

## Matlab Codes –

### 1) Fe-FeO equilibrium code –

```
T=linspace(300,1500,100);%Temperature
%% DeltaG= DeltaG0_net+ 8.314*T*log(Keq)
% Keq= pH2O/pH2 , since activity of pure solid Fe, FeO and Fe3O4 is 1.
%% For stability of Fe and FeO, Reaction:- FeO(s) + H2 = Fe(s) + H2O (g):
DeltaG0_1= 12300 - 6.65*T; % in J/mol
Keq1 = -(DeltaG0_1./(8.314*T));
m1=1./(1+exp(Keq1));
plot(T,m1,"*", "MarkerSize",5);
%% Labelling
xlabel("Temperature,K");
ylabel("p_{H2}/p_{H2O}+p_{H2}");
ylim([0 1]);
xlim([200 1600]);
title("Stability In different Region");
text(600,0.5,"Region I","Color","b")
text(570,0.45,"FeO is stable")
text(1200,0.9,"Region II","Color","b")
text(1170,0.85,"Fe is stable")
```

### 2) FeO-Fe<sub>3</sub>O<sub>4</sub> equilibrium code –

```
T=linspace(300,1500,100);%Temperature
%% DeltaG= DeltaG0_net+ 8.314*T*log(Keq)
% Keq= pH2O/pH2 , since activity of pure solid Fe, FeO and Fe3O4 is 1.
%% For stability of FeO and Fe3O4, Reaction:- Fe3O4 + H2 = 3FeO(s) + H2O(g)
DeltaG0_2= 64900 - 69.25*T; % in J/mol
Keq2 = -(DeltaG0_2./(8.314*T));
m2=1./(1+exp(Keq2));
plot(T,m2,"*", "MarkerSize",5);
%% Labelling
xlabel("Temperature,K");
ylabel("p_{H2}/p_{H2O}+p_{H2}");
ylim([0 1]);
xlim([200 1600]);
title("Stability In different Region");
text(600,0.5,"Region I","Color","b")
text(570,0.45,"Fe3O4 is stable")
text(1200,0.9,"Region II","Color","b")
text(1170,0.85,"FeO is stable")
```

### 3) Fe-Fe<sub>3</sub>O<sub>4</sub> equilibrium code –

```
T=linspace(300,1500,100);%Temperature
%% DeltaG= DeltaG0_net+ 8.314*T*log(Keq)
```

```

% Keq= (pH20/pH2)^4, factor of 4 taken in gibbs free energy equation, since activity
of pure solid Fe, Feo and Fe3O4 is 1.
%% For stability of Fe and Fe3O4, Reaction:- Fe3O4 + 4H2 = 3Fe(s) + 4H2O(g)
DeltaG0_3= 101800 - 89.2*T; % in J/mol
Keq3 = -(DeltaG0_3./(4*8.314*T));
m3=1./(1+exp(Keq3));
plot(T,m3,"*", "MarkerSize",5);
%% Labelling
xlabel("Temperature,K");
ylabel("p_{H2}/p_{H20}+p_{H2}");
ylim([0 1]);
xlim([200 1600]);
title("Stability In different Region");
text(600,0.5,"Region I", "Color", "b")
text(570,0.45,"Fe3O4 is stable")
text(1200,0.9,"Region II", "Color", "b")
text(1170,0.85,"Fe is stable")

```

#### 4) All in one stability plot –

```

T=linspace(300,845.455,70);%Temperature
T1=linspace(845.455,1500,70);
%% DeltaG= DeltaG0_net+ 8.314*T*log(Keq)
% Keq= pH20/pH2 , since activity of pure solid Fe, Feo and Fe3O4 is 1.
%% For stability of Fe and FeO, Reaction:- FeO(s) + H2 = Fe(s) + H2O (g):
DeltaG0_1= 12300 - 6.65*T1; % in J/mol
Keq1 = -(DeltaG0_1./(8.314*T1));
m1=1./(1+exp(Keq1));
plot(T1,m1,"*", "MarkerSize",5);
hold on;
%% For stability of FeO and Fe3O4, Reaction:- Fe3O4 + H2 = 3FeO(s) + H2O(g)
DeltaG0_2= 64900 - 69.25*T1; % in J/mol
Keq2 = -(DeltaG0_2./(8.314*T1));
m2=1./(1+exp(Keq2));
plot(T1,m2,"*", "MarkerSize",5);
hold on;
%% For stability of Fe and Fe3O4, Reaction:- Fe3O4 + 4H2 = 3Fe(s) + 4H2O(g)
DeltaG0_3= 101800 - 89.2*T; % in J/mol
Keq3 = -(DeltaG0_3./(4*8.314*T));
m3=1./(1+exp(Keq3));
plot(T,m3,"*", "MarkerSize",5);
hold off;
%% Labelling
xlabel("Temperature,K");
ylabel("p_{H2}/p_{H20}+p_{H2}");
ylim([0 1]);
xlim([200 1600]);
title("Stability In different Region");
legend(["FeO to Fe", "Fe3O4 to FeO", "Fe3O4 to Fe"])

```

```
text(550,0.5,"Region I","Color","b")
text(520,0.45,"Fe3O4 is stable")
text(1130,0.75,"Region II","Color","b")
text(1100,0.7,"Fe is stable")
text(1200,0.3,"Region II","Color","b")
text(1170,0.25,"FeO is stable")
```