))
40  MM = 1 / (AA(1) + AA(2) * SOX + AA(4) * SOX2) * (CW - AA(3) * Sat – (1 – AA
        (3)) * CBB) ' + (TRANS * CW * 2 * 96500 * (POT - OSPOT) / (8.314 * (TC
        + 273)) / (AA(1) * FDIF * op1 / TOR + AA(2) * op1 * FDIF / TOR * SOX))

  If (MM <= 0) Then
    MM = 0
  End If
  If (CBB >= Sat) Then
    CS = 1 / (HD - ELEKD * SA) * (0.476 * (1.101 + (op1 + SOX * PORCON)) * MM
        + HD * CBB - ELEKD * SA * Sat)
'  Falling if keeps CS negative
      If (CS <= 0) Then
          CS = 1E-300
      End If

    DD = 0.658 * (1 - (op1 + SOX * PORCON)) * MM
    DD2 = (-ELEKD * 35 * SA * (Sat - CS)) / FE
  Else
```

```
    CS = 1 / (HD + ELEKD * SA) * (0.476 * (1.101 + (op1 + SOX * PORCON))* MM+
        ELEKD * SA * Sat + HD * CBB)
'  Falling if keeps CS negative
      If (CS <= 0) Then
          CS = 1E-300
      End If

    If (SOX <> 0 And CS < Sat And SOX2 = 0) Then
      LAMBDA = 1#
    Else
      LAMBDA = 0#
    End If
    DD = 0.658 * (1 - (op1 + SOX * PORCON)) * MM - LAMBDA/ FE *ELEKD* SA*
        (Sat - CS)
    If (SOX2 > 0) Then
      DD2 = (-ELEKD * SA * (Sat - CS)) / FE
    End If
  End If
  H2W = H2 + 0.1 * (0.00566 * MM* (7.32 - (op1 +SOX * PORCON))* OX1 * TOR /
        (OXDEN * (op1 + SOX* PORCON)* (1 - (op1+ SOX* PORCON))) / H2DIF)
  H2OS = H2 + 0.1 * 0.00566 * MM * (7.32 - op1) / HDH

' TOTAL INNER LAYER AND METAL LOSS
  KK(ITER) = INCR * DD
  KK2(ITER) = INCR * DD2
  HH(ITER) = INCR * MM

  If ITER < 4 Then
    SOX = OX1 + KK(ITER) / 2#
    SOX2 = OX2 + KK2(ITER) / 2#
      If (SOX2 < 0) Then
        SOX2 = 0
      End If
    SMET = MET + HH(ITER) / 2#
  End If
```

```
Select Case ITER
Case Is = 1
   DOX = DD
   DC = MM
   GoTo 49
Case Is = 2
   GoTo 49
Case Is = 3
   GoTo 49
Case Is = 4
   OX1 = OX1 + (KK(1) + 2 * KK(2) + 2 * KK(3) + KK(4)) / 6#
   If (OX1 < 0) Then
      OX1 = 0
   End If
   OX2 = OX2 + (KK2(1) + 2 * KK2(2) + 2 * KK2(3) + KK2(4)) / 6#
   If (OX2 < 0) Then
      OX2 = 0
   End If
   MET = MET + (HH(1) + 2 * HH(2) + 2 * HH(3) + HH(4)) / 6#
   If (MET < 0) Then
      MET = 0
   End If
   DC = (HH(1) + 2 * HH(2) + 2 * HH(3) + HH(4)) / 6# / 3600
   If (CorrosionTime > (PERIOD - 2000)) Then
      AveOx = AveOx + OX1
      AveCorr = AveCorr + (HH(1) + 2 * HH(2) + 2 * HH(3) + HH(4)) / 6#
   End If
End Select

If (K <> 1) Then
   Call Potential(DC, OX1, op1, H2, H2W, H2OS, CKD, ELEKD, TC, di, CW,
                  CB, CS, Sat, POT, OSPOT, MOEXFE, EeFEFE, MOEeH2H,
                  EeFEOHFEO, MOEXFEOH, MOEXH)
End If
```

```
    Call Bulk(di, Velo, dis, HD, CB, CS)

End Sub

Sub Potential(CR, OX1, op1, H2, H2W, H2OS, CKD, KD, TC, di, CW, CB, CS, Sat,
            POT, OSPOT, MOEXFE, EeFEFE, MOEeH2H, EeFEOHFEO,
            MOEXFEOH, MOEXH)

    Dim OSEXFE, OSEXH As Double
    Dim EeFEOFE, EeHH2, Csol, KDMO
    Dim Tafel1, FEFEOH, FEFEOHR, FEOHFEO, FEOHFEOR, Tafel2, CorrCur,
          EeH2H, EeFEFEO
    Dim ExchangeCon, T, pHCal
    Dim PrecCorrCur, PrecPot

    If (CR > 0) Then
'COMPUTING THE EFFECT OF POTENTIAL AT THE METAL-OXIDE INTERFACE
'COMPUTING THE EQUILIBRIUM POTENTIAL FOR EACH REACTION AT M-O
INTERFACE
      EeFEFE = 0.14 - 0.000198 * (TC + 273) * pht + 0.0000431 * (TC + 273) * Log
              (11 *CW)
      EeFEOHFEO = -0.75 - 0.000198 * (TC + 273) * pht - 0.0001292 * Log(CW * 11)
                 * (TC + 273)
      MOEeH2H = -0.0000431* (TC + 273)* Log(H2W) - 0.000198* (TC + 273) * pht

'COMPUTING THE EXCHANGE CURRENT FOR EACH REACTION AT THE M-O
INTERFACE
      MOEXFE = 2.011E+15 * (TC + 273) * Exp(-AEFEFE / 8.314 / (TC + 273)) * CW *
              1000 / 89.9 * Exp(11607 * EeFEFE / (TC + 273))
      MOEXFEOH = 2.011E+15 * (TC + 273) * Exp(-AEFEOH / 8.314 / (TC + 273)) * CW
                 * 1000 / 89.9 * Exp(1934 * EeFEOHFEO / (TC + 273))
      MOEXH = 2.011E+15 * (TC + 273) * Exp(-AEHH / 8.314 / (TC + 273)) * H2W * 1000
              / 2.016 * Exp(5803 / 3 * 7 * MOEeH2H / (TC + 273))
```

```
'SETTING UP CONSTANTS FOR BUTLER-VOLMER EXPRESSION
    CorrCur = 2 * 96500 * CR / MW
    PrecCorrCur = 2 / 3 * 96500 * 0.476 * (1 - (op1 + OX1 * PORCON)) * CR / 89.9
    FEFEOH = MOEXFE / Exp(11607 / (TC + 273) * EeFEFE)
    FEFEOHR = MOEXFE * Exp(11607 / (TC + 273) * EeFEFE)
    Tafel1 = 11607 / (TC + 273)
    FEOHFEO = MOEXFEOH / Exp(1934 / (TC + 273) * EeFEOHFEO)
    FEOHFEOR = MOEXFEOH * Exp(1934 / (TC + 273) * EeFEOHFEO)
    Tafel2 = 1934 / (TC + 273)
    Call BisectPotential(FEFEOH, FEFEOHR, Tafel1, CorrCur, POT)
  End If

'COMPUTE THE EFFECT OF POTENTIAL AT THE OXIDE-SOLUTION INTERFACE
  EeH2H = -0.0000431 * (TC + 273) * Log(H2OS) - 0.000198 * (TC + 273) * pht
  EeFEFEO = -0.75 - 0.000198 * (TC + 273)* pht - 0.000129* (TC + 273) * Log(11* CS)
  OSEXFE = 2.011E+15 * (TC + 273)* Exp(-AEFEFEO / 8.314/ (TC + 273)) * CS *1000
           / 89.9 * di / 4 * Exp(5803 / 3 * EeFEFEO / (TC + 273))
  OSEXH = 2.011E+15* (TC + 273)* Exp(-AEHH / 8.314 / (TC + 273)) * H2OS *1000 /
          2.016 * di / 4 * Exp(5803 / 3 * EeH2H / (TC + 273))
  OSPOT = 0.000258 * (TC + 273) * Log((OSEXFE* Exp(1934/ (TC + 273) *EeFEFEO)
          +OSEXH * Exp(1934/ (TC + 273) *EeH2H)) / (OSEXFE * Exp(-1934 / (TC +
          273) * EeFEFEO) + OSEXH * Exp(-1934 / (TC + 273) * EeH2H)))

'CALCULATIONS FOR PRECIPITATION
  If (CB >= Sat) Then
    KD = CKD * Exp(-1934 * OSPOT / (TC + 273))
  Else
'CALCULATIONS FOR DISSOLUTION
    EeFEOFE = -EeFEFEO
    KD = CKD * Exp(1934 * OSPOT / (TC + 273))
  End If
'DETERMINE NEW ELECTROCHEMICAL SOLUBILITIES AT EACH INTERFACE
  KDMO = CKD * Exp(-1934 * POT / (TC + 273))
  Csol = (Exp((POT+ 0.75+ 0.000198 * (TC+ 273) * pht) / (-0.000129 * (TC+ 273))) /11)
  CW = Csol + 0.476 * (1 - (op1 + OX1 * PORCON)) * CR / KDMO / 90 / SA
```

```
  Sat = (Exp((OSPOT + 0.75 + 0.000198 * (TC + 273) * pht) / (-0.000129 * (TC+
       273)))/11)
End Sub

Sub BisectPotential(Forward, Reverse, ALPHA, ICorr, ECorr)

  Dim MAXITER, MAXERR, MID, EA, ITERATION, TEST

  MAXITER = 10000
  MAXERR = 0.000005
  LOWER = -1.5
  UPPER = 1#

  ITERATION = 0
  EA = 1000000 * MAXERR

10 If (EA > MAXERR And ITERATION < MAXITER) Then
    MID = (LOWER + UPPER) / 2
    ITERATION = ITERATION + 1
    If (LOWER + UPPER <> 0) Then
      EA = Abs((UPPER - LOWER) / (UPPER + LOWER)) * 100
    End If
    TEST = MOPOT(LOWER, Forward, Reverse, ALPHA, ICorr) * MOPOT (MID,
           Forward, Reverse, ALPHA, ICorr)
    If (TEST = 0) Then
      EA = 0
    Else
      If (TEST < 0) Then
        UPPER = MID
      Else
        LOWER = MID
      End If
    End If
    GoTo 10
  End If
```

```
    ECorr = MID
End Sub

Function MOPOT(P, Forward, Reverse, ALPHA, ICorr)
    MOPOT = Forward * Exp(ALPHA * P) - Reverse * Exp(-ALPHA * P) - ICorr
End Function

Sub Bulk(di, Velo, dis, HD, CB, CS)


'  SUB BULK: CALCULATE THE IRON BULK CONCENTRATION FOR
'  INLET AND OUTLET SECTIONS
    Z = 4 * HD / (Velo * di) * (CS - CB)
    CB = CB + Z * dis
End Sub

Sub OutputDataVariables(DC, CS, OX1, OX2, POT, OSPOT)
    MatDen = 7.86
    CRBox.Text = (DC * 8640000000#) * 36.5 / MatDen
    CSBox.Text = CS
    Thick1Box.Text = OX1 * 1000# / (OXDEN * (1 - (op1 + OX1 * PORCON)))
    Thick2Box.Text = OX2 * 1000# / (OXDEN * (1 - (op1 + OX1 * PORCON)))
    MOPotBox.Text = POT
    OSPotBox.Text = OSPOT
End Sub
```

Appendix D Samples of calculations

D.1 Dissolution rate constant calculations

At pH10.2, and T=250°C

Dissolution rate from Balakrishnan's work = $7.30*10^{-13}$g/cm^{2}s (D.1)

Oxide solubility from Tremaine and Leblanc's work = $6.20*10^{-10}$g/cm^3 (D.2)

$$\text{Dissolution rate constant} = \frac{7.30*10^{-13}\, g/cm^2 s}{6.20*10^{-10}\, g/cm^3} \tag{D.3}$$

D.2 Electrochemical calculations

For example, H_2 evolution

$$2H^+ + 2e^- \rightarrow H_2 \tag{D.4}$$

D.2.1 Nernst equation

From equation2.39,

$$E^e{}_{O/R} = E^\circ_{O/R} + \frac{RT}{nF}\ln\frac{a_{Ox}}{a_{\mathrm{Re}}} \tag{D.5}$$

$$E_{H^+/H_2} = E^\circ_{H^+/H_2} + \frac{RT}{nF}\ln\frac{[H^+]^2}{[H_2]} \tag{D.6}$$

$$= 0 + 2(2.303)\frac{RT}{nF}\log[H^+] - \frac{RT}{nF}\ln[H_2] \tag{D.7}$$

where:

R = 8.314 J/mol K

n = 2

F = Faraday constant (96480C/mol).

$$E^e_{H^+/H_2} = -1.98\times10^{-4}T\cdot pH - 4.31\times10^{-5}\ln[H_2] \tag{D.8}$$

D.2.2 Exchange current density

From equation3.22,

$$I_o = nF\frac{k}{h}T\exp\left(-\Delta G^{*}_{H_2/H^+}/RT\right)C_{H_2}\exp\left(-\frac{(1-\beta)nF}{RT}E_e\right) \quad (D.9)$$

where:

k = 1.38×10^{-23} J K^{-1}
h = 6.62×10^{-34} J s
β = 0.5

$$I_o = 2.011\times10^{15}T\cdot Exp\left(-\Delta G^{*}_{H_2/H^+}/8.314T\right)C_{H_2}Exp\left(5803/3\times E_e/T\right) \quad (D.10)$$

D.2.3 Mixed potential at oxide/solution interface

From equation2.84,

$$E_{mixed} = \frac{RT}{nF}\ln\left[\frac{I_{0,so}e^{nFE_{e,so}/2RT} + I_{0,M}e^{nFE_{e,M}/2RT}}{I_{0,so}e^{-nFE_{e,so}/2RT} + I_{0,M}e^{-nFE_{e,M}/2RT}}\right] \quad (D.11)$$

$$E_{mixed} = 4.308\times10^{-5}\ln\left[\frac{I_{0,H^+/H_2}e^{11603E_{e,H^+/H_2}/T} + I_{0,Fe_3O_4/Fe(OH)_2}e^{11603E_{e,Fe_3O_4/Fe(OH)_2}/T}}{I_{0,H^+/H_2}e^{-11603E_{e,H^+/H_2}/T} + I_{0,Fe_3O_4/Fe(OH)_2}e^{-11603E_{e,Fe_3O_4/Fe(OH)_2}/T}}\right] \quad (D.12)$$

Appendix E A simpler model

The simple model is based on chemical surface reaction and mass transfer. It is used to predict : 1) the corrosion rate, 2) the oxide thickness and 3) the metal penetration rate. The reaction is according to Eq.E.1.

$$3Fe + 4OH^- \rightarrow Fe_3O_4 + 2H_2 + 4e^- \quad \text{(E.1)}$$

$$\frac{3}{4}Fe + OH^- \rightarrow \frac{1}{4}Fe_3O_4 + \frac{1}{2}H_2 + e^- \quad \text{(E.2)}$$

General reaction,

$$aA + bB \rightarrow cC + dD \quad \text{(E.3)}$$

where A = OH^-

B = Fe

C = Fe_3O_4

D = H_2.

Rate of reaction,

$$-\frac{1}{a}\frac{dN_A}{dt} = -\frac{1}{b}\frac{dN_B}{dt} \quad \text{(E.4)}$$

$$-\frac{dN_B}{dt} = -\frac{bdN_A}{dt} = bk_{s,A}C_{Ao} - k_{sB}C_{Bo} \quad \text{(E.5)}$$

When C_{Bo} equals C_{Bosat}, the rate of reaction is zero.

Therefore,

$$bk_{s,A}C_{Ao} = k_{sB}C_{Bosat} \quad \text{(E.6)}$$

$$k_{sB} = \frac{bk_{s,A}C_{Ao}}{C_{Bosat}} \quad \text{(E.7)}$$

$$-\frac{dN_B}{dt} = -\frac{bdN_A}{dt} = bk_{s,A}C_{Ao}\left(1 - \frac{C_{Bo}}{C_{Bosat}}\right) \quad \text{(E.8)}$$

where $\frac{dN_B}{dt}$ = reaction rate of Fe (gmoles Fe/m^2 s)

b = stoichiometric coefficient for reaction between Fe and OH^- of boundary layer Fe_3O_4

= 3/4

C_{Bo} = concentration of Fe^{2+} at the metal/oxide interface (gmoles/m^3)

C_{Bosat} = concentration of Fe^{2+} at saturation (gmoles/m^3)

C_{B2} = concentration of Fe^{2+} in the bulk solution (gmoles/m^3)

C_{Ao} = concentration of OH^- in bulk solution (gmoles/m^3)

k_{sa} = reaction coefficient for reaction between OH^- and Fe at the surface (m/s).

Diffusion of Fe^{2+} through oxide layer,

$$-(1-f')\frac{dN_B}{dt} = -b(1-f')\frac{dN_A}{dt} = \frac{D\phi}{l}(C_{Bo} - C_{B1}) \qquad \text{(E.9)}$$

where C_{B1} = concentration of Fe^{2+} at the oxide/fluid interface (gmoles/m^3)

fÂ = fraction of Fe forming oxide(dimensionless)

= 0.428

D = Diffusivity of iron through the oxide layer(m^2/s)

f = porosity

l = oxide layer thickness(m).

Mass transfer of Fe^{2+} from the oxide/fluid interface to fluid,

$$-(1-f')\frac{dN_B}{dt} = -b(1-f')\frac{dN_A}{dt} = k_g(C_{B1} - C_{B2}) \qquad \text{(E.10)}$$

$$\frac{k_g dia}{D} 0.02\,\mathrm{Re}^{0.83}\,Sc^{1/3} \qquad \text{(E.11)}$$

where k_g = mass transfer coefficient between oxide surface and bulk fluid(m/s)

Re = Reynolds number

Sc = Schmidt number

dia = diameter of pipes.

Combine three effect on corrosion rate together,

$$-\frac{dN_B}{dt} = \frac{(C_{Bosat} - C_{B2})}{\frac{C_{Bosat}}{bk_{sa}C_{Ao}} + \frac{(1-f')l}{\phi D_{Fe}} + \frac{(1-f')}{k_g}} \tag{E.12}$$

Chemical reaction | Diffusion through layer | Mass transfer from oxide

Oxide layer growth rate ;

$$\frac{dl}{dt} = -\frac{f' M_{Bo}}{(1-p)\rho_{Bo}} \frac{dN_B}{dt'} - kE - kD \tag{E.13}$$

where M_{Bo} = molecular weight of iron oxide (g/gmole)

ρ_{Bo} = density of oxide layer (gmole/m^3)

kD = dissolution rate constant (m/s)

kE = erosion rate coefficient (m/s).

$$kE = kE' f \frac{1}{2} \rho V^2 \tag{E.14}$$

where f = the friction factor for turbulent flow.

For rough approximation,

$f = 0.04 / Re^{0.16}$ ...a rough approximation (E.15)

$$kD = kD'(C_{Bosat} - C_{B2}) \tag{E.16}$$

At pH of 10.2,

$$kD' = \exp(0.0879 - 3569/T) \tag{E.17}$$

where T = absolute temperature of system(K).

The metal penetration rate ;

$$\frac{dx}{dt} = -\frac{dN_B}{dt}\frac{M_B}{\rho_B} \qquad \text{(E.18)}$$

where M_B = molecular weight of carbon steel

ρ_B = density of carbon steel.

There are three differential equations in the model. These equations can be solved by the mathmetical tools such as POLYMATH program, MATLAB, or MAPLE program. The code for POLYMATH solver is in the attached diskette.

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