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Scientific Notebook # 213

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Initial Scientific notebook entry for Galvanic Corrosion calculations

Title: Galvanic corrosion

Tests Preformed by: Darrell S. Dunn

Objectives: Determine the potential for the galvanic couple of carbon steel and Ni base container materials.

Method: Calculate the galvanic corrosion potential based on the kinetics for the following reactions:

reduction of oxygen
reduction of water
passive dissolution of the inner Ni base material
active dissolution of the carbon steel overpack.

The sum of current densities for all anodic and cathodic reactions should equal zero

Parameters: Obtained through the literature or from previous laboratory tests.

Equipment: IBM compatable computer and Mathematica version 2.2.3

Uncertainty and Sources of Error: Values of some parameters such as exchange current densities are not well defined for the container materials.

4/24/94

GALVAN01

OBJECTIVE: CALCULATE GALVANIC POTENTIAL ASSUMING:
CARBON STEEL IS ACTIVE
ALLOY 825 IS PASSIVE
O_2 REDUCTION ON 825 ONLY
H_2O REDUCTION ON 825 ONLY

PARAMETERS DEFINED IN GALVAN01.MA

INPUT VALUES DEFINED IN GALVAN01.MA

CALCULATION GALVAN01.MA WHERE CALCULATED GALVANIC CORROSION POTENTIAL

OTHER PARAMETERS SEEN AS ~~THE~~ DD 4/24/97
THE REDUCTION OF O_2, N_2O, THE DIFFUSION COEFF FOR O_2 AND THE BULK CONCENTRATION OF O_2 WERE CALCULATED

GALVAN01.MA NOTEBOOK SHOWN ON PAGES 7-9

4/24/97

GALVANIC CORROSION

Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2)

PARAMETERS

carbon steel

istee=corrosion current density for carbon steel (not calculated)
arsteel=area of steel (input)
i0steel=exchange current density for steel (input)
ecorrsteel=corrosion potential for steel (input)
bfe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
ih2o825=current density from water reduction on alloy 825 (not calculated)
io2825=current density oxygen reduction on alloy 825 (not calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equlibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)

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4/24/97

hplusconc=concentration of H+ (calculated from pH)
k1h2o=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
egalv=potential of galvanic couple alloy 825, carbon steel (calculated)
ph=ph (-log[H+]) (input)
khenryconst=henry's constant (calculated)

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
i0steel=0.01;
ecorrsteel=-0.600;
bo2=0.750;
bh2o=0.5;
zfe=2;
ipass825=0.00001;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
delta=0.0005;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o=0.0000000518;
i0o2825at298k=0.000001;

Off[General::spell]
Off[General::spell1]

eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=1.47172-(0.000815*tempk);
```


4/24/97


```
eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

hplusconc=10^-ph;

i0h2o825at298k=(2*f*k1h2o)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

SetOptions[$Output, PageWidth->400]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," "," ","khenryconst"," "," ","cbulko2"," "," ","do2","
","i0o2825at298k"," ","i0o2825"," ","o2actenergy"," ","i0steel"," ","ecorrsteel"," ","bo2","
","bh2o"," ","afe"," ","hplusconc"," ","h2oactenergy"," ","i0h2o825at298k"," ","k1h2o","
","i0h2o825"," ","ipass825"," ","ar825"," ","arsteel"," ","temp"," ","ph"," ","egalv","
","delta"]
```


4/24/97

GALVANO2.MA

OBJECTIVE SAME AS GALVANO1.MA P6

PARAMETERS DEFINED IN GALVANO2

INPUT VALUES DEFINED IN GALVANO2

GALVANIC CORROSION POTENTIAL OF A516 AND ALLOY 825 COUPLE CALCULATED BY SUMMING ALL ANODIC CURRENTS AND ALL CATHODIC CURRENTS TO ZERO. FOR A GIVEN SET OF INPUT PARAMETERS ONLY ONE POTENTIAL EXISTS WHERE THE SUM OF THE CURRENTS IS EQUAL TO ZERO.

CHANGES FROM GALVAN01.MA

CORROSION POTENTIAL OF GALVANIC COUPLE CALCULATED ASSUMING PERFECT CONTACT BETWEEN THE TWO MATERIALS.

DIFFUSION LAYER THICKNESS, DELTA, VARIED

OUTPUT CONTINUED NOTATION OF GALVANO2.MA DATED 2/10/97, THE DATE THE NOTEBOOK WAS WRITTEN.

OUTPUT DATA PUT IN FORTRAN FORM

4/24/97

GALVANIC CORROSION

Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2)

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (not calculated)
arsteel=area of steel (input)
i0steel=exchange current density for steel (input)
ecorrsteel=corrosion potential for steel (input)
bfe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
ih2o825=current density from water reduction on alloy 825 (not calculated)
io2825=current density oxygen reduction on alloy 825 (not calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equlibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)

4/24/97

hplusconc=concentration of H+ (calculated from pH)
k1h2o=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
egalv=potential of galvanic couple alloy 825, carbon steel (calculated)
ph=ph (-log[H+]) (input)
khenryconst=henry's constant (calculated)

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
i0steel=0.01;
ecorrsteel=-0.600;
bo2=0.750;
bh2o=0.5;
zfe=2;
ipass825=0.00001;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o=0.0000000518;
i0o2825at298k=0.000001;


Off[General::spell]
Off[General::spell1]


eeqh2o=0-(((2.303*r*tempk)/f)*ph);


eeq0o2=1.47172-(0.000815*tempk);
```


4/24/97


```
eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

hplusconc=10^-ph;

i0h2o825at298k=(2*f*k1h2o)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

SetOptions[$Output, PageWidth->400]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," "," ","khenryconst"," "," ","cbulko2"," "," ","do2","
","i0o2825at298k"," ","i0o2825"," "," ","o2actenergy"," "," ","i0steel"," "," ","ecorrsteel"," "," ","bo2","
","bh2o"," "," ","afe"," "," ","hplusconc"," "," ","h2oactenergy"," "," ","i0h2o825at298k"," "," ","k1h2o","
","i0h2o825"," "," ","ipass825"," "," ","ar825"," "," ","arsteel"," "," ","temp"," "," ","ph"," "," ","egalv","
","delta"," "," ","isteel"," "," ","ih20825"," "," ","io2825"," "," ","tempk=",tempk," "," ","pH=",ph,"
","ar825=",ar825," "," ","arsteel=",arsteel," "," ","afe=",afe," "," ","bo2=",bo2," "," ","bh2o=",bh2o,"
","i0steel=",AccountingForm[i0steel]," "," ","ipass825=",AccountingForm[ipass825],"
","galvan02.ma"," "," ","2/10/97"]


Do[galv=egalv /. FindRoot[arsteel*i0steel*(Exp[(afe zfe f (egalv - ecorrsteel))/(r tempk)]) +
ipass825*ar825-(ar825*i0h2o825*(Exp[-(bh2o zh2o f (egalv - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (egalv - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (egalv - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{egalv,0}, MaxIterations->100];


isteel=i0steel*(Exp[(afe zfe f (galv - ecorrsteel))/(r tempk)]);
```


4/24/97

```
ih2o825=i0h2o825*(Exp[(bh2o zh2o f (galv - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (galv - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (galv - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," "
",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," "
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[o2actenergy]," "
",FortranForm[i0steel]," ",FortranForm[ecorrsteel]," ",FortranForm[bo2]," "
",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[hplusconc]," "
",FortranForm[h2oactenergy]," ",FortranForm[i0h2o825at298k]," ",FortranForm[k1h2o]," "
",FortranForm[i0h2o825]," ",FortranForm[ipass825]," ",FortranForm[ar825]," "
",FortranForm[arsteel]," ",FortranForm[tempk]," ",FortranForm[ph]," ",FortranForm[galv]," "
",FortranForm[delta]," ",FortranForm[isteel]," ",FortranForm[ih2o825]," "
",FortranForm[io2825]],{delta,0.00005,0.005,0.0001}]
```

4/24/97

GALVAN 03.MA

OBJECTIVE : SAME AS GALVAN 01.MA P 6

PARAMETERS AND INPUT VALUES DEFINED IN GALVAN03.MA

GALVAN03.MA CALCULATED CORROSION POTENTIAL OF GALVANIC COUPLE BETWEEN CARBON STEEL AND ALLOY 825 (ecouple)

- THE CORROSION POTENTIAL OF UNCOUPLED ALLOY 825 WAS ALSO CALCULATED.
- THE CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE WAS CALCULATED ACCORDING TO EQUATION 2-24 OF CNWRA 96-011 REPORT (CBSPAC 1.0 B MANUAL):

$$E_{corr}^{wp} = (1-\eta)\, E_{corr} + \eta\, E_{couple}$$

AFTER CALCULATING E_{corr}^{wp} (THE CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE) THE CATHODIC CURRENTS FOR THE REDUCTION OF WATER AND O_2 ARE CALCULATED FOR THE WASTE PACKAGE.

THE SUM OF THE CURRENTS IS THEN CALCULATED WHICH INCLUDES THE FOLLOWING VALUES

ANODIC CURRENTS:

- STEEL DISSOLUTION
- ~~ALLOY~~ 4/24/97 ALLOY 825 PASSIVE DISSOLUTION
- O_2 REDUCTION ON ALLOY 825 WASTE PACKAGE
- N_2O REDUCTION ON ALLOY 825 WASTE PACKAGE.

CHANGES FROM GALVAN02.MA

E_{corr} 825 (UNCOUPLED) CALCULATED

η EQUATION ADDED

CURRENT SUM CALCULATED.

GALVAN03.MA

PROBLEMS ENCOUNTERED.

IF $\eta = 1$ (PERFECT GALVANIC COUPLE) CODE WORKS FINE AND THE SUM OF THE CURRENTS = 0 AND $E^{WP}_{825} = E_{COUPLE}$

HOWEVER IF $\eta \neq 1$ THEN THE SUM OF THE CURRENTS DOES NOT = 0

IF $\eta = 0$ THEN $E^{WP}_{CORR\ 825} = E^{825}_{CORR}$ (THE CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE IS THE SAME AS THE CORROSION POTENTIAL OF THE UNCOUPLED ALLOY 825 MATERIAL) HOWEVER THE SUM OF THE CURRENTS $\neq 0$

SINCE CHARGE BALANCE MUST BE MAINTAINED THEN THE CALCULATED VALUES ARE NOT VALID.

GALVAN03.MA SHOWN ON PAGES 17-21

4/24/97

GALVANIC CORROSION
Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2). The coefficient of galvanic galvanic coupling is included.

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
arsteel=area of steel (input)
i0steel=exchange current density for steel (input)
ecorrsteel=corrosion potential for steel (input)
bfe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
io2825=current density oxygen reduction on alloy 825 (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)
ecorr825=corrosion potential of alloy 825 not in contact with other metals(calculated)

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contact(calculated)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equlibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
khenryconst=henry's constant (calculated)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecouple=potential of galvanic couple alloy 825, carbon steel (calculated)
galvaniccoeff=coefficient of galvainc coupling, 1=complete coupling, 0=complete insulation(input)
currentsum=sum of currents

Input


```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
i0steel=0.01;
ecorrsteel=-0.600;
bo2=0.750;
bh2o=0.5;
zfe=2;
ipass825=0.00001;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o=0.0000000518;
i0o2825at298k=0.000001;
galvaniccoeff=1;

Off[General::spell]
Off[General::spell1]

eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=1.47172-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;
```

```
i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

hplusconc=10^-ph;

i0h2o825at298k=(2*f*k1h2o)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

SetOptions[$Output, PageWidth->500]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2", " ","khenryconst"," ","cbulko2"," ","do2","
","i0o2825at298k"," ","i0o2825"," ","o2actenergy"," ","i0steel"," ","ecorrsteel"," ","bo2","
","bh2o"," ","afe"," ","hplusconc"," ","h2oactenergy"," ","i0h2o825at298k"," ","k1h2o","
","i0h2o825"," ","ipass825"," ","ar825"," ","arsteel"," ","temp"," ","ph"," ","delta","
","isteel","
","ih20825"," ","io2825"," ","currentsum"," ","Ecouple"," ","Ecorr825","
","E825wastepackage"," ","tempk=",tempk," ","pH=",ph," ","ar825=",ar825,"
","arsteel=",arsteel," ","afe=",afe," ","bo2=",bo2," ","bh2o=",bh2o,"
","i0steel=",AccountingForm[i0steel]," ","ipass825=",AccountingForm[ipass825],"
","galvan03.ma"," ","2/12/97"]

Do[couple=ecouple /. FindRoot[arsteel*i0steel*(Exp[(afe zfe f (ecouple - ecorrsteel))/(r
tempk)]) + ipass825*ar825-(ar825*i0h2o825*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecouple,0}, MaxIterations->100];

corr825=ecorr825 /. FindRoot[ ipass825*ar825-(ar825*i0h2o825*(Exp[-(bh2o zh2o f
(ecorr825 - eeqh2o))/(r tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (ecorr825 - eeqo2))/(r
tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr825 - eeqo2))/(r tempk)])/(cbulko2 4 f
do2)))))==0, {ecorr825,0}, MaxIterations->100];

e825wp=((1-galvaniccoeff)*corr825) + galvaniccoeff*couple;
```


4/24/97

4/24/97


```
ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

currentsum=arsteel*isteel+ar825*ipass825-ar825*ih2o825-ar825*io2825;

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2],"
",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2],"
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[o2actenergy],"
",FortranForm[i0steel]," ",FortranForm[ecorrsteel]," ",FortranForm[bo2],"
",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[hplusconc],"
",FortranForm[h2oactenergy]," ",FortranForm[i0h2o825at298k]," ",FortranForm[k1h2o],"
",FortranForm[i0h2o825]," ",FortranForm[ipass825]," ",FortranForm[ar825],"
",FortranForm[arsteel]," ",FortranForm[tempk]," ",FortranForm[ph]," ",FortranForm[delta],"
",FortranForm[isteel]," ",FortranForm[ih2o825]," ",FortranForm[io2825],"
",FortranForm[currentsum]," ",FortranForm[couple]," ",FortranForm[corr825],"
",FortranForm[e825wp]],{delta,0.00005,0.005,0.0001}]
^*)
```


4/24/97

4/24/97

GALVAN 04.MA

OBJECTIVE SAME AS GALVAN 01.MA P 6

PARAMETERS AND INPUT SHOWN IN GALVAN04.MA

SAME AS GALVAN 03.MA EXCEPT CORROSION POTENTIAL OF CARBON STEEL CALCULATED (UNCOUPLED CORROSION POTENTIAL OF CARBON STEEL) O_2 AND N_2O REDUCTION ON STEEL. INCLUDED CHARGE BALANCE IDENTIFIED AS A PROBLEM WITH GALVAN 03.MA WAS STILL OBSERVED TO BE A PROBLEM WITH GALVAN 04.MA

GALVAN 04.MA SHOWN ON PAGES 23 –

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GALVANIC CORROSION

Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2). The coefficient of galvanic galvanic coupling is included.

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
arsteel=area of steel (input)
i0steel=exchange current density for steel (input)
ecorrsteel=corrosion potential for steel (input)
bfe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h20steel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equlibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
io2825=current density oxygen reduction on alloy 825 (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)
ecorr825=corrosion potential of alloy 825 not in contact with other metals(calculated)
e825wp=corrosion potential of alloy 825 waste package barrier with or without galvanic contact(calculated)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)

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khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equlibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecouple=potential of galvanic couple alloy 825, carbon steel (calculated)
galvaniccoeff=coefficient of galvainc coupling, 1=complete coupling, 0=complete insulation(input)
currentsum=sum of currents

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.750;
bh2o=0.5;
zfe=2;
ipass825=0.00001;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc;
```



```
k1h2osteel;
i0o2steelat298k;
galvaniccoeff=1;


Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->500]


Print["eeqh2o"," ","eeq0o2"," ","eeqo2", " ","khenryconst"," ","cbulko2"," ","do2","
","temp"," ","ph"," ","hplusconc"," ","h2oactenergy"," ","o2actenergy"," ","bo2"," ","bh2o","
","afe"," ","arsteel"," ","ar825"," ","ferrousconc"," ","eferrous"," ","i0ferrous","
","k1h20steel"," ","i0o2steelat298k"," ","i0o2steel"," ","ih2osteelat298k"," ","i0h2osteel","
","isteel"," ","ih2osteel"," ","io2steel"," ","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825","
","i0o2825at298k"," ","i0o2825"," ","ipass825"," ","ih20825"," ","io2825","
","arsteel*isteel"," ","arsteel*ih20steel"," ","arsteel*io2steel"," ","ar825*ipass825","
","ar825*ih2o825"," ","ar825*io2825"," ","currentsum"," ","ecorrsteel"," ","Ecouple","
","Ecorr825"," ","E825wastepackage"," ","delta"," ","tempk=",tempk," ","pH=",ph,"
","ar825=",ar825," ","arsteel=",arsteel," ","afe=",afe," ","bo2=",bo2," ","bh2o=",bh2o,"
","ipass825=",AccountingForm[ipass825]," ","galvan03.ma"," ","2/12/97"]


Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=1.47172-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

hplusconc=10^-ph;
```

```
i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;

i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2o825at298k=(2*f*k1h2o)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

corrsteel=ecorrsteel /. FindRoot[ i0ferrous*(Exp[(afe zfe f (ecorrsteel - eferrous))/(r
tempk)]*-(i0h2osteel*(Exp[-(bh2o zh2o f (ecorrsteel - eeqh2o))/(r
tempk)])+i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteel - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteel - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorrsteel,0}, MaxIterations->100];

corr825=ecorr825 /. FindRoot[ ipass825*-(i0h2o825*(Exp[-(bh2o zh2o f (ecorr825 -
eeqh2o))/(r tempk)])+i0o2825*((Exp[-(bo2 zo2 f (ecorr825 - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorr825,0}, MaxIterations->100];

couple=ecouple /. FindRoot[arsteel*i0ferrous*(Exp[(afe zfe f (ecouple - eferrous))/(r
tempk)]) + ipass825*ar825-((arsteel*i0h2osteel*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+arsteel*i0o2steel*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f
do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0,
{ecouple,0}, MaxIterations->100];

e825wp=((1-galvaniccoeff)*corr825) + galvaniccoeff*couple;
```

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```
isteel=i0ferrous*(Exp[(afe zfe f (couple - corrsteel))/(r tempk)]);

ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (couple - eeqh2o))/(r tempk)]);

io2steel=i0o2steel*((Exp[-(bo2 zo2 f (couple - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (couple - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

currentsum=arsteel*isteel+ar825*ipass825-ar825*ih2o825-ar825*io2825-arsteel*ih2osteel-ar

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," "
",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," "
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[o2actenergy]," "
",FortranForm[i0steel]," ",FortranForm[ecorrsteel]," ",FortranForm[bo2]," "
",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[hplusconc]," "
",FortranForm[h2oactenergy]," ",FortranForm[i0h2o825at298k]," ",FortranForm[k1h2o]," "
",FortranForm[i0h2o825]," ",FortranForm[ipass825]," ",FortranForm[ar825]," "
",FortranForm[arsteel]," ",FortranForm[tempk]," ",FortranForm[ph]," ",FortranForm[delta]," "
",FortranForm[isteel]," ",FortranForm[ih2o825]," ",FortranForm[io2825]," "
",FortranForm[currentsum]," ",FortranForm[couple]," ",FortranForm[corr825]," "
",FortranForm[e825wp]],{delta,0.00005,0.005,0.0001}]
```

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GALVANOS.MA / ~~GALVANOS~~ GALVANSA.MA DW 4/24/97

OBJECTIVE SAME AS GALVANO1.MA WITH O_2 AND H_2O REDUCTION ON STEEL CONSIDERED THE EFFICIENCY OF GALVANIC CONTACT η IS ALSO CONSIDERED.

PARAMETERS AND INPUT IN GALVANOS.MA

GALVANOS.MA CALCULATES THE CORROSION POTENTIAL OF UNCOUPLED CARBON STEEL, UNCOUPLED ALLOY 825 AND THE GALVANIC CORROSION POTENTIAL OF A PERFECT GALVANIC COUPLE OF ALLOY 825 AND CARBON STEEL

THE CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE IS CALCULATED USING THE INPUT PARAMETER VALUE OF η (SAME EQUATION AS LISTED ON PAGE 15)

THE CORROSION POTENTIAL FOR THE CARBON STEEL WASTE PACKAGE IS THEN CALCULATED CONSIDERING THE FOLLOWING PARAMETERS

- CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE
- O_2 REDUCTION ON STEEL
- O_2 REDUCTION ON ALLOY 825 WASTE PACKAGE
- H_2O REDUCTION ON STEEL
- H_2O REDUCTION ON ALLOY 825 WASTE PACKAGE
- PASSIVE DISSOLUTION OF ALLOY 825 WASTE PACKAGE
- THE ACTIVE DISSOLUTION OF STEEL

AFTER THE CORROSION POTENTIAL OF THE ALLOY 825 WP AND THE CARBON STEEL WASTE PACKAGE ARE CALCULATED, THE REDUCTION CURRENT FOR H_2O AND O_2 ARE CALCULATED AND ALL ANODIC AND CATHODIC CURRENTS ARE SUMMED.

GALVANSA.MA IS THE SAME AS GALVANOS.MA EXCEPT THE GALVANIC COEFF (η) AND THE PARTIAL PRESSURE OF O_2 ARE IDENTIFIED IN THE FIRST PRINT STATEMENT ALL OTHER CALCULATIONS REMAINED THE SAME.

CHANGES FROM GALVANO4.MA

AFTER CALCULATING CORROSION POTENTIAL OF ALLOY 825 UNCOUPLED, THE CORROSION POTENTIAL OF THE PERFECT GALVANIC COUPLE BETWEEN 825 AND CARBON STEEL AND THE CORROSION POTENTIAL OF THE ALLOY 825 WASTE PACKAGE, THE CORROSION POTENTIAL OF THE CARBON STEEL OVERPACK IS CALCULATED. THIS METHOD CORRECTS THE ~~P~~ DW 4/24/97 PROBLEM ENCOUNTERED WITH GALVANO4.MA WHERE THE CURRENT SUM WAS NOT ZERO.

GALVANSA SHOWN ON PAGES 30-35

DW 4/24/97

GALVANIC CORROSION
Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2). The coefficient of galvanic galvanic coupling is included.

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
isteelwp=corrosion current density for carbon steel waste package (calculated)
arsteel=area of steel (input)
ecorrsteel=corrosion potential for steel (calculated)
ecorrsteelwp=corrosion potential of the carbon steel waste package (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
ih2osteelwp=current density from water reduction on carbon steel waste package (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
io2steelwp=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
io2825wp=current density oxygen reduction on alloy 825 waste package (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
ih2o825wp=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)

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ecorr825=corrosion potential of alloy 825 not in contact with other metals(calculated)
e825wp=corrosion potential of alloy 825 waste package barrier with or without galvanic contact(calculated)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecouple=potential of perfect galvanic couple of alloy 825and carbon steel (calculated)
galvaniccoeff=coefficient of galvainc coupling, 1=complete coupling, 0=complete insulation(input)
currentsum=sum of currents

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.750;
bh2o=0.5;
zfe=2;
ipass825=0.01;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
```


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```
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.000000003;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.5
galvaniccoeff=1;


Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]


Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","h2oactenergy","
","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","arsteel"," ","ar825"," ","ferrousconc","
","eferrous"," ","i0ferrous"," ","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel","
","i0h2osteelat298k"," ","i0h2osteel"," ","isteel"," ","ih2osteel"," ","io2steel","
","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825"," ","i0o2825at298k"," ","i0o2825","
","ipass825"," ","ih2o825"," ","io2825"," ","isteelwp"," ","ih2osteelwp"," ","io2steelwp","
","ih2o825wp"," ","io2825wp"," ","arsteel*isteelwp"," ","arsteel*ih2osteelwp","
","arsteel*io2steelwp"," ","ar825*ipass825"," ","ar825*ih2o825wp"," ","ar825*io2825wp","
","currentsum"," ","ecorrsteel"," ","Ecouple"," ","Ecorr825"," ","Ecorrsteelwp","
","E825wastepackage"," ","delta"," ","tempk=",tempk," ","pH=",ph," ","ar825=",ar825,"
","arsteel=",arsteel," ","galvaniccoeff=",galvaniccoeff," ","galvan05.ma"," ","po2=",po2,"
","Revised:4/3/97"," ","run:4/3/97"]


Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);


eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);


eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));


khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;
```

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```
do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;


hplusconc=10^-ph;


eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);


i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];


i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;


i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];


i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];


i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;


i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];


corrsteel=ecorrsteel /. FindRoot[i0ferrous*(Exp[(afe zfe f (ecorrsteel - eferrous))/(r
tempk)])-(i0h2osteel*(Exp[-(bh2o zh2o f (ecorrsteel - eeqh2o))/(r
tempk)])+i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteel - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteel - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorrsteel,0}, MaxIterations->100];


isteel=i0ferrous*(Exp[(afe zfe f (corrsteel - eferrous))/(r tempk)]);


ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (corrsteel - eeqh2o))/(r tempk)]);


io2steel=i0o2steel*((Exp[-(bo2 zo2 f (corrsteel - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteel - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));
```

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```
corr825=ecorr825 /. FindRoot[ipass825-(i0h2o825*(Exp[-(bh2o zh2o f (ecorr825 -
eeqh2o))/(r tempk)])+i0o2825*((Exp[-(bo2 zo2 f (ecorr825 - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorr825,0}, MaxIterations->100];


ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (corr825 - eeqh2o))/(r tempk)]);


io2825=i0o2825*((Exp[-(bo2 zo2 f (corr825 - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (corr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));


couple=ecouple /. FindRoot[arsteel*i0ferrous*(Exp[(afe zfe f (ecouple - eferrous))/(r
tempk)]) + ipass825*ar825-((arsteel*i0h2osteel*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+arsteel*i0o2steel*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f
do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0,
{ecouple,0}, MaxIterations->100];


e825wp=((1-galvaniccoeff)*corr825) + galvaniccoeff*couple;


corrsteelwp=ecorrsteelwp /. FindRoot[arsteel*i0ferrous*(Exp[(afe zfe f (ecorrsteelwp -
eferrous))/(r tempk)]) + ipass825*ar825-((arsteel*i0h2osteel*(Exp[-(bh2o zh2o f
(ecorrsteelwp - eeqh2o))/(r tempk)])+arsteel*i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteelwp -
eeqo2))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteelwp - eeqo2))/(r
tempk)])/(cbulko2 4 f do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0,
{ecorrsteelwp,0}, MaxIterations->100];


isteelwp=i0ferrous*(Exp[(afe zfe f (corrsteelwp - eferrous))/(r tempk)]);


ih2osteelwp=i0h2osteel*(Exp[-(bh2o zh2o f (corrsteelwp - eeqh2o))/(r tempk)]);


io2steelwp=i0o2steel*((Exp[-(bo2 zo2 f (corrsteelwp - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteelwp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));
```

4/24/97

4/24/97


```
ih2o825wp=i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)]);


io2825wp=i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));


currentsum=arsteel*isteelwp+ar825*ipass825-ar825*ih2o825wp-ar825*io2825wp-arsteel*ih


Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2],"
",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2],"
",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph],"
",FortranForm[hplusconc]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy],"
",FortranForm[bo2]," ",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[arsteel],"
",FortranForm[ar825]," ",FortranForm[ferrousconc]," ",FortranForm[eferrous],"
",FortranForm[i0ferrous]," ",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k],"
",FortranForm[i0o2steel]," ",FortranForm[i0h2osteelat298k]," ",FortranForm[i0h2osteel],"
",FortranForm[isteel]," ",FortranForm[ih2osteel]," ",FortranForm[io2steel],"
",FortranForm[k1h2o825]," ",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825],"
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[ipass825],"
",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[isteelwp],"
",FortranForm[ih2osteelwp]," ",FortranForm[io2steelwp]," ",FortranForm[ih2o825wp],"
",FortranForm[io2825wp]," ",FortranForm[arsteel*isteelwp],"
",FortranForm[arsteel*ih2osteelwp]," ",FortranForm[arsteel*io2steelwp],"
",FortranForm[ar825*ipass825]," ",FortranForm[ar825*ih2o825wp],"
",FortranForm[ar825*io2825wp]," ",FortranForm[currentsum]," ",FortranForm[corrsteel],"
",FortranForm[couple]," ",FortranForm[corr825]," ",FortranForm[corrsteelwp],"
",FortranForm[e825wp]," ",FortranForm[delta]],{delta,0.00005,0.005,0.0001}]
```

4/24/97

4/24/97

COROXRD1, MA

OBJECTIVE: CALCULATE THE CURRENT FOR THE REDUCTION OF O_2 AND WATER AND THE DISSOLUTION OF METAL. ANODIC DISSOLUTION OF ALLOY 825 ASSUMED TO BE CONTROLLED BY PASSIVE CURRENT DENSITY. ANODIC DISSOLUTION OF A516 CARBON STEEL ASSUMED TO BE ACTIVE.

PARAMETERS AND INPUT THE SAME AS GALVANSa EXCEPT THAT THE GALVANIC POTENTIALS AND CORROSION POTENTIALS ARE NOT CALCULATED. E_{corr} IS VARIED FROM $-1\ V_{SHE}$ TO $1\ V_{SHE}$. ALSO AN OXYGEN OVER POTENTIAL IS ADDED TO THE CALCULATION OF THE EQULIBRIUM POTENTIAL FOR OXYGEN REDUCTION.

VARIED PARAMETERS Ecorr, TEMP K, I PASS 825 PH, i0ferrous, o2overpotential.

COROXRD1 SHOWN ON PAGES 37-40

Dunn 4/25/97

Metal oxidation, Oxy Hyd reduction

Darrell S. Dunn

The corrosion rate of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 and carbon steel. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2).

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)

Dunn 4/25/97

Dunn 4/25/97

o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecorr= corrosion potential of alloy 825 and carbon steel

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.50;
bh2o=0.5;
zfe=2;
ipass825=0.01;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.000000003;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.0
```


4/25/97


```
delta=0.0001;

Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","h2oactenergy","
","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","ferrousconc"," ","eferrous"," ","i0ferrous","
","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel"," ","i0h2osteelat298k"," ","i0h2osteel","
","isteel"," ","ih2osteel"," ","io2steel"," ","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825","
","i0o2825at298k"," ","i0o2825"," ","ipass825"," ","ih2o825"," ","io2825"," ","Ecorr","
","delta"," ","tempk=",tempk," ","pH=",ph," ","galvaniccoeff=",galvaniccoeff,"
","coroxrd1.ma"," ","po2=",po2," ","Revised:4/12/97"," ","run:4/12/97"]

Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)-((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

hplusconc=10^-ph;

eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);

i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];
```


4/25/97

Coroxrd1

```
i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;

i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

isteel=i0ferrous*(Exp[(afe zfe f (ecorr - eferrous))/(r tempk)]);

ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2steel=i0o2steel*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));


Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," ",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph]," ",FortranForm[hplusconc]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy]," ",FortranForm[bo2]," ",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[ferrousconc]," ",FortranForm[eferrous]," ",FortranForm[i0ferrous]," ",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k]," ",FortranForm[i0o2steel]," ",FortranForm[i0h2osteelat298k]," ",FortranForm[i0h2osteel]," ",FortranForm[isteel]," ",FortranForm[ih2osteel]," ",FortranForm[io2steel]," ",FortranForm[k1h2o825]," ",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825]," ",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[ipass825]," ",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[ecorr]," ",
FortranForm[delta]],{ecorr,-1,1,0.05}]
```

1/25/97

4/25/97

O2H2ORED, MA

OBJECTIVE: DETERMINE EQULIBRIUM POTENTIAL FOR OXYGEN AS A FUNCTION OF THE OXYGEN PARTIAL PRESSURE

PARAMETERS AND INPUT: A LIMITED NUMBER OF PARAMETERS FROM GALVANSa, MA. ONLY THOSE PARAMETERS NECESSARY TO CALCULATE THE EQULIBRIUM POTENTIALS FOR WATER AND OXYGEN REDUCTION WERE INCLUDED. NO CALCULATION OF REDUCTION CURRENT DISSOLUTION CURRENT OR CORROSION POTENTIAL INCLUDED.

VARIED PARAMETER pO2 VARIED FROM 0.01 TO 0.21

O2H2ORED, MA SHOWN ON PAGES 42-44

OUTPUT GRAPH p 43

PROBLEMS ENCOUNTERED

EQULIBRIUM POTENTIAL OF O_2 REDUCTION INVERSLY ~~PORPORTIO~~ 4/25/95 RELATED TO PARTIAL PRESSURE OF OXYGEN. THIS OCCURS AS A RESULT OF A SIGN ERROR IN THE CALCULATION OF THE REDUCTION OF O_2 EQULIBRIUM POTENTIAL. THIS ERROR ALSO OCCURS IN ALL PREVIOUS CALCULATIONS INCLUDING GALVAN01.MA, GALVAN02.MA, GALVAN03.MA GALVAN04.MA GALVAN05.MA GALVANSa.MA AND COROXRD1.MA.

RESOLUTION. PROPER EQUATION WILL BE PLACED IN GALVANSa.MA, COROXRD1.MA AND THIS CALCULATION.

4/25/97

Oxygen/hydrogen reduction/concentration/diffusion

The purpose of this calculation is to determine the equlibrium potential for oxygen as a function of te partial pressure of oxygen in the system.

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

4/25/97

4/25/97

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.250;
bh2o=0.5;
zfe=2;
tempk=298;
ph=9;
o2actenergy=40;
h2oactenergy=20;
o2overpotential=0.0;
delta=0.0001;

Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst"," ","cbulko2"," ","do2"," ","temp"," ","po2"," ","ph"," ","o2h20red.ma"," ","4/23/97"," ","run:4/23/97"]

Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));
```

4/25/97

4/25/97

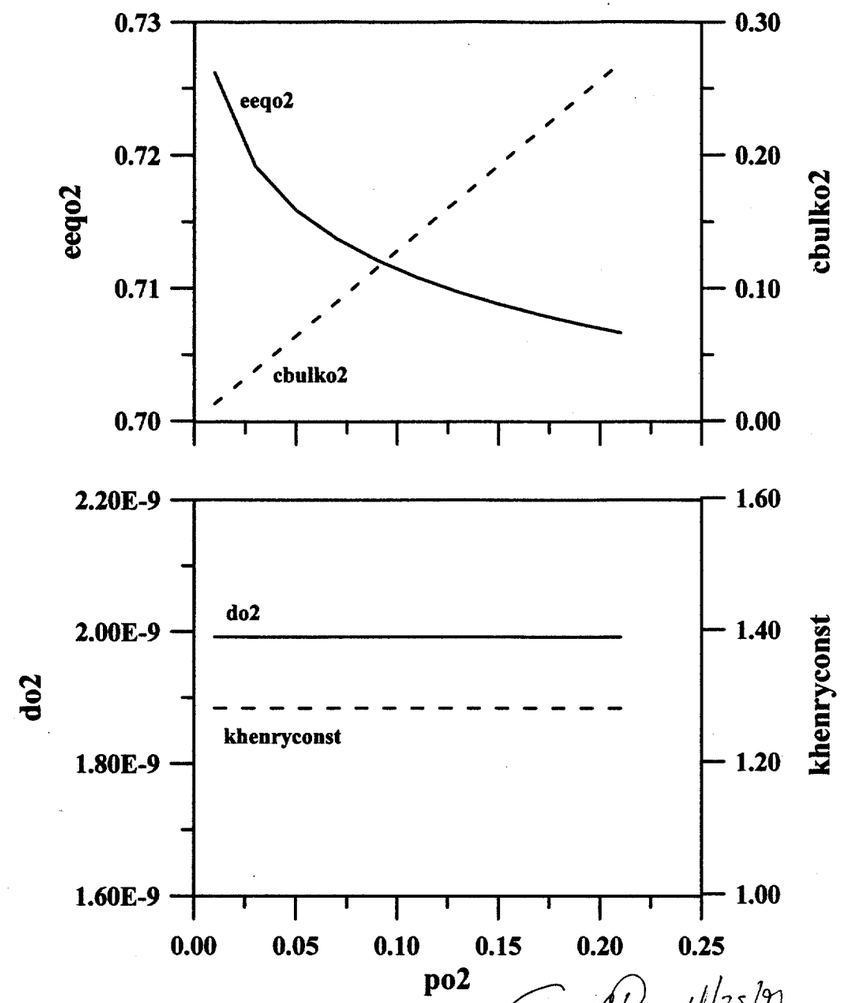
O2h2ored

```
cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," ",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[po2]," ",FortranForm[ph]],{po2,0.01,0.21,0.02}]
```

3

4/25/97

4/25/97



4/25/97

CALCULATED W O_2H_2O REP.MA
DATA FILE O2N2OR1.MA/XLS
GRAPH FILE O2N2OR1.GRF

4/25/97

O2H2ORX2.MA

OBJECTIVE CORRECT SIGN ERROR IN O2H2ORED.MA AND PLOT EQULIBRIUM POTENTIAL OF OXYGEN REDUCTION

PARAMETERS AND INPUT SHOWN IN O2H2ORX2.MA THE SAME AS O2H2ORED.MA EXCEPT FOR CORRECTED O_2 REDUCTION EQULIBRIUM POTENTIAL CALCULATION.

VARIED PARAMETER po2 FROM 0.01 TO 0.21
O2H2ORX2.MA SHOWN ON PAGE 47-49
OUTPUT GRAPH SHOWN ON PAGE. 50

4/25/97

Oxygen/hydrogen reduction/concentration/diffusion

The purpose of this calculation is to determine the equlibrium potential for oxygen as a function of te partial pressure of oxygen in the system.

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

4/25/97

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f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.250;
bh2o=0.5;
zfe=2;
tempk=298;
ph=9;
o2actenergy=40;
h2oactenergy=20;
o2overpotential=0.0;
delta=0.0001;

Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","po2"," ","ph"," ","o2h20rx2.ma"," ","4/23/97","
","run:m/d/97"]

Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));
```

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4/25/97

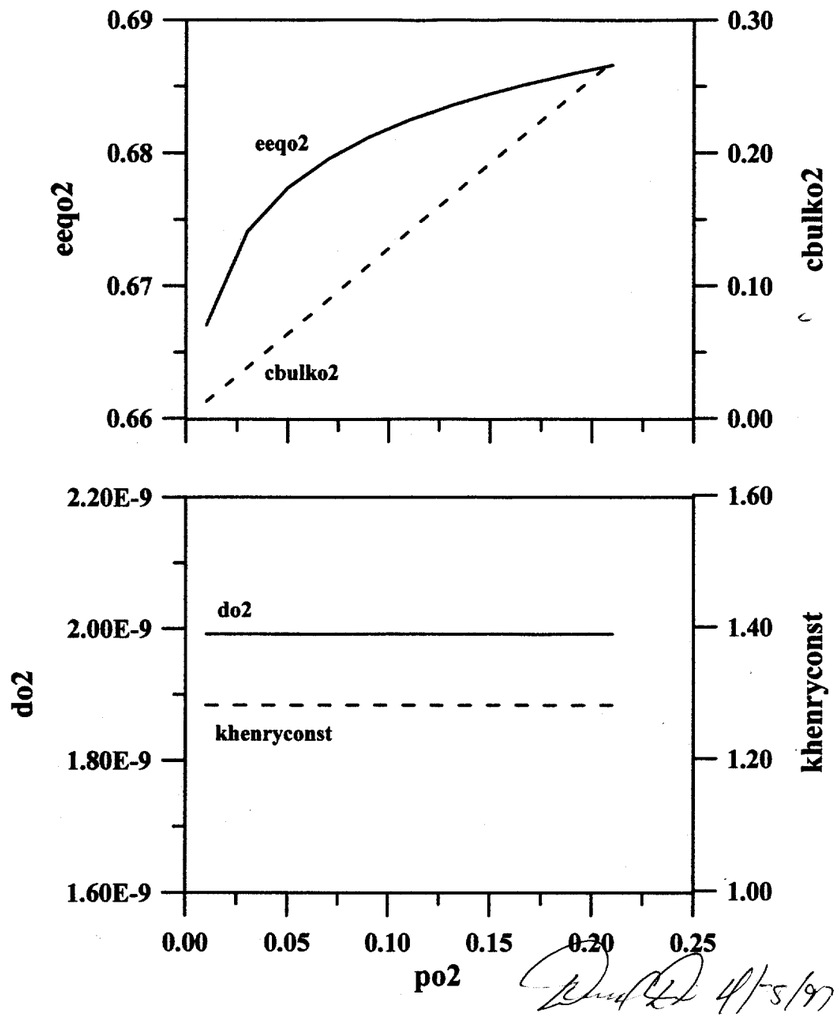

```
cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," ",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[po2]," ",FortranForm[ph]],{po2,0.01,0.21,0.02}]
```

4/25/97

4/25/97



4/25/97

CALCULATED W O2H2ORX2.MA
DATA FILE O2H2ORX2.MA/WLS
GRAPH FILE O2H2ORX2.GRF
4/28/97

COROXRD2.MA

OBJECTIVE. CALCULATE CURRENT DENSITY FOR REDUCTION REACTIONS AND DISSOLUTION REACTIONS AS A FUNCTION OF POTENTIAL

PARAMETERS AND INPUT SAME AS COROXRD1.MA

CHANGES FROM COROXRD1.MA THE EQULIBRIUM POTENTIAL FOR THE REDUCTION OF OXYGEN IS NOW CALCULATED ~~CORRECTLY~~ 4/25/97 USING THE CORRECT EQUATION.

COROXRD2.MA ON PAGES 52-55

4/25/97

Metal oxidation, Oxy Hyd reduction
Darrell S. Dunn

The corrosion rate of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 and carbon steel. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2).

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)

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o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecorr= corrosion potential of alloy 825 and carbon steel

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.50;
bh2o=0.5;
zfe=2;
ipass825=0.01;
ar825=1;
arsteel=1;
afe=0.2;
po2=0.21;
tempk=373;
ph=7;
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.000000003;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.0
```


4/25/97

4/25/97

```
delta=0.0001;

Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]

Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","h2oactenergy","
","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","ferrousconc"," ","eferrous"," ","i0ferrous","
","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel"," ","i0h2osteelat298k"," ","i0h2osteel","
","isteel"," ","ih2osteel"," ","io2steel"," ","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825","
","i0o2825at298k"," ","i0o2825"," ","ipass825"," ","ih2o825"," ","io2825"," ","Ecorr","
","delta"," ","tempk=",tempk," ","pH=",ph," ","galvaniccoeff=",galvaniccoeff,"
","coroxrd1.ma"," ","po2=",po2," ","Revised:4/23/97"," ","run:m/d/97"]

Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

hplusconc=10^-ph;

eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);

i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];
```

4/28/97

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```
i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;

i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

isteel=i0ferrous*(Exp[(afe zfe f (ecorr - eferrous))/(r tempk)]);

ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2steel=i0o2steel*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2],"
",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2],"
",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph],"
",FortranForm[hplusconc]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy],"
",FortranForm[bo2]," ",FortranForm[bh2o]," ",FortranForm[afe],"
",FortranForm[ferrousconc]," ",FortranForm[eferrous]," ",FortranForm[i0ferrous],"
",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k]," ",FortranForm[i0o2steel],"
",FortranForm[i0h2osteelat298k]," ",FortranForm[i0h2osteel]," ",FortranForm[isteel],"
",FortranForm[ih2osteel]," ",FortranForm[io2steel]," ",FortranForm[k1h2o825],"
",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825],"
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[ipass825],"
",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[ecorr]," ",
FortranForm[delta]],{ecorr,-1,1,0.05}]
```

4/25/97

4/28/97

CALCULATIONS WITH CORDXRD2.MA

OBJECTIVE CALCULATE THE CURRENT DENSITY FOR THE REDUCTION OF O_2 N_2O AND THE DISSOLUTION OF 825 AND CARBON STEEL

PARAMETERS:

TEMPERATURE VARIES FROM 273 TO 373 K

pH VARIED FROM 1 TO 13

O_2 OVERPOTENTIAL : 0.0 TO 1.0 VOLTS

DELTA : 0.0001 TO 0.005 m

b_{O_2} 0.250 TO 0.750

$i_{o\,Fe/Fe^{2+}}$ 10^{-8} TO 10^{-1} A/m^2

a_{Fe} 0.2 TO 0.5

pO_2 - 0.01 TO 0.21

E_{corr} VARIED FROM -1.5 V TO +1.5 V

RUNFILES	TEMP
COXRD043.MA	273 K
COXRD044.MA	298 K
COXRD045.MA	323 K
COXRD046.MA	353 K
COXRD047.MA	373 K

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RUNFILES	VARIABLE	VALUE
COXRD048.MA	pH	1
COXRD049.MA	pH	3
COXRD050.MA	pH	5
COXRD051.MA	pH	7
COXRD052.MA	pH	9
COXRD053.MA	pH	11
COXRD054.MA	pH	13

~~COXRD054.MA pH=9 T=273~~ 5/20/87

FILE	pH	T
COXRD055.MA	9	273
COXRD056.MA	9	298
COXRD057.MA	9	323
COXRD058.MA	9	353
COXRD059.MA	9	373

			O_2 OVERPOTENTIAL
COXRD060.MA	9	373	0.0
COXRD061.MA	9	373	0.2
COXRD062.MA	9	373	0.4
COXRD063.MA	9	373	0.6
COXRD064.MA	9	373	0.8
COXRD065.MA	9	373	1.0

FILE	pH	T	O_2 OP.	δ
COXRD066.MA	9	373	0.0	0.0001
COXRD067.MA	9	373	0.0	0.0005
COXRD068.MA	9	373	0.0	0.001
COXRD069.MA	9	373	0.0	0.002
COXRD070.MA	9	373	0.0	0.005

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FILE	pH	T	O_2 OP	δ	bO_2
COXRD071.MA	9	373	0.0	0.0001	0.250
COXRD072.MA	9	373	0.0	0.0001	0.500
COXRD073	9	373	0.0	0.0001	0.750

FILE	pH	T	O_2 OP	δ	bO_2	$i_{Fe/Fe^{2+}}$
COXRD074	9	373	0.0	0.0001	0.250	10^{-8}
COXRD075	9	373	0.0	0.0001	0.250	10^{-7}
COXRD076	9	373	0.0	0.0001	0.250	10^{-6}
COXRD077	9	373	0.0	0.0001	0.250	10^{-5}
COXRD078	9	373	0.0	0.0001	0.250	10^{-4}
COXRD079	9	373	0.0	0.0001	0.250	10^{-3}
COXRD080	9	373	0.0	0.0001	0.250	10^{-2}
COXRD081	9	373	0.0	0.0001	0.250	10^{-1}

DD 5/20/97

FILE	pH	T	O_2 OP	δ	bO_2	$i_{Fe/Fe^{2+}}$	α_{Fe}	pO_2
~~COXRD081~~								
COXRD082	"	"	"	"	"	"	0.2	0.21
COXRD083	"	"	"	"	"	"	0.3	0.21
COXRD084	"	"	"	"	"	"	0.4	0.21
COXRD085	"	"	"	"	"	"	0.5	0.21
COXRD086	"	"	"	"	"	"	0.2	0.21
COXRD087	"	"	"	"	"	"	0.2	0.15
COXRD088	"	"	"	"	"	"	0.2	0.10
COXRD089	"	"	"	"	"	"	0.2	0.05
COXRD090	"	"	"	"	"	"	0.2	0.01

5/20/97

CALCULATIONS WITH CORDXRD2.MA

OBJECTIVE CALCULATE CORROSION POTENTIAL OF STEEL AND ALLOYS

REFERENCE DATA BY HACK & SCULLY WHERE GALVANIC CORROSION OF ALLOY 625 & CARBON STEEL IN SEAWATER MEASURED TO BE -0.46 VSHE

DD 5/23/97

$$b_a = \cancel{\alpha_{Fe}} = \frac{2.303\,RT}{\beta n F} = \frac{2.303\,RT}{\alpha_{Fe} n F}$$

FOR $Fe \rightarrow Fe_{2+} + 2e^-$ $n = 2$

$$\alpha_{Fe} = \frac{2.303\,RT}{b_a\, 2F}$$

$$\frac{2.303\,RT}{F} = 0.059\,V \text{ AT } 298\,K$$

$$\alpha_{Fe} = \frac{0.059}{b_a(2)} \qquad b_a = 40 \text{ TO } 80\ mV/\text{DECADE}$$

DD 5/23/97

$$\cancel{\alpha_{Fe} = \frac{0.059}{(40)}} \qquad \alpha_{Fe} = \frac{0.059}{(0.040)2} = 0.750$$

$$\alpha_{Fe} = \frac{0.059}{(0.080)2} = 0.375$$

$$\alpha_{Fe} = 0.375 \text{ TO } 0.750$$

5/23/97

CALCULATIONS WITH COROXRD2.MA

FOR O_2 REDUCTION RX

$$O_2 + 2H_2O + 4e^- = 4OH^-$$

$$b_c = \frac{2.303\,RT}{B_{O_2}\,nF} \qquad n=4 \qquad \frac{2.303\,RT}{F} = 0.059 \text{ AT } 298K$$

$$b_c = \frac{0.059}{B_{O_2}(4)}$$

$$B_{O_2} = \frac{0.059}{b_c(4)}$$ FOR O_2 REDUCTION TAFEL SLOPE = 120 mV DECADE

$B_{O_2} = 0.125$

FOR $2H^+ + 2e^- \rightarrow H_2$

$$b_c = \frac{2.303\,RT}{B_{H_2}\,nF}$$

$$B_{H_2} = \frac{0.059}{b_{H_2}(2)}$$ FOR HYDROGEN REDUCTION b_{H_2} = 120 mV DECADE

$$B_{H_2} = \frac{0.059}{(0.120)(2)} = 0.250$$

i_0 Fe/Fe^{2+} GIVEN BY BOCKRIS ET AL 1961 ELECTROCHIM ACTA VOL 4 P 325 TO 361

= 0.1 TO 0.0001 A/m²

δ = 0.05 cm STAGNANT 0.005 cm FLOWING
BOCKRIS & REDDY MODERN ELECTROCHEM P 1058

5/23/97

RUN	α_{Fe}	$i_{0\,Fe/Fe^{2+}}$	TEMP	pH	O_2 OP	δ	pO_2	B_{O_2}
								5/23/97
~~COXRD091~~	~~10^{-4}~~							
COXRD091	0.75	10^{-4}	298	7	0	0.0005	0.21	0.125
COXRD092	0.75	10^{-4}	298	7	0	0.0001	0.21	
COXRD093	0.75	10^{-4}	298	7	0	0.001	0.21	
COXRD094	0.75	10^{-4}	298	7	0	0.005	0.21	
COXRD095	0.375	10^{-4}	298	7	0	0.0005	0.21	
COXRD096	0.500	10^{-4}	298	7	0	0.0005	0.21	
COXRD097	0.750	10^{-3}	298	7	0	0.0005	0.21	
COXRD098	0.750	10^{-2}	298	7	0	0.0005	0.21	
COXRD099	0.750	10^{-1}	298	7	0	0.0005	0.21	
COXRD100	0.750	10^{-4}	273	7	0	0.0005	0.21	
COXRD101	0.750	10^{-4}	373	7	0	0.0005	0.21	
COXRD102	0.750	10^{-4}	298	1	0	0.0005	0.21	
COXRD103	0.750	10^{-4}	298	3	0	0.0005	0.21	
COXRD104	0.750	10^{-4}	298	5	0	0.0005	0.21	
COXRD105	0.750	10^{-4}	298	7	0	0.0005	0.21	
COXRD106	0.750	10^{-4}	298	9	0	0.0005	0.21	
COXRD107	0.750	10^{-4}	298	11	0	0.0005	0.21	
COXRD108	0.750	10^{-4}	298	13	0	0.0005	0.21	
COXRD109	0.750	10^{-4}	298	7	0.2	0.0005	0.21	
COXRD110	0.750	10^{-4}	298	7	0.4	0.0005	0.21	
COXRD111	0.750	10^{-4}	298	7	0.6	0.0005	0.21	
COXRD112	0.750	10^{-4}	298	7	0.8	0.0005	0.21	
COXRD113	0.750	10^{-4}	298	7	1.0	0.0005	0.21	
COXRD114	0.750	10^{-4}	298	7	0.0	0.0005	0.15	
COXRD115	0.750	10^{-4}	298	7	0.0	0.0005	0.10	
COXRD116	0.750	10^{-4}	298	7	0.0	0.0005	0.05	
COXRD117	0.750	10^{-4}	298	7	0.0	0.0005	0.01	
COXRD118	0.750	10^{-4}	298	7	0.0	0.0005	0.001	

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RUN	α_{Fe}	$i_{o\,Fe/Fe^{2+}}$	TEMP	pH	O_2 OP	δ	pO_2	bO_2
COXRD1A	0.75	10^{-4}	298	7	0.0	0.0005	0.21	0.25
COXRD10	0.75	10^{-4}	298	7	0.0	0.0001	0.21	0.25
COXRD121	0.75	10^{-4}	298	7	0.0	0.001	0.21	0.25
COXRD122	0.75	10^{-4}	298	7	0.0	0.005	0.21	0.25
COXRD123	0.375	10^{-4}	298	7	0.0	0.0005	0.21	0.25
COXRD124	0.500	10^{-4}	298	7	0.0	0.0005	0.21	0.25
COXRD125	0.750	10^{-3}	298	7	0.0	0.0005	0.21	0.25
COXRD126	0.750	10^{-2}	298	7	0.0	0.0005	0.21	0.25
COXRD127	0.750	10^{-1}	298	7	0.0	0.0005	0.21	0.25
COXRD128	0.750	10^{-4}	273	7	0.0	0.0005	0.21	0.25
COXRD129	0.750	10^{-4}	373	7	0.0	0.0005	0.21	0.25
COXRD130	0.750	10^{-4}	298	1	0.0	0.0005	0.21	0.25
COXRD131	0.750	10^{-4}	298	3	0.0	0.0005	0.21	0.25
COXRD132	0.750	10^{-4}	298	5	0.0	0.0005	0.21	0.25
COXRD133	0.750	10^{-4}	298	7	0.0	0.0005	0.21	0.25
COXRD134	0.750	10^{-4}	298	9	0.0	0.0005	0.21	0.25
COXRD135	0.750	10^{-4}	298	11	0.0	0.0005	0.21	0.25
COXRD136	0.750	10^{-4}	298	13	0.0	0.0005	0.21	0.25
COXRD137	0.750	10^{-4}	298	7	0.2	0.0005	0.21	0.25
COXRD138	0.750	10^{-4}	298	7	0.4	0.0005	0.21	0.25
COXRD139	0.750	10^{-4}	298	7	0.6	0.0005	0.21	0.25
COXRD140	0.750	10^{-4}	298	7	0.8	0.0005	0.21	0.25
COXRD141	0.750	10^{-4}	298	7	1.0	0.0005	0.21	0.25
COXRD142	0.750	10^{-4}	298	7	0.0	0.0005	0.15	0.25
COXRD143	0.750	10^{-4}	298	7	0.0	0.0005	0.10	0.25
COXRD144	0.750	10^{-4}	298	7	0.0	0.0005	0.05	0.25
COXRD145	0.750	10^{-4}	298	7	0.0	0.0005	0.01	0.25
COXRD146	0.750	10^{-4}	298	7	0.0	0.0005	0.001	0.25
COXRD147*	0.750	10^{-4}	298	7	0.0	0.0005	0.0010	0.25
COXRD148*	0.750	10^{-4}	298	7	0.0	0.0005	0.0001	0.25
COXRD149*	0.750	10^{-4}	298	7	0.0	0.0005	0.01	0.25
COXRD150*	0.750	10^{-4}	298	7	0.0	0.0005	0.21	0.25

COXRD147 - COXRD150 $i_{pass\,825} = 0.001\ A/m^2$

5/27/97

CALCULATIONS WITH GALVAN06.MD

INITIAL CALCULATIONS RUN TO OBTAIN GALVANIC CORROSION POTENTIAL OF ALLOY 825 AND A 516 CARBON STEEL COUPLE

PARAMETERS:

$\alpha_{Fe} = 0.750$

O_2 OVER POTENTIAL $= 0.0$

$bO_2 = 0.250$

$bN_2 = 0.250$

RUN	TEMP	A_{825}	A_{516}	pH	$i_{o\,Fe/Fe^{2+}}$	$i_{pass\,825}$	δ
GV06R001	298	1	1	7	10^{-4}	10^{-2}	0.0005
GV06R002	273	1	1	7	10^{-4}	10^{-2}	0.0005
GV06R003	353	1	1	7	10^{-4}	10^{-2}	0.0005
GV06R004	373	1	1	7	10^{-4}	10^{-2}	0.0005
GV06R005	298	10	1	7	10^{-4}	10^{-2}	0.0005
GV06R006	298	1	10	7	10^{-4}	10^{-2}	0.0005
GV06R007	298	1	1	1	10^{-4}	10^{-2}	0.0005
GV06R008	298	1	1	3	10^{-4}	10^{-2}	0.0005
GV06R009	298	1	1	5	10^{-4}	10^{-2}	0.0005
GV06R010	298	1	1	7	10^{-4}	10^{-2}	0.0005
GV06R011	298	1	1	9	10^{-4}	10^{-2}	0.0005
GV06R012	298	1	1	11	10^{-4}	10^{-2}	0.0005
GV06R013	298	1	1	13	10^{-4}	10^{-2}	0.0005
GV06R014	298	1	1	7	10^{-1}	10^{-2}	0.0005
GV06R015	298	1	1	7	10^{-2}	10^{-2}	0.0005
GV06R016	298	1	1	7	10^{-3}	10^{-2}	0.0005
GV06R017	298	1	1	7	10^{-4}	10^{-5}	0.0005
GV06R018	298	1	1	7	10^{-4}	10^{-4}	0.0005
GV06R019	298	1	1	7	10^{-4}	10^{-3}	0.0005
GV06R020	298	1	1	7	10^{-4}	10^{-1}	0.0005
GV06R021	298	1	1	7	10^{-4}	10^{-2}	0.0001
GV06R022	298	1	1	7	10^{-4}	10^{-2}	0.001
GV06R023	298	1	1	7	10^{-4}	10^{-2}	0.005

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CALCULATIONS WITH GALVAN06

CALCULATIONS PERFORMED FOR η = 0 TO 1 IN 0.05 INCREMENTS δ VALUES WERE AS SHOWN IN TABLE ON ~~p63 Fa~~ DD 5/21/97 p63 FOR EACH RUN

ADDITIONAL CALCULATIONS PERFORMED WITH SAME PARAMETERS AS GV06001 WITH pO_2 VARIED FROM 0.21 TO 0.001

FILE	pO_2
~~GV0600~~ DD 5/27/97	
GV06R024	0.21
GV06R025	0.10
GV06R026	0.01
GV06R027	0.001

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GALVAN06.MA / GALVAN6a.MA

OBJECTIVE SAME AS GALVAN01.MA

PARAMETERS AND INPUT SAME AS GALVAN5a.MA p28

CHANGES FROM GALVAN5a.MA

RESISTANCE OF MGAIA BETWEEN ALLOY 825 AND CARBON STEEL ARE CALCULATED BY TAKING THE POTENTIAL DIFFERENCE BETWEEN 825 AND CARBON STEEL DIVIDED BY THE CATHODIC CURRENT DENSITY SUM AS SHOWN BELOW

$$\text{RESISTANCE} = \left| \frac{E^{wp}_{825} - E^{wp}_{STEEL}}{\Sigma i_c} \right|$$

RESISTANCE HAS UNITS OF $\Omega m \cdot m^2$

RESISTANCE / LENGTH = RESISTIVITY $\Omega m \cdot m$ WHICH CAN THEN BE COMPARED TO EITHER IMPEDANCE DATA OR SOLUTION CONDUCTIVITY DATA.

5/27/97

GALVANIC CORROSION
Darrell S. Dunn

The galvanic corrosion of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 only. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2). The coefficient of galvanic galvanic coupling is included.

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
isteelwp=corrosion current density for carbon steel waste package (calculated)
arsteel=area of steel (input)
ecorrsteel=corrosion potential for steel (calculated)
ecorrsteelwp=corrosion potential of the carbon steel waste package (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
ih2osteelwp=current density from water reduction on carbon steel waste package (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
io2steelwp=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
io2825wp=current density oxygen reduction on alloy 825 waste package (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
ih2o825wp=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)

ecorr825=corrosion potential of alloy 825 not in contact with other metals(calculated)
e825wp=corrosion potential of alloy 825 waste package barrier with or without galvanic contact(calculated)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecouple=potential of perfect galvanic couple of alloy 825and carbon steel (calculated)
galvaniccoeff=coefficient of galvainc coupling, 1=complete coupling, 0=complete insulation(input)
currentsum=sum of currents

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.125;
bh2o=0.250;
zfe=2;
ipass825=0.01;
ar825=1;
arsteel=1;
afe=0.75;
po2=0.21;
tempk=298;
```

```
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.1;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.0;
galvaniccoeff=0.6;


Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]


Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","h2oactenergy","
","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","arsteel"," ","ar825"," ","ferrousconc","
","eferrous"," ","i0ferrous"," ","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel","
","i0h2osteelat298k"," ","i0h2osteel"," ","isteel"," ","ih2osteel"," ","io2steel","
","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825"," ","i0o2825at298k"," ","i0o2825","
","ipass825"," ","ih2o825"," ","io2825"," ","isteelwp"," ","ih2osteelwp"," ","io2steelwp","
","ih2o825wp"," ","io2825wp"," ","arsteel*isteelwp"," ","arsteel*ih2osteelwp","
","arsteel*io2steelwp"," ","ar825*ipass825"," ","ar825*ih2o825wp"," ","ar825*io2825wp","
","currentsum"," ","cathcurrsum"," ","potentialdrop"," ","resistance"," ","ecorrsteel","
","Ecouple"," ","Ecorr825"," ","Ecorrsteelwp"," ","E825wastepackage"," ","delta","
","tempk=",tempk," ","pH=",ph," ","ar825=",ar825," ","arsteel=",arsteel,"
","galvaniccoeff=",galvaniccoeff," ","galvan06.ma"," ","po2=",po2,"
","5/23/97Revised:m/d/97"," ","run:5/23/97"]


Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);


eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);


eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));


khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;
```

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```
cbulko2=khenryconst*po2;


do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;


hplusconc=10^-ph;


eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);


i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];


i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;


i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];


i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];


i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;


i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];


corrsteel=ecorrsteel /. FindRoot[i0ferrous*(Exp[(afe zfe f (ecorrsteel - eferrous))/(r
tempk)])-(i0h2osteel*(Exp[-(bh2o zh2o f (ecorrsteel - eeqh2o))/(r
tempk)])+i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteel - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteel - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorrsteel,0}, MaxIterations->100];


isteel=i0ferrous*(Exp[(afe zfe f (corrsteel - eferrous))/(r tempk)]);


ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (corrsteel - eeqh2o))/(r tempk)]);


io2steel=i0o2steel*((Exp[-(bo2 zo2 f (corrsteel - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteel - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));
```

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```
corr825=ecorr825 /. FindRoot[ipass825-(i0h2o825*(Exp[-(bh2o zh2o f (ecorr825 -
eeqh2o))/(r tempk)])+i0o2825*((Exp[-(bo2 zo2 f (ecorr825 - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorr825,0}, MaxIterations->100];


ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (corr825 - eeqh2o))/(r tempk)]);


io2825=i0o2825*((Exp[-(bo2 zo2 f (corr825 - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (corr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));


couple=ecouple /. FindRoot[arsteel*i0ferrous*(Exp[(afe zfe f (ecouple - eferrous))/(r
tempk)]) + ipass825*ar825-((arsteel*i0h2osteel*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+arsteel*i0o2steel*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f
do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (ecouple - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0,
{ecouple,0}, MaxIterations->100];


e825wp=((1-galvaniccoeff)*corr825) + galvaniccoeff*couple;


corrsteelwp=ecorrsteelwp /. FindRoot[arsteel*i0ferrous*(Exp[(afe zfe f (ecorrsteelwp -
eferrous))/(r tempk)]) + ipass825*ar825-((arsteel*i0h2osteel*(Exp[-(bh2o zh2o f
(ecorrsteelwp - eeqh2o))/(r tempk)])+arsteel*i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteelwp -
eeqo2))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteelwp - eeqo2))/(r
tempk)])/(cbulko2 4 f do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0,
{ecorrsteelwp,0}, MaxIterations->100];


isteelwp=i0ferrous*(Exp[(afe zfe f (corrsteelwp - eferrous))/(r tempk)]);


ih2osteelwp=i0h2osteel*(Exp[-(bh2o zh2o f (corrsteelwp - eeqh2o))/(r tempk)]);


io2steelwp=i0o2steel*((Exp[-(bo2 zo2 f (corrsteelwp - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteelwp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));
```

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```
ih2o825wp=i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)]);


io2825wp=i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));


currentsum=arsteel*isteelwp+ar825*ipass825-ar825*ih2o825wp-ar825*io2825wp-arsteel*ih


cathcurrsum=ar825*ih2o825wp-ar825*io2825wp-arsteel*ih2osteelwp-arsteel*io2steelwp;


potentialdrop=e825wp-corrsteelwp;


resistance=Abs[potentialdrop/cathcurrsum];


Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2],"
",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2],"
",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph],"
",FortranForm[hplusconc]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy],"
",FortranForm[bo2]," ",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[arsteel],"
",FortranForm[ar825]," ",FortranForm[ferrousconc]," ",FortranForm[eferrous],"
",FortranForm[i0ferrous]," ",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k],"
",FortranForm[i0o2steel]," ",FortranForm[i0h2osteelat298k]," ",FortranForm[i0h2osteel],"
",FortranForm[isteel]," ",FortranForm[ih2osteel]," ",FortranForm[io2steel],"
",FortranForm[k1h2o825]," ",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825],"
",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[ipass825],"
",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[isteelwp],"
",FortranForm[ih2osteelwp]," ",FortranForm[io2steelwp]," ",FortranForm[ih2o825wp],"
",FortranForm[io2825wp]," ",FortranForm[arsteel*isteelwp],"
",FortranForm[arsteel*ih2osteelwp]," ",FortranForm[arsteel*io2steelwp],"
",FortranForm[ar825*ipass825]," ",FortranForm[ar825*ih2o825wp],"
",FortranForm[ar825*io2825wp]," ",FortranForm[currentsum],"
",FortranForm[cathcurrsum]," ",FortranForm[potentialdrop]," ",FortranForm[resistance],"
",FortranForm[corrsteel]," ",FortranForm[couple]," ",FortranForm[corr825],"
",FortranForm[corrsteelwp]," ",FortranForm[e825wp],"
",FortranForm[delta]],{delta,0.0001,0.001,0.0001}]
```

5/26/97

GALVANGA. CALCULATIONS

CALCULATION OF GALVANIC CORROSION POTENTIAL USING SAMG ~~EXCHANGE~~ DD 5/29/97
i_{pass} 825 AS IN EBSPAL 10^{-3} A/m²

RUN	TEMP	A_{825}	A_{516}	pH	$i_0 Fe/Fe^{2+}$	δ	pO_2	O_2 OP
GV06R028	298	1	1	7	10^{-4}	0.0005	0.21	0.0
GV06R029	273	1	1	7	10^{-4}	0.0005	0.21	0.0
GV06R030	373	1	1	7	10^{-4}	0.0005	0.21	0.0
GV06R031	298	10	1	7	10^{-4}	0.0005	0.21	0.0
GV06R032	298	1	10	7	10^{-4}	0.0005	0.21	0.0
GV06R033	298	1	1	1	10^{-4}	0.0005	0.21	0.0
GV06R034	298	1	1	3	10^{-4}	0.0005	0.21	0.0
GV06R035	298	1	1	5	10^{-4}	0.0005	0.21	0.0
GV06R036	298	1	1	9	10^{-4}	0.0005	0.21	0.0
GV06R037	298	1	1	11	10^{-4}	0.0005	0.21	0.0
GV06R038	298	1	1	13	10^{-4}	0.0005	0.21	0.0
GV06R039	298	1	1	7	10^{-1}	0.0005	0.21	0.0
GV06R040	298	1	1	7	10^{-4}	0.0001	0.21	0.0
GV06R041	298	1	1	7	10^{-4}	0.001	0.21	0.0
GV06R042	298	1	1	7	10^{-4}	0.005	0.21	0.0
GV06R043	298	1	1	7	10^{-4}	0.0005	0.10	0.0
GV06R044	298	1	1	7	10^{-4}	0.0005	0.01	0.0
GV06R045	298	1	1	7	10^{-4}	0.0005	0.002	0.0
GV06R046	298	1	1	7	10^{-4}	0.0005	0.21	0.2
GV06R047	298	1	1	7	10^{-4}	0.0005	0.21	0.4
GV06R048	298	1	1	7	10^{-4}	0.0005	0.21	0.6
GV06R049	298	1	1	7	10^{-4}	0.0005	0.21	0.8
GV06R050	298	1	1	7	10^{-4}	0.0005	0.21	1.0
GV06R051	298	1	1	7	10^{-4}	0.0005	0.0001	0.0
GV06R052*								
GV06R053*								
GV06R054	298	1	1	7	10^{-4}	0.0005	0.001	0.0

* RUN ABORTED

5/29/97

NOTE ON CALCULATIONS

UNABLE TO OBTAIN SOLUTION WHEN $pO_2 = 0.001$

SOLUTION WAS OBTAINED FOR $pO_2 = 0.002$ AND $pO_2 = 0.0001$

ADDITIONAL RUNS

$A_{825} = 1$ $A_{516} = 1$ pH = 7 $i_0 Fe/Fe^{2+}$ 0.0001
$\delta = 0.0005$ ~~$pO_2 = 0.21$~~ O_2 OP = 0.0
DD 5/29/97

	pO_2
GV06R055	0.0005
GV06R056	0.0008
GV06R057	0.0007
GV06R058	0.0006
GV06R059	0.00055
GV06R060	0.00052
GV06R061	0.000505
GV06R062	0.00051
GV06R063	0.000507
GV06R064	0.000508
GV06R065	0.000509
GV06R066	0.0005085
GV06R067	0.0005083
GV06R068	0.00050825

5/29/97

GALVANIC GA CALCULATIONS

ADDITIONAL CALCULATIONS PERFORMED AT ~~373K~~ 5/30/97 368K (95°C) WITH GALVANIC GA.

RUN	A_{825}	A_{516}	pH	$i_{pass\,825}$	$i_0 Fe/Fe^{2+}$	δ	pO_2	O_2 OP
GV06R069	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R070	10	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R071	0.1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R072	1	1	1	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R073	1	1	3	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R074	1	1	5	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R075	1	1	9	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R076	1	1	11	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R077	1	1	13	10^{-3}	10^{-4}	0.0005	0.21	0.0
GV06R078	1	1	7	10^{-5}	10^{-4}	0.0005	0.21	0.0
GV06R079	1	1	7	10^{-4}	10^{-4}	0.0005	0.21	0.0
GV06R080	1	1	7	10^{-2}	10^{-4}	0.0005	0.21	0.0
GV06R081	1	1	7	10^{-1}	10^{-4}	0.0005	0.21	0.0
GV06R082	1	1	7	10^{-3}	10^{-1}	0.0005	0.21	0.0
GV06R083	1	1	7	10^{-3}	10^{-2}	0.0005	0.21	0.0
GV06R084	1	1	7	10^{-3}	10^{-3}	0.0005	0.21	0.0
GV06R085	1	1	7	10^{-3}	10^{-5}	0.0005	0.21	0.0
GV06R086	1	1	7	10^{-3}	10^{-4}	0.0001	0.21	0.0
GV06R087	1	1	7	10^{-3}	10^{-4}	0.001	0.21	0.0
GV06R088	1	1	7	10^{-3}	10^{-4}	0.005	0.21	0.0
GV06R089	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.2
GV06R090	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.4
GV06R091	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.6
GV06R092	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	0.8
GV06R093	1	1	7	10^{-3}	10^{-4}	0.0005	0.21	1.0
GV06R094	1	1	7	10^{-3}	10^{-4}	0.0005	0.10	0.0
GV06R095	1	1	7	10^{-3}	10^{-4}	0.0005	0.01	0.0
GV06R096	1	1	7	10^{-3}	10^{-4}	0.0005	0.001	0.0
GV06R097	1	1	7	10^{-3}	10^{-4}	0.0005	0.0001	0.0

5/30/97

RUN	A_{825}	A_{516}	pH	$i_{pass\,825}$	$i_0 Fe/Fe^{2+}$	δ	pO_2	O_2 OP
GV06R098	1	1	7	0.001	10^{-4}	0.0005	0.0004	0.0
GV06R099	1	1	7	0.001	10^{-4}	0.0005	0.0003	0.0
GV06R100	1	1	7	0.001	10^{-4}	0.0005	0.0002	0.0
GV06R101	1	1	7	0.001	10^{-4}	0.0005	0.00021	0.0
GV06R102	1	1	7	0.001	10^{-4}	0.0005	0.00023	0.0
GV06R103	1	1	7	0.001	10^{-4}	0.0005	0.00026	0.0
GV06R104	1	1	7	0.001	10^{-4}	0.0005	0.00028	0.0
GV06R105	1	1	7	0.001	10^{-4}	0.0005	0.00027	0.0
GV06R106	1	1	7	0.001	10^{-4}	0.0005	2.75×10^{-4}	0.0
GV06R107	1	1	7	0.001	10^{-4}	0.0005	2.73×10^{-4}	0.0
GV06R108	1	1	7	0.001	10^{-4}	0.0005	2.72×10^{-4}	0.0
GV06R109	1	1	7	0.001	10^{-4}	0.0005	2.725×10^{-4}	0.0
GV06R110	1	1	7	0.001	10^{-4}	0.0005	2.723×10^{-4}	0.0
GV06R111	1	1	7	0.001	10^{-4}	0.0005	2.722×10^{-4}	0.0

5/30/97

CALCULATIONS W/ ~~COROXRD2.MA~~ COROXRD3.MA DD 6/21/97

~~RUN T pH A825 A516~~ DD 6/21/97

PURPOSE OF COROXRD3.MA
AND EFFECT OF AREA

CHANGES FROM COROXRD2.MA

CURRENT SUMMATION AND CATHODIC CURRENT SUMMATION

ANODIC AND CATHODIC CURRENTS CALCULATED BY MULTIPLYING O_2 AND H_2O REDUCTION BY AREA, AND PASSIVE CURRENT DENSITY OF ALLOY 825 X AREA AND DISSOLUTION OF CARBON STEEL X AREA

DD 6/21/97

RUN	T	pH	A_{825}	A_{516}	pO_2	pH	i_{pass} 825	DELTA
COXRD151	298							0.0005
COXRD152	298							0.0005
COXRD153	298	5	1	1	0.21	5	0.001	0.0005
COXRD154	298	5	10	1	0.21	5	0.001	0.0005
COXRD155	298	5	1	10	0.21	5	0.001	0.0005
COXRD156	273	5	1	1	0.21	5	0.001	0.0005
COXRD157	368	5	1	1	0.21	5	0.001	0.0005
COXRD158	368	5	10	1	0.21	5	0.001	0.0005
COXRD159	368	5	1	10	0.21	5	0.001	~~0.005~~ DD 6/21/97 0.0005
COXRD160	368	3	1	1	0.21	5	0.001	0.0005
COXRD161	368	7	1	1	0.21	5	0.001	0.0005
COXRD162	368	11	1	1	0.21	5	0.001	0.0005
COXRD163	368	5	1	1	0.21	5	0.001	0.0001
COXRD164	368	5	1	1	0.21	5	0.001	0.005
COXRD165	368	5	1	1	0.21	5	0.1	0.0005
COXRD166	368	5	1	1	0.21	5	0.00001	0.0005
COXRD167	368	5	1	1	0.00021	5	0.001	0.0005
COXRD175	368	5	1	1	0.000021	5	0.001	0.0005

DD 6/21/97

THE FOLLOWING RUNS DONE WITH

$T = 368\,K$ $A_{SiO_2} = 1$ $p_{O_2} = 0.21$ $\delta = 0.0005$

p_{N_2} 5 $A_{BaO} = 1$ $i_{pass\ BaO} = 0.001$

RUN	$i_{o\,Fe/Fe^{2+}}$	α_{Fe}	β_{O_2}	$i_{o\,O_2}$ (STEGL, 825) AT 298 K
COXRD168	0.1	0.750	0.250	10^{-6}
COXRD169	0.00001	0.750	0.250	10^{-6}
COXRD170	0.0001	0.375	0.250	10^{-6}
COXRD171	0.0001	0.750	0.125	10^{-6}
COXRD172	0.0001	0.750	0.500	10^{-6}
COXRD173	0.0001	0.750	0.250	10^{-5}
COXRD174	0.0001	0.750	0.250	10^{-8}

ALL RUNS COXRD151, MA – COXRD175

$i_{h2o\ 825\ amp}$ NOT CALCULATED CORRECTLY

Daniel D 6/22/97

ADDITIONAL CALCULATIONS W GALVANGM.MA

$\alpha_{Fe} = 0.750$ $\beta_{O_2} = 0.250$ O_2 OVERPOTENTIAL = 0

RUN	A_{BaO}	A_{SiO_2}	pH	$i_{pass\ BaO}$	$i_{o\,Fe/Fe^{2+}}$	δ	p_{O_2}	$i_{o\,O_2}$	T
GV06R112	1	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R113	10	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R114	1	10	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R115	1	1	3	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R116	1	1	7	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R117	1	1	11	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R118	1	1	5	0.1	0.0001	0.0005	0.21	10^{-6}	368
GV06R119	1	1	5	0.00001	0.0001	0.0005	0.21	10^{-6}	368
GV06R120	1	1	5	0.0001	0.0001	0.0005	0.21	10^{-6}	368
GV06R121	1	1	5	0.001	0.1	0.0005	0.21	10^{-6}	368
GV06R122	1	1	5	0.001	0.00001	0.0005	0.21	10^{-6}	368
GV06R123	1	1	5	0.001	0.0001	0.0001	0.21	10^{-6}	368
GV06R124	1	1	5	0.001	0.0001	0.005	0.21	10^{-6}	368
GV06R125	1	1	5	0.001	0.0001	0.0005	0.21	10^{-5}	368
GV06R126	1	1	5	0.001	0.0001	0.0005	0.21	10^{-8}	368
GV06R127	1	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	273
GV06R128	1	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	298
GV06R129	1	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	373
GV06R130	1	1	5	0.001	0.0001	0.0005	0.00021	10^{-6}	368
GV06R131	1	1	5	0.001	0.0001	0.0005	0.000021	10^{-6}	368
GV06R132	1	1	5	0.001	0.0001	0.0005	0.00026	10^{-6}	368
GV06R133	1	1	5	0.001	0.0001	0.0005	0.00027	10^{-6}	368
GV06R134	1	1	5	0.001	0.0001	0.0005	0.000275	10^{-6}	368
GV06R135	1	1	5	0.001	0.0001	0.0005	0.00028	10^{-6}	368
GV06R136	1	1	5	0.001	0.0001	0.0005	0.000272	10^{-6}	368
GV06R137	1	1	5	0.001	0.0001	0.0005	0.000271	10^{-6}	368
GV06R138	1	1	5	0.001	0.0001	0.0005	0.0002715	10^{-6}	368
GV06R139	1	1	5	0.0001	0.0001	0.0005	0.0002718	10^{-6}	368
GV06R140	1	1	5	0.001	0.0001	0.0005	0.0002719	10^{-6}	368
GV06R144	0.10	1	5	0.001	0.0001	0.0005	0.21	10^{-6}	368

Daniel D 6/22/97

ADDITIONAL CALCULATIONS W GALVANGA.MA

FOLLOWING CALCULATIONS DONE W/

$A_{825} = 1$ $A_{316} = 1$
$pH = 5$ i_{pass} 825 = 0.001
$i_0 Fe/Fe^{2+} = 0.0001$ $\delta = 0.0005$

$pO_2 = 0.21$ $i_{0O_2} = 10^{-6}$
$T = 368K$ O_2 OVERPOTENTIAL = 0

RUN	α_{Fe}	β_{O_2}
~~GALVAN~~ DL	6/22/97	
GV06R141	0.375	0.250
GV06R142	0.750	0.125
GV06R143	0.750	0.500

6/22/97

CORROXRD4.MA

OBJECTIVE FIX CALCULATION ERROR IN CORROXRD3.MA

ADD CATHODIC CURRENT SUM FOR STEEL AND ALLOY 825

RUNS W CORROXRD4.MA

RUN	T	pH	A_{825}	A_{316}	pO_2	i_{pass} 825	δ	i_{0O_2}	O_2 OVERPOT
COXRD176	368	5	1	1	0.21	0.001	0.0005	10^{-6}	
COXRD177	368	9	1	1	0.21	0.001	0.0005	10^{-6}	
COXRD178	368	9	1	1	0.00021	0.001	0.0005	10^{-6}	
COXRD179	368	9	1	1	0.0021	0.001	0.0005	10^{-6}	
COXRD180	368	9	1	1	0.0008	0.001	0.0005	10^{-6}	
COXRD181	368	9	1	1	0.0003	0.001	0.0005	10^{-6}	
COXRD182	368	9	1	1	0.0003	0.001	0.0005	10^{-6}	
COXRD183	368	9	1	1	0.00025	0.001	0.0005	10^{-6}	
COXRD184	368	9	1	1	0.00027	0.001	0.0005	10^{-6}	
COXRD185	368	9	1	1	0.000265	0.001	0.0005	10^{-6}	
COXRD186	368	9	1	1	0.00026	0.001	0.0005	10^{-6}	
COXRD187	368	5	1	1	0.21	0.001	0.0005	10^{-6}	0.2

7/16/97

ADDITIONAL CALCULATIONS W CALVANGA.MA

$\alpha_{Fe} = 0.750$ $\beta_{O_2} = 0.250$ O_2 OVERPOTENTIAL = 0

RUN	A_{825}	A_{316}	pH	$i_{pass\,825}$	$i_{0\,Fe/Fe^{2+}}$	δ	pO_2	i_{0,O_2}	T
GV06R145	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R146	7.85×10^{-3}	6.28×10^{-4}	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R147	7.85×10^{-5}	3.14×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R148	1×10^{-3}	1×10^{-3}	3	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R149	1×10^{-3}	1×10^{-3}	7	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R150	1×10^{-3}	1×10^{-3}	11	0.001	0.0001	0.0005	0.21	10^{-6}	368
GV06R151	1×10^{-3}	1×10^{-3}	5	0.1	0.0001	0.0005	0.21	10^{-6}	368
GV06R152	1×10^{-3}	1×10^{-3}	5	0.00001	0.0001	0.0005	0.21	10^{-6}	368
GV06R153	1×10^{-3}	1×10^{-3}	5	0.001	0.1	0.0005	0.21	10^{-6}	368
GV06R154	1×10^{-3}	1×10^{-3}	5	0.001	0.00001	0.0005	0.21	10^{-6}	368
GV06R155	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0001	0.21	10^{-6}	368
GV06R156	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.005	0.21	10^{-6}	368
GV06R157	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-5}	368
GV06R158	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-8}	368
GV06R159	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-6}	273
GV06R160	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-6}	298
GV06R161	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.21	10^{-6}	373
GV06R162	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.021	10^{-6}	368
GV06R163	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.0021	10^{-6}	368
GV06R164	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.00021	10^{-6}	368
GV06R165	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.000021	10^{-6}	368
GV06R166	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.00027	10^{-6}	368
GV06R167	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.000272	10^{-6}	368
GV06R168	1×10^{-3}	1×10^{-3}	5	0.001	0.0001	0.0005	0.0002719	10^{-6}	368

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CALCULATIONS W GALVANGA.MA

$A_{825} = 1\times10^{-3}\ m^2$
$A_{316} = 1\times10^{-3}\ m^2$
pH = 5
$i_{pass\,825} = 0.001$
$i_{0\,Fe/Fe^{2+}} = 0.0001$
$\delta = 0.0005$
$pO_2 = 0.21$
i_{0,O_2} 10^{-6}
T = 368K
O_2 OVERPOTENTIAL = 0

RUN	α_{Fe}	β_{O_2}
GV06R169	0.375	0.250
GV06R170	0.750	0.125
GV06R171	0.750	0.500

7/16/97

GV06R172

SAME CONDITIONS AS GV06R148

BUT T=298 K

2/15/98

ADDITIONAL CALCULATIONS W COROXRD4.MA

RUN	T	pH	APS	ASIL	pO_2	$i_{PAN\,PS}$	δ	i_{O_2}	$[Fe^{2+}]$
COXRD188	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-5}
COXRD189	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-4}
COXRD190	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-3}
COXRD191	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-7}
COXRD192	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-8}
COXRD193	368	5	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-9}
COXRD194	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-9}
COXRD195	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-8}
COXRD196	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-7}
COXRD197	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-6}
COXRD198	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-5}
COXRD199	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-4}
COXRD200	368	5	1	1	2.1×10^{-5}	10^{-3}	0.0005	10^{-6}	10^{-3}
COXRD201	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-3}
COXRD202	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-4}
COXRD203	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-5}
COXRD204	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-6}
COXRD205	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-7}
COXRD206	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-8}
COXRD207	368	3	1	1	0.21	10^{-3}	0.0005	10^{-6}	10^{-9}

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CALCULATIONS W GALVAN06

RUN	A_{825}	A_{S16}	pH	PO_2	$i_{pass\,825}$	δ	$i_{o\,O_2}$	T	$[Fe^{2+}]$
GV06R173	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	10^{-5}
GV06R174	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	10^{-4}
GV06R175	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	~~10^{-8}~~ DD 2/16/98 10^{-3}
GV06R176	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	10^{-7}
GV06R177	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	10^{-6}
GV06R178	1×10^{-3}	1×10^{-3}	3	0.21	~~0.0001~~ 0.001	0.0005	10^{-6}	368	10^{-6}
GV06R179	1×10^{-3}	1×10^{-3}	3	0.21	0.001	0.0005	10^{-6}	368	10^{-7}
GV06R180	1×10^{-3}	1×10^{-3}	3	0.21	0.001	0.0005	10^{-6}	368	10^{-5}
GV06R181	1×10^{-3}	1×10^{-3}	3	0.21	0.001	0.0005	10^{-6}	368	10^{-4}
GV06R182	1×10^{-3}	1×10^{-3}	3	0.21	0.001	0.0005	10^{-6}	368	10^{-3}
GV06R183	1×10^{-3}	1×10^{-3}	5	0.000021	0.001	0.0005	10^{-6}	368	10^{-3}
GV06R184	1×10^{-3}	1×10^{-3}	5	0.000021	0.001	0.0005	10^{-6}	368	10^{-4}
GV06R185	1×10^{-3}	1×10^{-3}	5	0.000021	0.001	0.0005	10^{-6}	368	10^{-5}
~~GV06R186~~	DD	2/16/98							
GV06R186	1×10^{-3}	1×10^{-3}	5	0.000021	~~0.0001~~ 0.001	0.0005	10^{-6}	368	10^{-6}
GV06R187	1×10^{-3}	1×10^{-3}	5	0.000021	0.001	0.0005	10^{-6}	368	10^{-7}
GV06R188	1×10^{-3}	1×10^{-3}	3	0.21	0.001	0.0005	10^{-6}	368	5×10^{-4}
GV06R189	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	5×10^{-4}
GV06R190	1×10^{-3}	1×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	298	5×10^{-4}
GV06R191	7.85×10^{-3}	6.28×10^{-4}	5	0.21	0.001	0.0005	10^{-6}	368	5×10^{-4}
GV06R192	7.85×10^{-3}	3.14×10^{-3}	5	0.21	0.001	0.0005	10^{-6}	368	5×10^{-4}
GV06R193	4×10^{-3}	1×10^{-3}	5	0.0002719	0.001	0.0005	10^{-6}	368	5×10^{-4}

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EXAMPLE CALCULATION

EXAMPLE CALCULATION, OUTPUT AND HAND CALCULATION CHECK OF COXRD160.

Coxrd160

Metal oxidation, Oxy Hyd reduction

Darrell S. Dunn

The corrosion rate of carbon steel and alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen on the surface of alloy 825 and carbon steel. The rate of oxygen reduction is assumed to diffusion limited. This calculation assumes that carbon steel is pure iron which is active and the dissolution rate is controlled by Tafel kinetics. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2).

PARAMETERS

carbon steel

isteel=corrosion current density for carbon steel (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
i0h2osteel=exchange current density water reduction on carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)
isteelamp=anodic current density times area of steel (calculated)
ih2osteelamp=cathodic current density for water reduction times area of steel (calculated)
io2steelamp=cathodic current density for oxygen reduction times area of steel (calculated)
arsteel=area of carbon steel

alloy 825

ipass825=passive current density of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)
ipass825amp=anodic current density times area of alloy 825 (calculated)
ih2o825amp=cathodic current density for water reduction times area of alloy 825 (calculated)
io2825amp=cathodic current density for oxygen reduction times area of alloy 825 (calculated)
ar825=area of alloy 825

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zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph (-log[H+]) (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecorr= corrosion potential of alloy 825 and carbon steel
currentsum=sum of all anodic and cathodic current
cathcurrsum=sum of all the cathodic current

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.250;
bh2o=0.250;
zfe=2;
ipass825=0.001;
ar825=1;
arsteel=1;
afe=0.750;
po2=0.21;
tempk=368;
ph=3;
o2actenergy=40;
```


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```
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.0001;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.0;
galvaniccoeff=1;
delta=0.0005;


Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1000]


Print["eeqh2o"," ","eeq0o2"," ","eeqo2"," ","o2overpotential"," ","khenryconst","
","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","h2oactenergy","
","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","ferrousconc"," ","eferrous"," ","i0ferrous","
","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel"," ","i0h2osteelat298k"," ","i0h2osteel","
","isteel"," ","ih2osteel"," ","io2steel"," ","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825","
","i0o2825at298k"," ","i0o2825"," ","ipass825"," ","ih2o825"," ","io2825"," ","isteelamp","
","ih2osteelamp"," ","io2steelamp"," ","ipass825amp"," ","io2825amp"," ","ih2o825amp","
","currentsum"," ","cathcurrentsum"," ","Ecorr"," ","delta"," ","tempk=",tempk," ","pH=",ph,"
","galvaniccoeff=",galvaniccoeff," ","coroxrd3.ma"," ","po2=",po2," ","Revised:6/21/97","
","run:6/21/97"]


Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);


eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);


eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));


khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;


cbulko2=khenryconst*po2;


do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;
```


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```
hplusconc=10^-ph;

eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);

i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;

i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

isteel=i0ferrous*(Exp[(afe zfe f (ecorr - eferrous))/(r tempk)]);

ih2osteel=i0h2osteel*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2steel=i0o2steel*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (ecorr - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (ecorr - eeqo2))/(r tempk)])/(1 +
((i0o2825*delta*Exp[-(zo2 bo2 f (ecorr - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

isteelamp=arsteel*isteel;

ih2osteelamp=arsteel*ih2osteel;
```


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```
io2steelamp=arsteel*io2steel;

ipass825amp=ar825*ipass825;

io2825amp=ar825*io2825;

ih2o825amp=ih2o825-ar825;

currentsum=arsteel*isteel+ar825*ipass825-ar825*ih2o825-ar825*io2825-arsteel*ih2osteel-ar

cathcurrsum=ar825*ih2o825+ar825*io2825+arsteel*ih2osteel+arsteel*io2steel;

Print[FortranForm[eeqh2o]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2],"
",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2],"
",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph],"
",FortranForm[hplusconc]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy],"
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",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k]," ",FortranForm[i0o2steel],"
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",FortranForm[ih2ostee1]," ",FortranForm[io2steel]," ",FortranForm[k1h2o825],"
",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825],"
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",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[isteelamp],"
",FortranForm[ih2osteelamp]," ",FortranForm[io2steelamp]," ",FortranForm[ipass825amp],"
",FortranForm[io2825amp]," ",FortranForm[ih2o825amp]," ",FortranForm[currentsum],"
",FortranForm[cathcurrsum]," ",FortranForm[ecorr],"
",FortranForm[delta]],{ecorr,-1.5,1.5,0.02}]
```


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EXAMPLE CALCULATION

OUTPUT OF COXRD160 PRINTED WITH EXCEL 97
NO CALCULATIONS PERFORMED IN EXCEL
COLUMN HEADINGS PLACED IN FIRST AND LAST
ROWS.

COMPLETE OUTPUT IS 51 COLUMNS WIDE
AND 153 ROWS.

INPUT & CALCULATED PARAMETERS INCLUDED
IN OUTPUT FILE.

INPUT VALUES LISTED ON p 88 & 89.

OUTPUT PASTED ON PAGES 94-
SO THAT VALUES OF AN ENTIRE COLUMN
CAN BE VIEWED ON FACING PAGES.

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COXRD160

eeqh2o	eeq0o2	eeqo2	o2overpotential	khenryconst	cbulko2	do2	temp	ph	hplusconc	h2oactenergy	o2actenergy	bo2	bh2o	afe	ferrousconc
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06

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COXRD160

eeqh2o	eeq0o2	eeqo2	o2overpotential	khenryconst	cbulko2	do2	temp	ph	hplusconc	h2oactenergy	o2actenergy	bo2	bh2o	afe	ferrousconc
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06
-0.219085296	1.1718	0.940337246	0	0.778926233	0.163574509	6.12E-09	368	3	1/1000	20	40	0.25	0.25	0.75	1.00E-06

6/26/98

COXRD160

eferrous	i0ferrous	k1h2osteel	i0o2steelat298k	i0o2steel	i0h2osteelat298k	i0h2osteel	isteel	ih2osteel	io2steel	k1h2o825	i0h2o825at298k
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.23E-23	4.88E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.86E-22	3.56E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.80E-22	2.60E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.24E-21	1.89E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.18E-21	1.38E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.20E-21	1.01E+06	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.11E-20	735346.6762	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.44E-20	536456.4739	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.40E-19	391360.3714	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.61E-19	285508.6066	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	9.29E-19	208286.7106	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.39E-18	151951.1245	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.16E-18	110852.6999	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.59E-17	80870.22139	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.09E-17	58997.14408	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.05E-16	43040.10735	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.71E-16	31398.99175	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.98E-16	22906.46432	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.80E-15	16710.92217	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.63E-15	12191.09662	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.19E-14	8893.75436	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.07E-14	6488.248683	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.92E-14	4733.363354	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.04E-13	3453.124215	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.25E-13	2519.153075	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.35E-12	1837.794362	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.48E-12	1340.723654	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.97E-12	978.0963284	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.31E-11	713.5493018	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.95E-11	520.5546646	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.53E-10	379.7595458	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.95E-10	277.0454718	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.02E-09	202.1126113	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.62E-09	147.4469421	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.75E-09	107.5667698	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.74E-08	78.47304119	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.47E-08	57.24833243	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.15E-07	41.76429913	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.97E-07	30.46825309	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.64E-07	22.22746379	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.97E-06	16.21557183	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.07E-06	11.82972435	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.30607E-05	8.630122933	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.36388E-05	6.295922001	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.66391E-05	4.593055528	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.000223145	3.350765636	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.000574725	2.444479557	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.001480242	1.783317891	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.003812463	1.300981508	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.009819257	0.949103293	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.025290158	0.692398052	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.065136507	0.505124222	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.167763468	0.368502596	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	0.432086129	0.268833204	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.112866972	0.196121527	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.86626396	0.143076274	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.382256182	0.104378242	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	19.01349879	0.076146919	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	48.97054877	0.05555136	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	126.1269518	0.040526309	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	324.8484728	0.029565104	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	836.6691556	0.02156859	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2154.897851	0.015734905	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5550.084781	0.011479064	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	14294.61776	0.008374306	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	36816.75232	0.006109296	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	94824.02922	0.004456907	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	244225.684	0.003251441	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	629019.7242	0.00237202	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.62E+06	0.001730456	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.17E+06	0.001262417	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.07E+07	0.00092097	0.77218732	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.77E+07	0.000671874	0.772187319	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.13E+07	0.000490151	0.772187319	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.84E+08	0.000357579	0.772187318	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.73E+08	0.000260864	0.772187316	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.22E+09	0.000190308	0.772187313	5.18E-08	0.001777541

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-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.14E+09	0.000138835	0.772187307	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.08E+09	0.000101284	0.772187296	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.08E+10	7.38897E-05	0.772187274	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.36E+10	5.39047E-05	0.772187234	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.38E+11	3.9325E-05	0.772187159	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.56E+11	2.86887E-05	0.772187018	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	9.16E+11	2.09292E-05	0.772186752	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.36E+12	1.52685E-05	0.772186253	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.07E+12	1.11388E-05	0.772185314	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.56E+13	8.13E-06	0.772183552	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.03E+13	5.93E-06	0.77218024	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.04E+14	4.32E-06	0.772174016	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.67E+14	3.16E-06	0.772162324	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.88E+14	2.30E-06	0.772140354	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.77E+15	1.68E-06	0.772099079	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.57E+15	1.22E-06	0.772021536	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.18E+16	8.94E-07	0.771875878	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.03E+16	6.52E-07	0.771602344	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.80E+16	4.76E-07	0.77108891	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.01E+17	3.47E-07	0.770126039	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.18E+17	2.53E-07	0.768323341	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.33E+18	1.85E-07	0.764958888	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.43E+18	1.35E-07	0.758716294	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.84E+18	9.83E-08	0.747258184	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.28E+19	7.17E-08	0.72663918	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.87E+19	5.23E-08	0.690823015	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.51E+20	3.82E-08	0.632266438	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.89E+20	2.78E-08	0.545402192	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.00E+21	2.03E-08	0.433498624	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.58E+21	1.48E-08	0.312878842	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.65E+21	1.08E-08	0.205461151	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.71E+22	7.89E-09	0.124894172	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.41E+22	5.75E-09	0.071910998	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.14E+23	4.20E-09	0.040015094	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.93E+23	3.06E-09	0.021825589	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.53E+23	2.23E-09	0.011771483	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.94E+24	1.63E-09	0.006309922	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.00E+24	1.19E-09	0.003371103	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.29E+25	8.67E-10	0.001797813	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.32E+25	6.33E-10	0.000957861	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.54E+25	4.62E-10	0.000510081	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.20E+26	3.37E-10	0.000271555	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.66E+26	2.46E-10	0.000144549	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.46E+27	1.79E-10	7.69373E-05	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.76E+27	1.31E-10	4.09489E-05	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	9.68E+27	9.54E-11	2.1794E-05	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.49E+28	6.96E-11	1.15992E-05	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.42E+28	5.08E-11	6.17E-06	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.65E+29	3.70E-11	3.29E-06	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.26E+29	2.70E-11	1.75E-06	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.10E+30	1.97E-11	9.31E-07	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.83E+30	1.44E-11	4.95E-07	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.28E+30	1.05E-11	2.64E-07	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.87E+31	7.65E-12	1.40E-07	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.83E+31	5.58E-12	7.47E-08	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.24E+32	4.07E-12	3.97E-08	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.20E+32	2.97E-12	2.11E-08	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	8.25E+32	2.17E-12	1.13E-08	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.12E+33	1.58E-12	5.99E-09	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	5.47E+33	1.15E-12	3.19E-09	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.41E+34	8.41E-13	1.70E-09	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.63E+34	6.14E-13	9.03E-10	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	9.35E+34	4.48E-13	4.81E-10	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.41E+35	3.27E-13	2.56E-10	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	6.20E+35	2.38E-13	1.36E-10	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.60E+36	1.74E-13	7.25E-11	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.11E+36	1.27E-13	3.86E-11	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.06E+37	9.25E-14	2.05E-11	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	2.73E+37	6.75E-14	1.09E-11	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	7.03E+37	4.93E-14	5.81E-12	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.81E+38	3.59E-14	3.09E-12	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	4.66E+38	2.62E-14	1.65E-12	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	1.20E+39	1.91E-14	8.76E-13	5.18E-08	0.001777541
-0.616968112	0.0001	5.18E-08	1.00E-06	2.15641E-05	0.001777541	0.008254391	3.09E+39	1.40E-14	4.66E-13	5.18E-08	0.001777541
eferrous	i0ferrous	k1h2osteel	i0o2steelat298k	i0o2steel	i0h2osteelat298k	i0h2osteel	isteel	ih2osteel	io2steel	k1h2o825	i0h2o825at298k

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i0h2o825	i0o2825at298k	i0o2825	ipass825	ih2o825	io2825	isteelamp	ih2osteelamp	io2steelamp	ipass825amp	io2825amp	ih2o825amp
0.008254391	1.00E-06	2.15641E-05	0.001	4.88E+06	0.772187327	7.23E-23	4.88E+06	0.772187327	0.001	0.772187327	4.88E+06
0.008254391	1.00E-06	2.15641E-05	0.001	3.56E+06	0.772187327	1.86E-22	3.56E+06	0.772187327	0.001	0.772187327	3.56E+06
0.008254391	1.00E-06	2.15641E-05	0.001	2.60E+06	0.772187327	4.80E-22	2.60E+06	0.772187327	0.001	0.772187327	2.60E+06
0.008254391	1.00E-06	2.15641E-05	0.001	1.89E+06	0.772187327	1.24E-21	1.89E+06	0.772187327	0.001	0.772187327	1.89E+06
0.008254391	1.00E-06	2.15641E-05	0.001	1.38E+06	0.772187327	3.18E-21	1.38E+06	0.772187327	0.001	0.772187327	1.38E+06
0.008254391	1.00E-06	2.15641E-05	0.001	1.01E+06	0.772187327	8.20E-21	1.01E+06	0.772187327	0.001	0.772187327	1.01E+06
0.008254391	1.00E-06	2.15641E-05	0.001	735346.6762	0.772187327	2.11E-20	735346.6762	0.772187327	0.001	0.772187327	735345.6762
0.008254391	1.00E-06	2.15641E-05	0.001	536456.4739	0.772187327	5.44E-20	536456.4739	0.772187327	0.001	0.772187327	536455.4739
0.008254391	1.00E-06	2.15641E-05	0.001	391360.3714	0.772187327	1.40E-19	391360.3714	0.772187327	0.001	0.772187327	391359.3714
0.008254391	1.00E-06	2.15641E-05	0.001	285508.6066	0.772187327	3.61E-19	285508.6066	0.772187327	0.001	0.772187327	285507.6066
0.008254391	1.00E-06	2.15641E-05	0.001	208286.7106	0.772187327	9.29E-19	208286.7106	0.772187327	0.001	0.772187327	208285.7106
0.008254391	1.00E-06	2.15641E-05	0.001	151951.1245	0.772187327	2.39E-18	151951.1245	0.772187327	0.001	0.772187327	151950.1245
0.008254391	1.00E-06	2.15641E-05	0.001	110852.6999	0.772187327	6.16E-18	110852.6999	0.772187327	0.001	0.772187327	110851.6999
0.008254391	1.00E-06	2.15641E-05	0.001	80870.22139	0.772187327	1.59E-17	80870.22139	0.772187327	0.001	0.772187327	80869.22139
0.008254391	1.00E-06	2.15641E-05	0.001	58997.14408	0.772187327	4.09E-17	58997.14408	0.772187327	0.001	0.772187327	58996.14408
0.008254391	1.00E-06	2.15641E-05	0.001	43040.10735	0.772187327	1.05E-16	43040.10735	0.772187327	0.001	0.772187327	43039.10735
0.008254391	1.00E-06	2.15641E-05	0.001	31398.99175	0.772187327	2.71E-16	31398.99175	0.772187327	0.001	0.772187327	31397.99175
0.008254391	1.00E-06	2.15641E-05	0.001	22906.46432	0.772187327	6.98E-16	22906.46432	0.772187327	0.001	0.772187327	22905.46432
0.008254391	1.00E-06	2.15641E-05	0.001	16710.92217	0.772187327	1.80E-15	16710.92217	0.772187327	0.001	0.772187327	16709.92217
0.008254391	1.00E-06	2.15641E-05	0.001	12191.09662	0.772187327	4.63E-15	12191.09662	0.772187327	0.001	0.772187327	12190.09662
0.008254391	1.00E-06	2.15641E-05	0.001	8893.75436	0.772187327	1.19E-14	8893.75436	0.772187327	0.001	0.772187327	8892.75436
0.008254391	1.00E-06	2.15641E-05	0.001	6488.248683	0.772187327	3.07E-14	6488.248683	0.772187327	0.001	0.772187327	6487.248683
0.008254391	1.00E-06	2.15641E-05	0.001	4733.363354	0.772187327	7.92E-14	4733.363354	0.772187327	0.001	0.772187327	4732.363354
0.008254391	1.00E-06	2.15641E-05	0.001	3453.124215	0.772187327	2.04E-13	3453.124215	0.772187327	0.001	0.772187327	3452.124215
0.008254391	1.00E-06	2.15641E-05	0.001	2519.153075	0.772187327	5.25E-13	2519.153075	0.772187327	0.001	0.772187327	2518.153075
0.008254391	1.00E-06	2.15641E-05	0.001	1837.794362	0.772187327	1.35E-12	1837.794362	0.772187327	0.001	0.772187327	1836.794362
0.008254391	1.00E-06	2.15641E-05	0.001	1340.723654	0.772187327	3.48E-12	1340.723654	0.772187327	0.001	0.772187327	1339.723654
0.008254391	1.00E-06	2.15641E-05	0.001	978.0963284	0.772187327	8.97E-12	978.0963284	0.772187327	0.001	0.772187327	977.0963284
0.008254391	1.00E-06	2.15641E-05	0.001	713.5493018	0.772187327	2.31E-11	713.5493018	0.772187327	0.001	0.772187327	712.5493018
0.008254391	1.00E-06	2.15641E-05	0.001	520.5546646	0.772187327	5.95E-11	520.5546646	0.772187327	0.001	0.772187327	519.5546646
0.008254391	1.00E-06	2.15641E-05	0.001	379.7595458	0.772187327	1.53E-10	379.7595458	0.772187327	0.001	0.772187327	378.7595458
0.008254391	1.00E-06	2.15641E-05	0.001	277.0454718	0.772187327	3.95E-10	277.0454718	0.772187327	0.001	0.772187327	276.0454718
0.008254391	1.00E-06	2.15641E-05	0.001	202.1126113	0.772187327	1.02E-09	202.1126113	0.772187327	0.001	0.772187327	201.1126113
0.008254391	1.00E-06	2.15641E-05	0.001	147.4469421	0.772187327	2.62E-09	147.4469421	0.772187327	0.001	0.772187327	146.4469421
0.008254391	1.00E-06	2.15641E-05	0.001	107.5667698	0.772187327	6.75E-09	107.5667698	0.772187327	0.001	0.772187327	106.5667698
0.008254391	1.00E-06	2.15641E-05	0.001	78.47304119	0.772187327	1.74E-08	78.47304119	0.772187327	0.001	0.772187327	77.47304119
0.008254391	1.00E-06	2.15641E-05	0.001	57.24833243	0.772187327	4.47E-08	57.24833243	0.772187327	0.001	0.772187327	56.24833243
0.008254391	1.00E-06	2.15641E-05	0.001	41.76429913	0.772187327	1.15E-07	41.76429913	0.772187327	0.001	0.772187327	40.76429913
0.008254391	1.00E-06	2.15641E-05	0.001	30.46825309	0.772187327	2.97E-07	30.46825309	0.772187327	0.001	0.772187327	29.46825309
0.008254391	1.00E-06	2.15641E-05	0.001	22.22746379	0.772187327	7.64E-07	22.22746379	0.772187327	0.001	0.772187327	21.22746379
0.008254391	1.00E-06	2.15641E-05	0.001	16.21557183	0.772187327	1.97E-06	16.21557183	0.772187327	0.001	0.772187327	15.21557183
0.008254391	1.00E-06	2.15641E-05	0.001	11.82972435	0.772187327	5.07E-06	11.82972435	0.772187327	0.001	0.772187327	10.82972435
0.008254391	1.00E-06	2.15641E-05	0.001	8.630122933	0.772187327	1.30607E-05	8.630122933	0.772187327	0.001	0.772187327	7.630122933
0.008254391	1.00E-06	2.15641E-05	0.001	6.295922001	0.772187327	3.36388E-05	6.295922001	0.772187327	0.001	0.772187327	5.295922001
0.008254391	1.00E-06	2.15641E-05	0.001	4.593055528	0.772187327	8.66391E-05	4.593055528	0.772187327	0.001	0.772187327	3.593055528
0.008254391	1.00E-06	2.15641E-05	0.001	3.350765636	0.772187327	0.000223145	3.350765636	0.772187327	0.001	0.772187327	2.350765636
0.008254391	1.00E-06	2.15641E-05	0.001	2.444479557	0.772187327	0.000574725	2.444479557	0.772187327	0.001	0.772187327	1.444479557
0.008254391	1.00E-06	2.15641E-05	0.001	1.783317891	0.772187327	0.001480242	1.783317891	0.772187327	0.001	0.772187327	0.783317891
0.008254391	1.00E-06	2.15641E-05	0.001	1.300981508	0.772187327	0.003812463	1.300981508	0.772187327	0.001	0.772187327	0.300981508
0.008254391	1.00E-06	2.15641E-05	0.001	0.949103293	0.772187327	0.009819257	0.949103293	0.772187327	0.001	0.772187327	-0.050896707
0.008254391	1.00E-06	2.15641E-05	0.001	0.692398052	0.772187327	0.025290158	0.692398052	0.772187327	0.001	0.772187327	-0.307601948
0.008254391	1.00E-06	2.15641E-05	0.001	0.505124222	0.772187327	0.065136507	0.505124222	0.772187327	0.001	0.772187327	-0.494875778
0.008254391	1.00E-06	2.15641E-05	0.001	0.368502596	0.772187327	0.167763468	0.368502596	0.772187327	0.001	0.772187327	-0.631497404
0.008254391	1.00E-06	2.15641E-05	0.001	0.268833204	0.772187327	0.432086129	0.268833204	0.772187327	0.001	0.772187327	-0.731166796
0.008254391	1.00E-06	2.15641E-05	0.001	0.196121527	0.772187327	1.112866972	0.196121527	0.772187327	0.001	0.772187327	-0.803878473
0.008254391	1.00E-06	2.15641E-05	0.001	0.143076274	0.772187327	2.86626396	0.143076274	0.772187327	0.001	0.772187327	-0.856923726
0.008254391	1.00E-06	2.15641E-05	0.001	0.104378242	0.772187327	7.382256182	0.104378242	0.772187327	0.001	0.772187327	-0.895621758
0.008254391	1.00E-06	2.15641E-05	0.001	0.076146919	0.772187327	19.01349879	0.076146919	0.772187327	0.001	0.772187327	-0.923853081
0.008254391	1.00E-06	2.15641E-05	0.001	0.05555136	0.772187327	48.97054877	0.05555136	0.772187327	0.001	0.772187327	-0.94444864
0.008254391	1.00E-06	2.15641E-05	0.001	0.040526309	0.772187327	126.1269518	0.040526309	0.772187327	0.001	0.772187327	-0.959473691
0.008254391	1.00E-06	2.15641E-05	0.001	0.029565104	0.772187327	324.8484728	0.029565104	0.772187327	0.001	0.772187327	-0.970434896
0.008254391	1.00E-06	2.15641E-05	0.001	0.02156859	0.772187327	836.6691556	0.02156859	0.772187327	0.001	0.772187327	-0.97843141
0.008254391	1.00E-06	2.15641E-05	0.001	0.015734905	0.772187327	2154.897851	0.015734905	0.772187327	0.001	0.772187327	-0.984265095
0.008254391	1.00E-06	2.15641E-05	0.001	0.011479064	0.772187327	5550.084781	0.011479064	0.772187327	0.001	0.772187327	-0.988520936
0.008254391	1.00E-06	2.15641E-05	0.001	0.008374306	0.772187327	14294.61776	0.008374306	0.772187327	0.001	0.772187327	-0.991625694
0.008254391	1.00E-06	2.15641E-05	0.001	0.006109296	0.772187327	36816.75232	0.006109296	0.772187327	0.001	0.772187327	-0.993890704
0.008254391	1.00E-06	2.15641E-05	0.001	0.004456907	0.772187327	94824.02922	0.004456907	0.772187327	0.001	0.772187327	-0.995543093
0.008254391	1.00E-06	2.15641E-05	0.001	0.003251441	0.772187327	244225.684	0.003251441	0.772187327	0.001	0.772187327	-0.996748559
0.008254391	1.00E-06	2.15641E-05	0.001	0.00237202	0.772187327	629019.7242	0.00237202	0.772187327	0.001	0.772187327	-0.99762798
0.008254391	1.00E-06	2.15641E-05	0.001	0.001730456	0.772187327	1.62E+06	0.001730456	0.772187327	0.001	0.772187327	-0.998269544
0.008254391	1.00E-06	2.15641E-05	0.001	0.001262417	0.772187327	4.17E+06	0.001262417	0.772187327	0.001	0.772187327	-0.998737583
0.008254391	1.00E-06	2.15641E-05	0.001	0.00092097	0.772187327	1.07E+07	0.00092097	0.772187327	0.001	0.772187327	-0.99907903
0.008254391	1.00E-06	2.15641E-05	0.001	0.000671874	0.772187319	2.77E+07	0.000671874	0.772187319	0.001	0.772187319	-0.999328126
0.008254391	1.00E-06	2.15641E-05	0.001	0.000490151	0.772187319	7.13E+07	0.000490151	0.772187319	0.001	0.772187319	-0.999509849
0.008254391	1.00E-06	2.15641E-05	0.001	0.000357579	0.772187318	1.84E+08	0.000357579	0.772187318	0.001	0.772187318	-0.999642421
0.008254391	1.00E-06	2.15641E-05	0.001	0.000260864	0.772187316	4.73E+08	0.000260864	0.772187316	0.001	0.772187316	-0.999739136
0.008254391	1.00E-06	2.15641E-05	0.001	0.000190308	0.772187313	1.22E+09	0.000190308	0.772187313	0.001	0.772187313	-0.999809692

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0.008254391	1.00E-06	2.15641E-05	0.001	0.000138835	0.772187307	3.14E+09	0.000138835	0.772187307	0.001	0.772187307	-0.999861165
0.008254391	1.00E-06	2.15641E-05	0.001	0.000101284	0.772187296	8.08E+09	0.000101284	0.772187296	0.001	0.772187296	-0.999898716
0.008254391	1.00E-06	2.15641E-05	0.001	7.38897E-05	0.772187274	2.08E+10	7.38897E-05	0.772187274	0.001	0.772187274	-0.99992611
0.008254391	1.00E-06	2.15641E-05	0.001	5.39047E-05	0.772187234	5.36E+10	5.39047E-05	0.772187234	0.001	0.772187234	-0.999946095
0.008254391	1.00E-06	2.15641E-05	0.001	3.9325E-05	0.772187159	1.38E+11	3.9325E-05	0.772187159	0.001	0.772187159	-0.999960675
0.008254391	1.00E-06	2.15641E-05	0.001	2.86887E-05	0.772187018	3.56E+11	2.86887E-05	0.772187018	0.001	0.772187018	-0.999971311
0.008254391	1.00E-06	2.15641E-05	0.001	2.09292E-05	0.772186752	9.16E+11	2.09292E-05	0.772186752	0.001	0.772186752	-0.999979071
0.008254391	1.00E-06	2.15641E-05	0.001	1.52685E-05	0.772186253	2.36E+12	1.52685E-05	0.772186253	0.001	0.772186253	-0.999984732
0.008254391	1.00E-06	2.15641E-05	0.001	1.11388E-05	0.772185314	6.07E+12	1.11388E-05	0.772185314	0.001	0.772185314	-0.999988861
0.008254391	1.00E-06	2.15641E-05	0.001	8.13E-06	0.772183552	1.56E+13	8.13E-06	0.772183552	0.001	0.772183552	-0.999991874
0.008254391	1.00E-06	2.15641E-05	0.001	5.93E-06	0.77218024	4.03E+13	5.93E-06	0.77218024	0.001	0.77218024	-0.999994072
0.008254391	1.00E-06	2.15641E-05	0.001	4.32E-06	0.772174016	1.04E+14	4.32E-06	0.772174016	0.001	0.772174016	-0.999995675
0.008254391	1.00E-06	2.15641E-05	0.001	3.16E-06	0.772162324	2.67E+14	3.16E-06	0.772162324	0.001	0.772162324	-0.999996845
0.008254391	1.00E-06	2.15641E-05	0.001	2.30E-06	0.772140354	6.88E+14	2.30E-06	0.772140354	0.001	0.772140354	-0.999997698
0.008254391	1.00E-06	2.15641E-05	0.001	1.68E-06	0.772099079	1.77E+15	1.68E-06	0.772099079	0.001	0.772099079	-0.999998321
0.008254391	1.00E-06	2.15641E-05	0.001	1.22E-06	0.772021536	4.57E+15	1.22E-06	0.772021536	0.001	0.772021536	-0.999998775
0.008254391	1.00E-06	2.15641E-05	0.001	8.94E-07	0.771875878	1.18E+16	8.94E-07	0.771875878	0.001	0.771875878	-0.999999106
0.008254391	1.00E-06	2.15641E-05	0.001	6.52E-07	0.771602344	3.03E+16	6.52E-07	0.771602344	0.001	0.771602344	-0.999999348
0.008254391	1.00E-06	2.15641E-05	0.001	4.76E-07	0.77108891	7.80E+16	4.76E-07	0.77108891	0.001	0.77108891	-0.999999524
0.008254391	1.00E-06	2.15641E-05	0.001	3.47E-07	0.770126039	2.01E+17	3.47E-07	0.770126039	0.001	0.770126039	-0.999999653
0.008254391	1.00E-06	2.15641E-05	0.001	2.53E-07	0.768323341	5.18E+17	2.53E-07	0.768323341	0.001	0.768323341	-0.999999747
0.008254391	1.00E-06	2.15641E-05	0.001	1.85E-07	0.764958888	1.33E+18	1.85E-07	0.764958888	0.001	0.764958888	-0.999999815
0.008254391	1.00E-06	2.15641E-05	0.001	1.35E-07	0.758716294	3.43E+18	1.35E-07	0.758716294	0.001	0.758716294	-0.999999865
0.008254391	1.00E-06	2.15641E-05	0.001	9.83E-08	0.747258184	8.84E+18	9.83E-08	0.747258184	0.001	0.747258184	-0.999999902
0.008254391	1.00E-06	2.15641E-05	0.001	7.17E-08	0.72663918	2.28E+19	7.17E-08	0.72663918	0.001	0.72663918	-0.999999928
0.008254391	1.00E-06	2.15641E-05	0.001	5.23E-08	0.690823015	5.87E+19	5.23E-08	0.690823015	0.001	0.690823015	-0.999999948
0.008254391	1.00E-06	2.15641E-05	0.001	3.82E-08	0.632266438	1.51E+20	3.82E-08	0.632266438	0.001	0.632266438	-0.999999962
0.008254391	1.00E-06	2.15641E-05	0.001	2.78E-08	0.545402192	3.89E+20	2.78E-08	0.545402192	0.001	0.545402192	-0.999999972
0.008254391	1.00E-06	2.15641E-05	0.001	2.03E-08	0.433498624	1.00E+21	2.03E-08	0.433498624	0.001	0.433498624	-0.99999998
0.008254391	1.00E-06	2.15641E-05	0.001	1.48E-08	0.312878842	2.58E+21	1.48E-08	0.312878842	0.001	0.312878842	-0.999999985
0.008254391	1.00E-06	2.15641E-05	0.001	1.08E-08	0.205461151	6.65E+21	1.08E-08	0.205461151	0.001	0.205461151	-0.999999989
0.008254391	1.00E-06	2.15641E-05	0.001	7.89E-09	0.124894172	1.71E+22	7.89E-09	0.124894172	0.001	0.124894172	-0.999999992
0.008254391	1.00E-06	2.15641E-05	0.001	5.75E-09	0.071910998	4.41E+22	5.75E-09	0.071910998	0.001	0.071910998	-0.999999994
0.008254391	1.00E-06	2.15641E-05	0.001	4.20E-09	0.040015094	1.14E+23	4.20E-09	0.040015094	0.001	0.040015094	-0.999999996
0.008254391	1.00E-06	2.15641E-05	0.001	3.06E-09	0.021825589	2.93E+23	3.06E-09	0.021825589	0.001	0.021825589	-0.999999997
0.008254391	1.00E-06	2.15641E-05	0.001	2.23E-09	0.011771483	7.53E+23	2.23E-09	0.011771483	0.001	0.011771483	-0.999999998
0.008254391	1.00E-06	2.15641E-05	0.001	1.63E-09	0.006309922	1.94E+24	1.63E-09	0.006309922	0.001	0.006309922	-0.999999998
0.008254391	1.00E-06	2.15641E-05	0.001	1.19E-09	0.003371103	5.00E+24	1.19E-09	0.003371103	0.001	0.003371103	-0.999999999
0.008254391	1.00E-06	2.15641E-05	0.001	8.67E-10	0.001797813	1.29E+25	8.67E-10	0.001797813	0.001	0.001797813	-0.999999999
0.008254391	1.00E-06	2.15641E-05	0.001	6.33E-10	0.000957861	3.32E+25	6.33E-10	0.000957861	0.001	0.000957861	-0.999999999
0.008254391	1.00E-06	2.15641E-05	0.001	4.62E-10	0.000510081	8.54E+25	4.62E-10	0.000510081	0.001	0.000510081	-1
0.008254391	1.00E-06	2.15641E-05	0.001	3.37E-10	0.000271555	2.20E+26	3.37E-10	0.000271555	0.001	0.000271555	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.46E-10	0.000144549	5.66E+26	2.46E-10	0.000144549	0.001	0.000144549	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.79E-10	7.69373E-05	1.46E+27	1.79E-10	7.69373E-05	0.001	7.69373E-05	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.31E-10	4.09489E-05	3.76E+27	1.31E-10	4.09489E-05	0.001	4.09489E-05	-1
0.008254391	1.00E-06	2.15641E-05	0.001	9.54E-11	2.1794E-05	9.68E+27	9.54E-11	2.1794E-05	0.001	2.1794E-05	-1
0.008254391	1.00E-06	2.15641E-05	0.001	6.96E-11	1.15992E-05	2.49E+28	6.96E-11	1.15992E-05	0.001	1.15992E-05	-1
0.008254391	1.00E-06	2.15641E-05	0.001	5.08E-11	6.17E-06	6.42E+28	5.08E-11	6.17E-06	0.001	6.17E-06	-1
0.008254391	1.00E-06	2.15641E-05	0.001	3.70E-11	3.29E-06	1.65E+29	3.70E-11	3.29E-06	0.001	3.29E-06	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.70E-11	1.75E-06	4.26E+29	2.70E-11	1.75E-06	0.001	1.75E-06	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.97E-11	9.31E-07	1.10E+30	1.97E-11	9.31E-07	0.001	9.31E-07	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.44E-11	4.95E-07	2.83E+30	1.44E-11	4.95E-07	0.001	4.95E-07	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.05E-11	2.64E-07	7.28E+30	1.05E-11	2.64E-07	0.001	2.64E-07	-1
0.008254391	1.00E-06	2.15641E-05	0.001	7.65E-12	1.40E-07	1.87E+31	7.65E-12	1.40E-07	0.001	1.40E-07	-1
0.008254391	1.00E-06	2.15641E-05	0.001	5.58E-12	7.47E-08	4.83E+31	5.58E-12	7.47E-08	0.001	7.47E-08	-1
0.008254391	1.00E-06	2.15641E-05	0.001	4.07E-12	3.97E-08	1.24E+32	4.07E-12	3.97E-08	0.001	3.97E-08	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.97E-12	2.11E-08	3.20E+32	2.97E-12	2.11E-08	0.001	2.11E-08	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.17E-12	1.13E-08	8.25E+32	2.17E-12	1.13E-08	0.001	1.13E-08	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.58E-12	5.99E-09	2.12E+33	1.58E-12	5.99E-09	0.001	5.99E-09	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.15E-12	3.19E-09	5.47E+33	1.15E-12	3.19E-09	0.001	3.19E-09	-1
0.008254391	1.00E-06	2.15641E-05	0.001	8.41E-13	1.70E-09	1.41E+34	8.41E-13	1.70E-09	0.001	1.70E-09	-1
0.008254391	1.00E-06	2.15641E-05	0.001	6.14E-13	9.03E-10	3.63E+34	6.14E-13	9.03E-10	0.001	9.03E-10	-1
0.008254391	1.00E-06	2.15641E-05	0.001	4.48E-13	4.81E-10	9.35E+34	4.48E-13	4.81E-10	0.001	4.81E-10	-1
0.008254391	1.00E-06	2.15641E-05	0.001	3.27E-13	2.56E-10	2.41E+35	3.27E-13	2.56E-10	0.001	2.56E-10	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.38E-13	1.36E-10	6.20E+35	2.38E-13	1.36E-10	0.001	1.36E-10	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.74E-13	7.25E-11	1.60E+36	1.74E-13	7.25E-11	0.001	7.25E-11	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.27E-13	3.86E-11	4.11E+36	1.27E-13	3.86E-11	0.001	3.86E-11	-1
0.008254391	1.00E-06	2.15641E-05	0.001	9.25E-14	2.05E-11	1.06E+37	9.25E-14	2.05E-11	0.001	2.05E-11	-1
0.008254391	1.00E-06	2.15641E-05	0.001	6.75E-14	1.09E-11	2.73E+37	6.75E-14	1.09E-11	0.001	1.09E-11	-1
0.008254391	1.00E-06	2.15641E-05	0.001	4.93E-14	5.81E-12	7.03E+37	4.93E-14	5.81E-12	0.001	5.81E-12	-1
0.008254391	1.00E-06	2.15641E-05	0.001	3.59E-14	3.09E-12	1.81E+38	3.59E-14	3.09E-12	0.001	3.09E-12	-1
0.008254391	1.00E-06	2.15641E-05	0.001	2.62E-14	1.65E-12	4.66E+38	2.62E-14	1.65E-12	0.001	1.65E-12	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.91E-14	8.76E-13	1.20E+39	1.91E-14	8.76E-13	0.001	8.76E-13	-1
0.008254391	1.00E-06	2.15641E-05	0.001	1.40E-14	4.66E-13	3.09E+39	1.40E-14	4.66E-13	0.001	4.66E-13	-1
i0h2o825	i0o2825at298k	i0o2825	ipass825	ih2o825	io2825	isteelamp	ih2osteelamp	io2steelamp	ipass825amp	io2825amp	ih2o825amp

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currentsum	cathcurrentsum	Ecorr	delta	tempk=368	pH=3	galvaniccoeff=1	coroxrd3.ma	po2=0.21	Revised:6/21/97	run:6/21/97
-9.76E+06	9.76E+06	-1.5	0.0005							
-7.12E+06	7.12E+06	-1.48	0.0005							
-5.19E+06	5.19E+06	-1.46	0.0005							
-3.79E+06	3.79E+06	-1.44	0.0005							
-2.76E+06	2.76E+06	-1.42	0.0005							
-2.02E+06	2.02E+06	-1.4	0.0005							
-1.47E+06	1.47E+06	-1.38	0.0005							
-1.07E+06	1.07E+06	-1.36	0.0005							
-782722.2863	782722.2873	-1.34	0.0005							
-571018.7565	571018.7575	-1.32	0.0005							
-416574.9646	416574.9656	-1.3	0.0005							
-303903.7923	303903.7933	-1.28	0.0005							
-221706.9432	221706.9442	-1.26	0.0005							
-161741.9862	161741.9872	-1.24	0.0005							
-117995.8315	117995.8325	-1.22	0.0005							
-86081.75807	86081.75907	-1.2	0.0005							
-62799.52688	62799.52788	-1.18	0.0005							
-45814.472	45814.473	-1.16	0.0005							
-33423.38772	33423.38872	-1.14	0.0005							
-24383.73662	24383.73762	-1.12	0.0005							
-17789.05209	17789.05309	-1.1	0.0005							
-12978.04074	12978.04174	-1.08	0.0005							
-9468.270083	9468.271083	-1.06	0.0005							
-6907.791806	6907.792806	-1.04	0.0005							
-5039.849524	5039.850524	-1.02	0.0005							
-3677.132098	3677.133098	-1	0.0005							
-2682.990684	2682.991684	-0.98	0.0005							
-1957.736031	1957.737031	-0.96	0.0005							
-1428.641978	1428.642978	-0.94	0.0005							
-1042.652704	1042.653704	-0.92	0.0005							
-761.0624663	761.0634663	-0.9	0.0005							
-555.6343183	555.6353183	-0.88	0.0005							
-405.7685972	405.7695972	-0.86	0.0005							
-296.4372588	296.4382588	-0.84	0.0005							
-216.6769142	216.6779142	-0.82	0.0005							
-158.489457	158.490457	-0.8	0.0005							
-116.0400394	116.0410395	-0.78	0.0005							
-85.07197278	85.07297289	-0.76	0.0005							
-62.47988053	62.48088083	-0.74	0.0005							
-45.99830146	45.99930222	-0.72	0.0005							
-33.97451633	33.9755183	-0.7	0.0005							
-25.20281828	25.20382335	-0.68	0.0005							
-18.80360744	18.80462051	-0.66	0.0005							
-14.135185	14.13621864	-0.64	0.0005							
-10.72939906	10.7304857	-0.62	0.0005							
-8.244682766	8.245905911	-0.6	0.0005							
-6.43175903	6.433333755	-0.58	0.0005							
-5.10853018	5.111010422	-0.56	0.0005							
-4.141525192	4.146337655	-0.54	0.0005							
-3.43176197	3.442581227	-0.52	0.0005							
-2.902880586	2.929170744	-0.5	0.0005							
-2.488486576	2.554623083	-0.48	0.0005							
-2.112616363	2.281379831	-0.46	0.0005							
-1.648954919	2.082041048	-0.44	0.0005							
-0.822750721	1.936617693	-0.42	0.0005							
1.036736772	1.830527188	-0.4	0.0005							
5.630125058	1.753131124	-0.38	0.0005							
17.31783032	1.696668478	-0.36	0.0005							
47.31607141	1.655477359	-0.34	0.0005							
124.5025246	1.625427258	-0.32	0.0005							
323.245968	1.603504847	-0.3	0.0005							
835.0826438	1.587511821	-0.28	0.0005							
2153.323006	1.57584445	-0.26	0.0005							
5548.518448	1.567332768	-0.24	0.0005							
14293.05763	1.561123252	-0.22	0.0005							
36815.19673	1.556593233	-0.2	0.0005							
94822.47693	1.553288453	-0.18	0.0005							
244224.1341	1.550877522	-0.16	0.0005							
629018.176	1.549118679	-0.14	0.0005							
1.62E+06	1.547835552	-0.12	0.0005							
4.17E+06	1.546899474	-0.1	0.0005							
1.07E+07	1.546216579	-0.08	0.0005							
2.77E+07	1.545718386	-0.06	0.0005							
7.13E+07	1.54535494	-0.04	0.0005							
1.84E+08	1.545089795	-0.02	0.0005							
4.73E+08	1.544896361	1.06E-15	0.0005							
1.22E+09	1.544755242	0.02	0.0005							

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3.14E+09	1.544652284	0.04	0.0005							
8.08E+09	1.54457716	0.06	0.0005							
2.08E+10	1.544522328	0.08	0.0005							
5.36E+10	1.544482278	0.1	0.0005							
1.38E+11	1.544452968	0.12	0.0005							
3.56E+11	1.544431413	0.14	0.0005							
9.16E+11	1.544415362	0.16	0.0005							
2.36E+12	1.544403042	0.18	0.0005							
6.07E+12	1.544392906	0.2	0.0005							
1.56E+13	1.544383356	0.22	0.0005							
4.03E+13	1.544372336	0.24	0.0005							
1.04E+14	1.544356682	0.26	0.0005							
2.67E+14	1.544330957	0.28	0.0005							
6.88E+14	1.544285312	0.3	0.0005							
1.77E+15	1.544201516	0.32	0.0005							
4.57E+15	1.544045521	0.34	0.0005							
1.18E+16	1.543753544	0.36	0.0005							
3.03E+16	1.543205991	0.38	0.0005							
7.80E+16	1.542178771	0.4	0.0005							
2.01E+17	1.540252772	0.42	0.0005							
5.18E+17	1.536647189	0.44	0.0005							
1.33E+18	1.529918146	0.46	0.0005							
3.43E+18	1.517432857	0.48	0.0005							
8.84E+18	1.494516564	0.5	0.0005							
2.28E+19	1.453278504	0.52	0.0005							
5.87E+19	1.381646135	0.54	0.0005							
1.51E+20	1.264532951	0.56	0.0005							
3.89E+20	1.090804439	0.58	0.0005							
1.00E+21	0.866997288	0.6	0.0005							
2.58E+21	0.625757714	0.62	0.0005							
6.65E+21	0.410922323	0.64	0.0005							
1.71E+22	0.249788359	0.66	0.0005							
4.41E+22	0.143822008	0.68	0.0005							
1.14E+23	0.080030196	0.7	0.0005							
2.93E+23	0.043651185	0.72	0.0005							
7.53E+23	0.02354297	0.74	0.0005							
1.94E+24	0.012619847	0.76	0.0005							
5.00E+24	0.006742208	0.78	0.0005							
1.29E+25	0.003595628	0.8	0.0005							
3.32E+25	0.001915723	0.82	0.0005							
8.54E+25	0.001020163	0.84	0.0005							
2.20E+26	0.000543111	0.86	0.0005							
5.66E+26	0.000289098	0.88	0.0005							
1.46E+27	0.000153875	0.9	0.0005							
3.76E+27	8.1898E-05	0.92	0.0005							
9.68E+27	4.35883E-05	0.94	0.0005							
2.49E+28	2.31985E-05	0.96	0.0005							
6.42E+28	1.23467E-05	0.98	0.0005							
1.65E+29	6.57E-06	1	0.0005							
4.26E+29	3.50E-06	1.02	0.0005							
1.10E+30	1.86E-06	1.04	0.0005							
2.83E+30	9.91E-07	1.06	0.0005							
7.28E+30	5.27E-07	1.08	0.0005							
1.87E+31	2.81E-07	1.1	0.0005							
4.83E+31	1.49E-07	1.12	0.0005							
1.24E+32	7.95E-08	1.14	0.0005							
3.20E+32	4.23E-08	1.16	0.0005							
8.25E+32	2.25E-08	1.18	0.0005							
2.12E+33	1.20E-08	1.2	0.0005							
5.47E+33	6.38E-09	1.22	0.0005							
1.41E+34	3.40E-09	1.24	0.0005							
3.63E+34	1.81E-09	1.26	0.0005							
9.35E+34	9.62E-10	1.28	0.0005							
2.41E+35	5.12E-10	1.3	0.0005							
6.20E+35	2.73E-10	1.32	0.0005							
1.60E+36	1.45E-10	1.34	0.0005							
4.11E+36	7.74E-11	1.36	0.0005							
1.06E+37	4.12E-11	1.38	0.0005							
2.73E+37	2.20E-11	1.4	0.0005							
7.03E+37	1.17E-11	1.42	0.0005							
1.81E+38	6.26E-12	1.44	0.0005							
4.66E+38	3.35E-12	1.46	0.0005							
1.20E+39	1.79E-12	1.48	0.0005							
3.09E+39	9.61E-13	1.5	0.0005							
currentsum	cathcurrentsum	Ecorr	delta	tempk=368	pH=3	galvaniccoeff=1	coroxrd3.ma	po2=0.21	Revised:6/21/97	run:6/21/97

6/26/98

HAND CHECK OF CALCULATIONS

eeqh2o = 0-(((2.303 x r x tempk)/f) x ph)

FROM FIRST LINE OF COXRD160 OUTPUT

eeqh2o = -0.2190

HAND CALCULATION

$$= 0 - \left(\left[\frac{2.303 \times r \times tempk}{f} \right] \times ph \right)$$

$$= 0 - \left(\left[\frac{2.303 \times 8.314 \times 368}{96485} \right] \times 3 \right)$$

$$= -0.2190$$

CALCULATED OUTPUT SAME AS HAND CALCULATION

6/26/98

HAND CHECK OF CALCULATIONS

eeqO2 = (1.47172 - O2overpotential) - (0.000815 x tempk)

O2overpotential = 0.0
tempk = 368

FROM COXRD160 OUTPUT P94 COL 2 ROW 2

eeqO2 = 1.1718

HAND CALCULATION

~~eeqO2 = 1.47172~~ 6/26/98

eeqO2 = (1.47172 - 0.0) - (0.000815 * 368)

eeqO2 = 1.47172 - (0.29992)

eeqO2 = 1.1718

CALCULATED OUTPUT FROM COXRD160 SAME AS HAND CALCULATION.

6/26/98

HANDCALCULATION)

ecqO2 = ecqOo2-((2.303 × r × tempk × ph)/f) +

(((0.576 × r × tempk × Log[pO2])/(2.303 × f))

r = 8.314
ph = 3
f = 96485
pO2 = 0.21
ecqOo2 = 1.1718 FROM P 103

note that Log IN MATHEMATICA 2.2.3 IS REALLY LN

ecqO2 = 1.1718-((2.303 × 8.314 × 368 × 3)/96485) +

(((0.576 × 8.314 × 368 × -1.560)/(2.303 × 96485)))

ecqO2 = 1.1718-(21,138)/96485)

+(-2,763 / 222,204)

ecqO2 = 1.1718 - 0.2190 - 0.0124

ecqO2 = 0.9403

FROM COXRD160 COL 3 ROW 2 ON P 94
ecqO2 IS CALCULATED TO BE 0.9403

CALCULATED OUTPUT FROM COXRD160 SAME AS HAND CALCULATION.

6/26/98

HAND CALCULATION)

khenryconst = Exp[0.2984 - (5596.17/TEMPK) +

1049670/(tempk × tempk)] * 1000

tempk = 368

khenryconst = Exp[0.2984 - 5596.17/368) +

1049670/368 × 368)] 1000

khenryconst = Exp[(0.2984 - 15.206) + 7.7509]*1000

khenryconst = Exp[-7.1576] 1000

khenryconst = 0.7789

VALUE CALCULATED IN COXRD160 IS 0.7789
P 94 COL 5 ROW 2

CALCULATED OUTPUT FROM COXRD160 AND HAND CALCULATION ARE THE SAME

cbulkO2 = khenryconst · pO2

cbulkO2 = 0.7789 × 0.21 = 0.1635

FROM COXRD160 COL 6 ROW 2 PAGE 94
cbulkO2 = 0.1635

CALCULATED VALUE OF cbulkO2 FROM COXRD160 SAME AS HAND CALCULATION.

6/26/98

HAND CALCULATION

do2 = (0.063 * Exp[(14.612/(r/1000)) x

((1/298.15) − (1/tempk))])/31536000

r = 8.314

tempk = 368

do2 = (0.063 x Exp[(14.612/(8.314/1000)) x

((1/298.15) − (1/368))])/31536000

6/26/98 ~~do2 = (0.063 x Exp[0.12148 x 0.000636]) 31536000~~

do2 = (0.063 x Exp[1703.39 x 0.000636]) 31536000

do2 = 6.10×10^{-9}

FROM COXRD160 do2 = 6.12×10^{-9}

CALCULATED VALUES FROM COXRD160 SAME AS HAND CALCULATED VALUES

hplusConc = 10^{-ph}

ph = 3

hplusconc = 10^{-3}

VALUE OF hplusConc SAME AS HAND CALCULATED VALUE

6/26/98

HAND CALCULATION

eferrous = −0.440 + ((0.0295 * LN[ferrous conc]/2.303)

ferrousconc = 1.0 E-6

eferrous = −0.440 + ((0.0295 * LN[1.0×10^{-6}]/2.303)

eferrous = −0.61696

FROM COXRD160 OUTPUT P 96 COL 1 ROW 2
eferrous = −0.61696

CALCULATED VALUE FROM COXRD160 SAME AS HAND CALCULATION.

i O o2 steel = i O o2 steel at 298K * Exp [(O2actenergy/(r/1000)) * ((1/298) − (1/tempk

WHERE
tempk = 368
i O o2 steel at 298k = 1×10^{-6}
o2 act energy = 40
r = 8.314

$$i\,O_o2\,steel = 10^{-6} \exp\left[\frac{40}{\frac{8.314}{1000}} \times \left(\frac{1}{298} - \frac{1}{368}\right)\right]$$

i O o2 steel = 2.15×10^{-5}

FROM COXRD160 iO_2 Steel = 2.15×10^{-5}
PAGE 96 COL 5 ROW 1

VALUE CALCULATED IN COXRD160 SAME AS HAND CALCULATION

7/7/98

HAND CALCULATION)

$iOh2osteelat298k = (2 \times f \times k1h2osteel) * hplusconc^{bh2o}$

k1 h2osteel = 5.18×10^{-8}
hplusconc = 0.001
bh2o = 0.250
f = 96485

$iOh2osteelat298k = (2 \times 96485 \times 5.18 \times 10^{-8}) * 0.001^{(0.250)}$

iOh2osteel at 298k = 0.00177

VALUE FROM COXRD160 FOR iOh2osteelat298k = 0.00177
P 96 COL 6 ROW 2
VALUE CALCULATED IN COXRD160 SAME AS
HAND CALCULATION.

$iOh2osteel = iOh2osteelat298k \times Exp[(h2oactenergy/(r/1000)) * ((1/298) - (1/tempk))]$

iOh2osteelat298k = 0.00177
r = 8.314
tempk = 368
h2oactenergy = 20

$iOh2osteel = 0.00177 \times Exp\left[\frac{20}{\frac{8.314}{1000}} \times \frac{1}{298} - \frac{1}{368}\right]$

iOh2osteel = 0.0082

VALUE FROM COXRD160 = 0.0082
PAGE 96 COL 7 ROW 2

VALUE CALCULATED BY COXRD160 AND
HAND CALCULATION ARE THE SAME

Daniel D 7/8/98

$iOh2o825at298k = (2 * f * k1h2o825) hplusconc^{bh2o}$

f = 96485
k1h2o825 = 5.18×10^{-8}
hplusconc = 0.001
bh2o = 0.250

$iOh2o825at298k = (2 \times 96485 \times 5.18 \times 10^{-8}) * 0.001^{0.250}$

iOh2o825 at 298k = 0.00177

VALUE FROM COXRD160 = 0.00177 P96 COL 12 ROW 2

VALUE CALCULATED BY COXRD160 AND HAND CALCULATION
ARE THE SAME:

$iOo2825 = iOo2825at298k \times Exp[(o2actenergy/(r/1000)) \times ((1/298) - (1/tempk))]$

o2actenergy = 40
r = 8.314
iOo2825at298k = 10^{-6}
tempk = 368

$iOo2825 = 10^{-6} \times Exp\left[\left(\frac{40}{\frac{8.314}{1000}}\right) \times \frac{1}{298} - \frac{1}{368}\right]$

iOo2825 = 2.15×10^{-5}

VALUE CALCULATED IN COXRD160 = 2.15×10^{-5}
P 98 COL 3 ROW 2

VALUE CALCULATED IN COXRD160 AND HAND
CALCULATION ARE THE SAME.

Daniel Dunn 7/8/98

$iOh2o825 = iOh2o825 at 298k * Exp[(h2oactenergy/(r/1000)) * ((1/298) - (1/tempk))]$

iOh2o825at298k = 0.00177
h2oactenergy = 20
r = 8.314
tempk = 368

$$iOh2o825 = 0.00177 * Exp\left[\left(\frac{20}{\frac{8.314}{1000}}\right) * \frac{1}{298} - \frac{1}{368}\right]$$

iOh2o825 = 0.0082

VALUE CALCULATED BY CORROD160 = 0.0082
P 98 COL 1 ROW 2

VALUE CALCULATED BY CORROD160 AND HAND CALCULATION ARE THE SAME.

$istel = iOferrous * (Exp[(afe \times zfe \times f(ecorr - eferrous))/(r\ tempk)])$

iOferrous = 0.0001
afe = 0.750
zfe = 2
f = 96485
eferrous = -0.6169
ecorr = -0.6 (ROW 47)

$istel = 0.0001 * (Exp[(0.750 \times 2 \times 96485(-0.6 - (-0.6169)))/8.314(368)])$

$istel = 2.2 \times 10^{-4}$

VALUE FROM CORROD160 = 2.2×10^{-4}
P 96 COL 7 ROW 47

7/8/98

GALVAN07 / GALVAN08 / GALVAN08b

OBJECTIVE SAME AS GALVAN01.MA

Parameters and input: same as galvan06

Changes from GALVAN06

The passive surface of steel is considered and the reduction of O_2 is assumed to occur on the passive steel fraction. No reduction reactions occur on the active steel fraction

RUNS

A TOTAL OF 31 RUNS SAVED AS GV8***.ma
OUTPUTS ALSO CONVERTED TO EXCEL FILES

3/1/2001

GALVAN08b

GALVANIC CORROSION
Darrell S. Dunn

The galvanic corrosion of carbon steel and Alloy 825 are addressed on the basis of the kinetics of electrochemical reactions including the reduction of water and oxygen. This calculation assumes that carbon steel is pure iron. A fraction of the carbon steel area is active and the remainder is passive. The active dissolution rate is controlled by Tafel kinetics. The passive dissolution rate of both carbon steel and Alloy 825 are specified as input parameters. The reduction of oxygen and water occur only on the surface of Alloy 825 and the passive surface of carbon steel. The rate of oxygen reduction is assumed to diffusion limited. The kinetics of water reduction are modeled after Bockris and Reddy (Modern Electrochemistry Vol. 2). The coefficient of galvanic galvanic coupling is included.

PARAMETERS

carbon steel

ipasssteel=corrosion current density for passive carbon steel (input)
isteelactive=corrosion current density for active carbon steel (calculated)
isteel=corrosion current density for carbon steel both active and passive (calculated)
isteelwp=corrosion current density for carbon steel waste package (calculated)
arsteel=area of steel (input)
arsteelpass=area of steel that is passive (calculated)
arsteelactive=area of steel that is active (calculated)
arfractsteelpassive=area fraction of steel that is passive (input)
ecorrsteelactive=corrosion potential for steel under active conditions (calculated)
ecorrsteelpassive=corrosion potential for steel under passive conditions (calculated)
ecorrsteel=corrosion potential for steel including both active and passive surfaces (calculated)
ecorrsteelwp=corrosion potential of the carbon steel waste package (calculated)
afe=beta or partition coefficient for iron dissolution (input)
zfe=number of electrons from corrosion of iron (2)
ih2osteel=current density from water reduction on carbon steel (calculated)
ih2osteelwp=current density from water reduction on carbon steel waste package (calculated)
i0h2osteel=exchange current density water reduction on active carbon steel (calculated)
i0h2osteelpassive=exchange current density water reduction on passive carbon steel (calculated)
i0h2osteelat298k=exchange current density water reduction on active steel at 298 K (literature)
i0h2opassivesteelat298k=exchange current density water reduction on passive steel at 298 K (literature)
k1h2osteel=constant for water reduction on steel (input)
io2steel=cathodic current density from the reduction of oxygen on steel (calculated)

3/1/2000

GALVAN08b

io2steelwp=cathodic current density from the reduction of oxygen on steel (calculated)
i0o2steel=exchange current density for the reduction of oxygen (calculated)
i0o2steelat298k=exchange current density oxygen reduction on steel at 298 K (literature)
i0ferrous=exchange current density for the dissolution of iron (literature)
ferrousconc=concentration of ferrous iron in mol/liter (input)
eferrous=equilibrium potential for the dissolution of iron (calculated)

alloy 825

ipass825=passive current density of alloy 825 (input)
ar825=area of alloy 825 (input)
io2825=current density oxygen reduction on alloy 825 (calculated)
io2825wp=current density oxygen reduction on alloy 825 waste package (calculated)
i0o2825=exchange current density oxygen reduction alloy 825 (calculated)
i0o2825at298k=exchange current density oxygen reduction alloy 825 at 298K (input)
ih2o825=current density from water reduction on alloy 825 (calculated)
ih2o825wp=current density from water reduction on alloy 825 (calculated)
i0h2o825=exchange current density water reduction alloy 825 (calculated)
i0h2o825at298k=exchange current density water reduction alloy 825 at 298 K (literature)
ecorr825=corrosion potential of alloy 825 not in contact with other metals(calculated)
e825wp=corrosion potential of alloy 825 waste package barrier with or without galvanic contact(calculated)

oxygen reduction

zo2=number of electrons in the reduction of oxygen (4) (input)
bo2=beta or partition coeff for the reduction of oxygen (input)
khenryconst=henry's constant (calculated)
cbulko2=bulk concentration of oxygen (calculated)
do2=diffusion coeff for oxygen (calculated)
eeq0o2=standard potential for the reduction of oxygen (calculated)
eeqo2=equilibrium potential for the reduction of oxygen (calculated)
eeqo2passivesteel=equilibrium potential for the reduction of oxygen on passive steel (calculated)
po2=partial pressure of oxygen (0.21) (input)
o2actenergy=activation energy for the reduction of oxygen (literature) (input)
o2overpotential=overpoential for the reduction of oxygen

water reduction

zh2o=number of electrons in the reduction of water (2) (input)
bh2o=beta or partition coeff for the reduction of water (input)
eeqh2o=equlibrium potential for water reduction (calculated)
eeqh2opassivesteel=equlibrium potential for water reduction (calculated)
h2oactenergy=activation energy for the reduction of water (input)
hplusconc=concentration of H+ (calculated from pH)
hplusconcpassivesteel=concentration of H+ (calculated from pH)
k1h2o825=constant for water reduction (input)
k1h2osteel=constant for water reduction (input)

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GALVAN08b

other parameters

f=faradays constant (input)
r=gas constant (input)
ph=ph of solution contacting Alloy 825 and A516 steel(-log[H+]) (input)
phpassivesteel=ph (-log[H+]) on the passive steel surface (input)
tempk=temperature in degrees kelvin (input)
delta=diffision layer thickness (input)
ecouple=potential of perfect galvanic couple of alloy 825and carbon steel (calculated)
galvaniccoeff=coefficient of galvainc coupling, 1=complete coupling, 0=complete insulation(input)
currentsum=sum of currents

Input

```
zh2o=2;
f=96485;
r=8.314;
zo2=4;
bo2=0.250;
bh2o=0.250;
zfe=2;
ipass825=0.001;
ipasssteel=0.001;
ar825=0.000314;
arsteel=0.00251;
arfractsteelpassive=0.90909;
afe=0.75;
po2=0.21;
tempk=368;
ph=5;
phpassivesteel=10;
o2actenergy=40;
h2oactenergy=20;
k1h2o825=0.0000000518;
i0o2825at298k=0.000001;
ferrousconc=0.000001;
i0ferrous=0.0001;
k1h2osteel=0.0000000518;
i0o2steelat298k=0.000001;
o2overpotential=0.0;
delta=0.0005;
```

3/1/2000

GALVAN08b

```
Off[General::spell]
Off[General::spell1]
SetOptions[$Output, PageWidth->1200]

Print["eeqh2o","","eeqh2opassivesteel","","eeq0o2","","eeqo2","","eeqo2passivesteel","","o2overpotential","
","khenryconst"," ","cbulko2"," ","do2"," ","temp"," ","ph"," ","hplusconc"," ","phpassivesteel","
","hplusconcpassivesteel"," ","h2oactenergy"," ","o2actenergy"," ","bo2"," ","bh2o"," ","afe"," ","arsteel","
","arsteelpass"," ","arsteelactive"," ","arfractsteelpassive"," ","ar825"," ","ferrousconc"," ","eferrous","
","i0ferrous"," ","k1h2osteel"," ","i0o2steelat298k"," ","i0o2steel"," ","i0h2osteelat298k","
","i0h2opassivesteelat298k"," ","i0h2osteel"," ","i0h2osteelpassive"," ","isteel"," ","isteelpass","
","isteelactive"," ","ih2osteel"," ","io2steel"," ","k1h2o825"," ","i0h2o825at298k"," ","i0h2o825","
","i0o2825at298k","","i0o2825","","ipass825","","ih2o825","","io2825","","isteelwp","","isteelactivewp","
","ih2osteelwp"," ","io2steelwp"," ","ih2o825wp"," ","io2825wp"," ","arsteel*isteelwp","
","arsteel*ih2osteelwp"," ","arsteel*io2steelwp"," ","ar825*ipass825"," ","ar825*ih2o825wp","
","ar825*io2825wp","","currentsum","","cathcurrsum","","potentialdrop","","resistance","","ecorrsteel","
","ecorrsteelpassive"," ","ecorrsteelactive"," ","Ecouple"," ","Ecorr825"," ","Ecorrsteelwp","
","E825wastepackage"," ","galvaniccoeff"," ","istp"," ","tempk=",tempk," ","pH=",ph,"
","pHpassivesteel=",phpassivesteel," ","ar825=",ar825," ","arsteel=",arsteel," ","delta=",delta,"
","galvan08.ma","","po2=",po2,"","2/07/2000Revised:2/07/2000","","run:2/7/2000"]

Do[
eeqh2o=0-(((2.303*r*tempk)/f)*ph);

eeqh2opassivesteel=0-(((2.303*r*tempk)/f)*phpassivesteel);

eeq0o2=(1.47172-o2overpotential)-(0.000815*tempk);

eeqo2=eeq0o2-((2.303*r*tempk*ph)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));

eeqo2passivesteel=eeq0o2-
((2.303*r*tempk*phpassivesteel)/f)+((0.576*r*tempk*Log[po2])/(2.303*f));

khenryconst=Exp[0.2984-(5596.17/tempk)+(1049670/(tempk*tempk))]*1000;

cbulko2=khenryconst*po2;

do2=(0.063*Exp[(14.612/(r/1000))*((1/298.15)-(1/tempk))])/31536000;

hplusconc=10^-ph;

hplusconcpassivesteel=10^-phpassivesteel;
```

3/1/2000

GALVAN 08a

```
eferrous=-0.440+((0.0295*Log[ferrousconc])/2.303);

i0o2steel=i0o2steelat298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2osteelat298k=(2*f*k1h2osteel)*hplusconc^bh2o;

i0h2opassivesteelat298k=(2*f*k1h2osteel)*hplusconcpassivesteel^bh2o;

i0h2osteel=i0h2osteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2osteelpassive=i0h2opassivesteelat298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

i0o2825=i0o2825at298k*Exp[(o2actenergy/(r/1000))*((1/298)-(1/tempk))];

i0h2o825at298k=(2*f*k1h2o825)*hplusconc^bh2o;

i0h2o825=i0h2o825at298k*Exp[(h2oactenergy/(r/1000))*((1/298)-(1/tempk))];

arsteelpass=arfractsteelpassive*arsteel;

arsteelactive=(1-arfractsteelpassive)*arsteel;

corrsteelactive=ecorrsteelactive /. FindRoot[i0ferrous*(Exp[(afe zfe f (ecorrsteelactive - eferrous))/(r tempk)])-
(i0h2osteel*(Exp[-(bh2o zh2o f (ecorrsteelactive - eeqh2o))/(r tempk)])+i0o2steel*((Exp[-(bo2 zo2 f
(ecorrsteelactive - eeqo2))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteelactive - eeqo2))/(r
tempk)])/(cbulko2 4 f do2)))))==0, {ecorrsteelactive,0}, MaxIterations->500];

corrsteelpassive=ecorrsteelpassive /. FindRoot[ipasssteel-(i0h2osteelpassive*(Exp[-(bh2o zh2o f
(ecorrsteelpassive - eeqh2opassivesteel))/(r tempk)])+i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteelpassive -
eeqo2passivesteel))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteelpassive - eeqo2passivesteel))/(r
tempk)])/(cbulko2 4 f do2)))))==0, {ecorrsteelpassive,0}, MaxIterations->500];

corrsteelpass=ecorrsteelpass /. FindRoot[i0ferrous*(Exp[(afe zfe f (ecorrsteelpass - eferrous))/(r tempk)])-
(ipasssteel)==0, {ecorrsteelpass,0}, MaxIterations->500];

isteelpassivearea=((i0ferrous*(Exp[(afe zfe f (corrsteelpass- eferrous))/(r tempk)]))*(arfractsteelpassive));

isteelp=((i0ferrous*(Exp[(afe zfe f (corrsteelpassive - eferrous))/(r tempk)]))*(arfractsteelpassive));

If[isteelpassivearea>isteelp,istp=isteelp,istp=isteelpassivearea];
```

3/1/2000

GALVAN 08b

```
corrsteel=ecorrsteel /. FindRoot[arsteelactive*i0ferrous*(Exp[(afe zfe f (ecorrsteel - eferrous))/(r tempk)]) +
istp*arsteelpass-((arsteelpass*i0h2osteelpassive*(Exp[-(bh2o zh2o f (ecorrsteel - eeqh2opassivesteel))/(r
tempk)])+arsteelpass*i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteel - eeqo2passivesteel))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteel - eeqo2passivesteel))/(r tempk)])/(cbulko2 4 f do2)))))==0,
{ecorrsteel,0}, MaxIterations->500];

isteelactive=((i0ferrous*(Exp[(afe zfe f (corrsteel - eferrous))/(r tempk)]))*(1-arfractsteelpassive));

isteel=((i0ferrous*(Exp[(afe zfe f (corrsteel - eferrous))/(r tempk)]))*(1-
arfractsteelpassive))+(ipasssteel*arfractsteelpassive);

ih2osteel=(i0h2osteelpassive*(Exp[-(bh2o zh2o f (corrsteel - eeqh2opassivesteel))/(r
tempk)])*(arfractsteelpassive));

io2steel=((i0o2steel*((Exp[-(bo2 zo2 f (corrsteel - eeqo2passivesteel))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-
(zo2 bo2 f (corrsteel - eeqo2passivesteel))/(r tempk)])/(cbulko2 4 f do2)))))*(arfractsteelpassive));

corr825=ecorr825 /. FindRoot[ipass825-(i0h2o825*(Exp[-(bh2o zh2o f (ecorr825 - eeqh2o))/(r
tempk)])+i0o2825*((Exp[-(bo2 zo2 f (ecorr825 - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f
(ecorr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))))==0, {ecorr825,0}, MaxIterations->500];

ih2o825=i0h2o825*(Exp[-(bh2o zh2o f (corr825 - eeqh2o))/(r tempk)]);

io2825=i0o2825*((Exp[-(bo2 zo2 f (corr825 - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f
(corr825 - eeqo2))/(r tempk)])/(cbulko2 4 f do2))));

couple=ecouple /. FindRoot[arsteelactive*i0ferrous*(Exp[(afe zfe f (ecouple - eferrous))/(r tempk)])
+ipass825*ar825 + istp*arsteelpass-((arsteelpass*i0h2osteelpassive*(Exp[-(bh2o zh2o f (ecouple -
eeqh2opassivesteel))/(r tempk)])+arsteelpass*i0o2steel*((Exp[-(bo2 zo2 f (ecouple - eeqo2passivesteel))/(r
tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2passivesteel))/(r tempk)])/(cbulko2 4 f
do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (ecouple - eeqh2o))/(r tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2
f (ecouple - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f (ecouple - eeqo2))/(r tempk)])/(cbulko2
4 f do2)))))==0, {ecouple,0}, MaxIterations->500];

e825wp=((1-galvaniccoeff)*corr825) + galvaniccoeff*couple;
```

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```
corrsteelwp=ecorrsteelwp /. FindRoot[arsteelactive*i0ferrous*(Exp[(afe zfe f (ecorrsteelwp - eferrous))/(r
tempk)]) + istp*arsteelpass+ipass825*ar825-((arsteelpass*i0h2osteelpassive*(Exp[-(bh2o zh2o f (ecorrsteelwp
- eeqh2opassivesteel))/(r tempk)])+arsteelpass*i0o2steel*((Exp[-(bo2 zo2 f (ecorrsteelwp -
eeqo2passivesteel))/(r tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (ecorrsteelwp - eeqo2passivesteel))/(r
tempk)])/(cbulko2 4 f do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r
tempk)])+ar825*i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2
f (e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2))))))==0, {ecorrsteelwp,0}, MaxIterations->500];

isteelactivewp=((i0ferrous*(Exp[(afe zfe f (corrsteelwp - eferrous))/(r tempk)]))*(1-arfractsteelpassive));

isteelwp=((i0ferrous*(Exp[(afe zfe f (corrsteelwp - eferrous))/(r tempk)]))*(1-
arfractsteelpassive))+istp*arfractsteelpassive;


ih2osteelwp=(i0h2osteelpassive*(Exp[-(bh2o zh2o f (corrsteelwp - eeqh2opassivesteel))/(r
tempk)])*(arfractsteelpassive));

io2steelwp=((i0o2steel*((Exp[-(bo2 zo2 f (corrsteelwp - eeqo2passivesteel))/(r tempk)])/(1 +
((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteelwp - eeqo2passivesteel))/(r tempk)])/(cbulko2 4 f
do2)))))*(arfractsteelpassive));

ih2o825wp=i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)]);

io2825wp=i0o2825*((Exp[-(bo2 zo2 f (e825wp - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f
(e825wp - eeqo2))/(r tempk)])/(cbulko2 4 f do2)))));

currentsum=arsteelactive*i0ferrous*(Exp[(afe zfe f (corrsteelwp - eferrous))/(r tempk)]) +
istp*arsteelpass+ipass825*ar825-((arsteelpass*i0h2osteelpassive*(Exp[-(bh2o zh2o f (corrsteelwp -
eeqh2opassivesteel))/(r tempk)])+arsteelpass*i0o2steel*((Exp[-(bo2 zo2 f (corrsteelwp - eeqo2passivesteel))/(r
tempk)])/(1 + ((i0o2steel*delta*Exp[-(zo2 bo2 f (corrsteelwp - eeqo2passivesteel))/(r tempk)])/(cbulko2 4 f
do2)))))+(ar825*i0h2o825*(Exp[-(bh2o zh2o f (e825wp - eeqh2o))/(r tempk)])+ar825*i0o2825*((Exp[-(bo2
zo2 f (e825wp - eeqo2))/(r tempk)])/(1 + ((i0o2825*delta*Exp[-(zo2 bo2 f (e825wp - eeqo2))/(r
tempk)])/(cbulko2 4 f do2))))));

cathcurrsum=ar825*ih2o825wp-ar825*io2825wp-arsteel*ih2osteelwp-arsteel*io2steelwp;

anodiccurrsum=arsteel*isteelactivewp+istp*arsteelpass+ar825*ipass825;

potentialdrop=e825wp-corrsteelwp;

resistance=Abs[potentialdrop/anodiccurrsum];
```

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```
Print[FortranForm[eeqh2o]," ",FortranForm[eeqh2opassivesteel]," ",FortranForm[eeq0o2]," ",FortranForm[eeqo2]," ",FortranForm[eeqo2passivesteel]," ",FortranForm[o2overpotential]," ",FortranForm[khenryconst]," ",FortranForm[cbulko2]," ",FortranForm[do2]," ",FortranForm[tempk]," ",FortranForm[ph]," ",FortranForm[hplusconc]," ",FortranForm[phpassivesteel]," ",FortranForm[hplusconcpassivesteel]," ",FortranForm[h2oactenergy]," ",FortranForm[o2actenergy]," ",FortranForm[bo2]," ",FortranForm[bh2o]," ",FortranForm[afe]," ",FortranForm[arsteel]," ",FortranForm[arsteelpass]," ",FortranForm[arsteelactive]," ",FortranForm[arfractsteelpassive]," ",FortranForm[ar825]," ",FortranForm[ferrousconc]," ",FortranForm[eferrous]," ",FortranForm[i0ferrous]," ",FortranForm[k1h2osteel]," ",FortranForm[i0o2steelat298k]," ",FortranForm[i0o2steel]," ",FortranForm[i0h2osteelat298k]," ",FortranForm[i0h2opassivesteelat298k]," ",FortranForm[i0h2osteel]," ",FortranForm[i0h2osteelpassive]," ",FortranForm[isteel]," ",FortranForm[ipasssteel]," ",FortranForm[isteelactive]," ",FortranForm[ih2osteel]," ",FortranForm[io2steel]," ",FortranForm[k1h2o825]," ",FortranForm[i0h2o825at298k]," ",FortranForm[i0h2o825]," ",FortranForm[i0o2825at298k]," ",FortranForm[i0o2825]," ",FortranForm[ipass825]," ",FortranForm[ih2o825]," ",FortranForm[io2825]," ",FortranForm[isteelwp]," ",FortranForm[isteelactivewp]," ",FortranForm[ih2osteelwp]," ",FortranForm[io2steelwp]," ",FortranForm[ih2o825wp]," ",FortranForm[io2825wp]," ",FortranForm[arsteel*isteelwp]," ",FortranForm[arsteel*ih2osteelwp]," ",FortranForm[arsteel*io2steelwp]," ",FortranForm[ar825*ipass825]," ",FortranForm[ar825*ih2o825wp]," ",FortranForm[ar825*io2825wp]," ",FortranForm[currentsum]," ",FortranForm[cathcurrsum]," ",FortranForm[potentialdrop]," ",FortranForm[resistance]," ",FortranForm[corrsteel]," ",FortranForm[corrsteelpassive]," ",FortranForm[corrsteelactive]," ",FortranForm[couple]," ",FortranForm[corr825]," ",FortranForm[corrsteelwp]," ",FortranForm[e825wp]," ",FortranForm[galvaniccoeff]," ",FortranForm[istp]],{galvaniccoeff,0.0,1.0,0.05}]
```

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I have reviewed this notebook and find it in compliance with QAP-001. There is sufficient information regarding procedures used for conducting tests, acquiring and analyzing data so than another qualified individual could repeat the activity.

N. Sridhar 6/8/2000

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 213

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File Types: (.exe, .bat, .zip, etc.)	xls, ma, mb
Remarks: (computer runs, etc.)	Media contains: Calculations for galvanic corrosion potential based on kinetics for reduction of oxygen and water, passive dissolution of inner Ni base material and active dissolution of the carbon steel overpack to determine the potential for galvanic couple of carbon steel and Ni base container materials.