MM209

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PROBLEM

Write a program which will give the CO/CO_2 composition and total pressure to achieve desired carbon concentration at the surface of the steel. Please note that the steel should not get oxidized.

OBJECTIVE

C's activity is initially zero as we flush the CO and CO_2 mixture on a pure steel surface. $\Delta G \to -\infty$, and hence C starts spontaneously depositing on the surface. We can get the desired concentration of C deposited by adjusting total Pressure and CO/CO_2 composition in the gas that is being flushed.

When a_c on the surface and in the gas will be equal, carburization will stop. Thermodynamically, soot will be formed till activity becomes 1. Still, due to kinetic reasons such as nucleation and surface energy, soot can be created for activity greater than one as well.

In the process, O_2 is also formed, and we need to make sure that it does not oxidize Fe to FeO.

APPROACH

First, we solve the following equilibrium reaction:

$$C + CO_2 = 2CO$$

$K_{eq} = (P_{CO})^2/((P_{CO2})*(a_c))$; where a_c is activity of C in gaseous phase

$K_{eq} = e^{-\Delta G°/RT}$

$\Delta G° = 2\Delta G°_{CO} - \Delta G°_{CO2}$

$P_{CO} + P_{CO2} = P_{Total}$

We find a_c for a range of values of P_{Total} and P_{CO}/P_{CO2} and calculate the mole fraction of C on a Steel surface using the following equation:

$$a_c = k \cdot X_c \cdot (1+2X_c)/(1-X_c-12X_c^2)$$

$$\log_{10}k = (2000/T) - 0.8$$

We solve the above equation in an iterative manner to find the value of X_c from k and a_c From X_c , we calculate Wt% of C using the following equation:

$$Wt\% \ C = X_c \cdot 100 \cdot MW_{Fe} / MW_c \text{ where MW = Molecular weight}$$

Note: that this equation can only be used for dilute solutions.

Now we check the values of Wt % C, which satisfy our requirement and corresponding P_{CO}/P_{CO2} values.

To check FeO's oxidation, we first find partial pressure of O_2 from the following equilibrium reaction.

$$CO + 0.5O_2 = CO_2$$

$K_{eq} = (P_{CO2})/((P_{CO})^2 * (P_{O2})^{0.5})$
$K_{eq} = e^{-\Delta G°/RT}$
$\Delta G° = \Delta G°_{CO2} - \Delta G°_{CO}$

We check whether the O_2 composition can oxidize Fe.

$$Fe + 0.5O_2 = FeO \leftarrow \Delta G°_f$$

$K_{eq} = (a_{FeO})/((a_{Fe}) * (P_{O2})^{0.5})$

We consider Fe and FeO to be pure and hence their activities to be equal to 1

$\Delta G = \Delta G°_f + RT \ln (1/(P_{O2})^{0.5})$

If $\Delta G<0$, then oxidation would occur, and hence we would reject the value of CO/CO_2 composition and PTotal
If $\Delta G > 0$, we accept the value of CO/CO_2 composition and PTotal

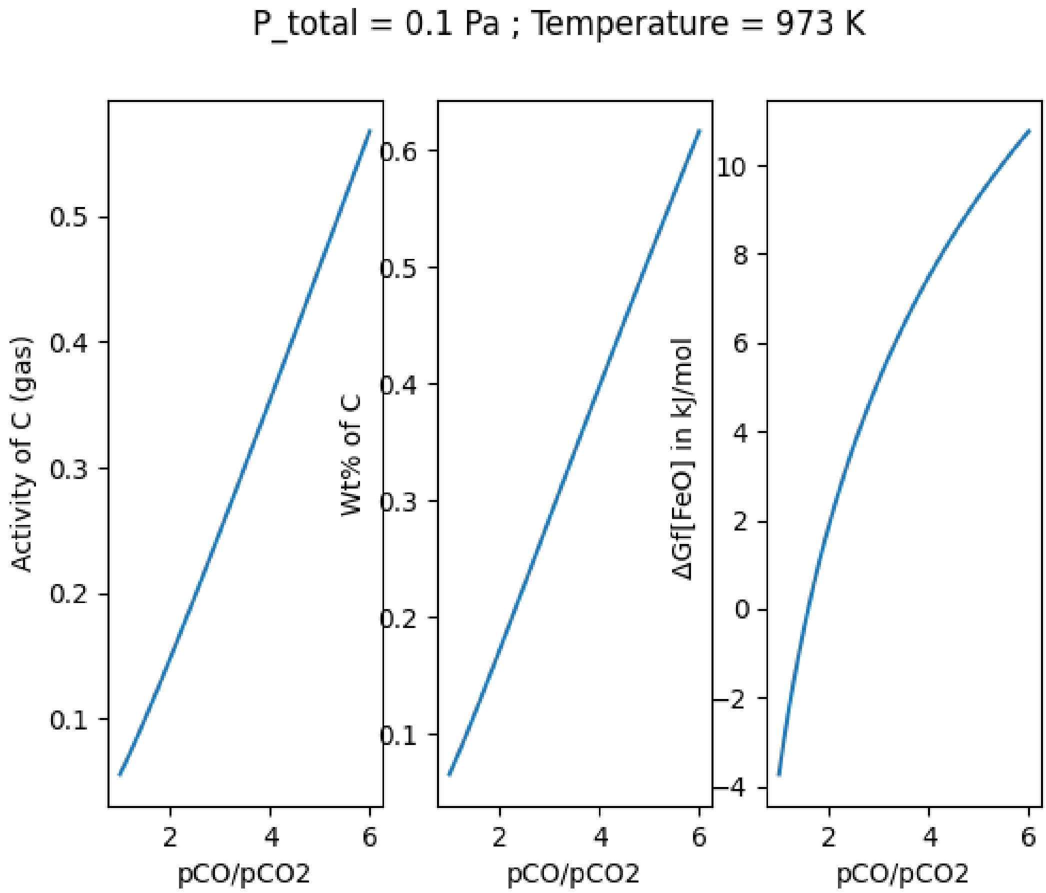
RESULTS

We ran the code for different values of Total pressure at a temperature of 973 K and desired Wt% of C between 0.2 and 0.4. We have plotted the graph for P_{CO}/P_{CO2} ranging from 1 to 6

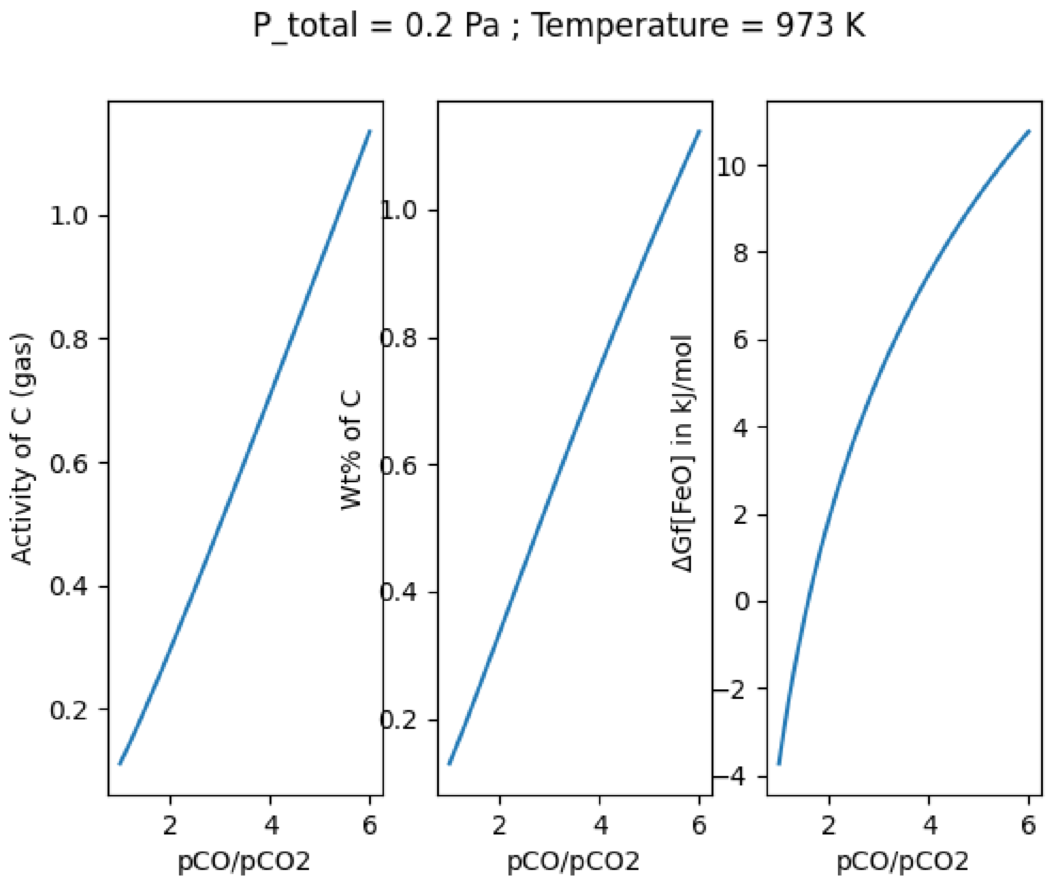
1st graph: Activity of C v/s P_{CO}/P_{CO2}
2nd graph: Wt% of C v/s P_{CO}/P_{CO2}
3rd graph: ΔG formation of FeO v/s P_{CO}/P_{CO2}

Following are some of the results that we obtained:

1. For Total pressure of 0.1 pascals
   The lower limit of desired Wt% of Carbon 0.2
   The upper limit of desired Wt% of Carbon 0.4
   Allowed values of CO/CO_2 composition ratio are from 2.326 to 3.959



2. For Total pressure of 0.2 pascals
   The lower limit of desired Wt% of Carbon 0.2
   The upper limit of desired Wt% of Carbon 0.4
   Allowed values of CO/CO_2 composition ratio are from 1.612 to 2.224

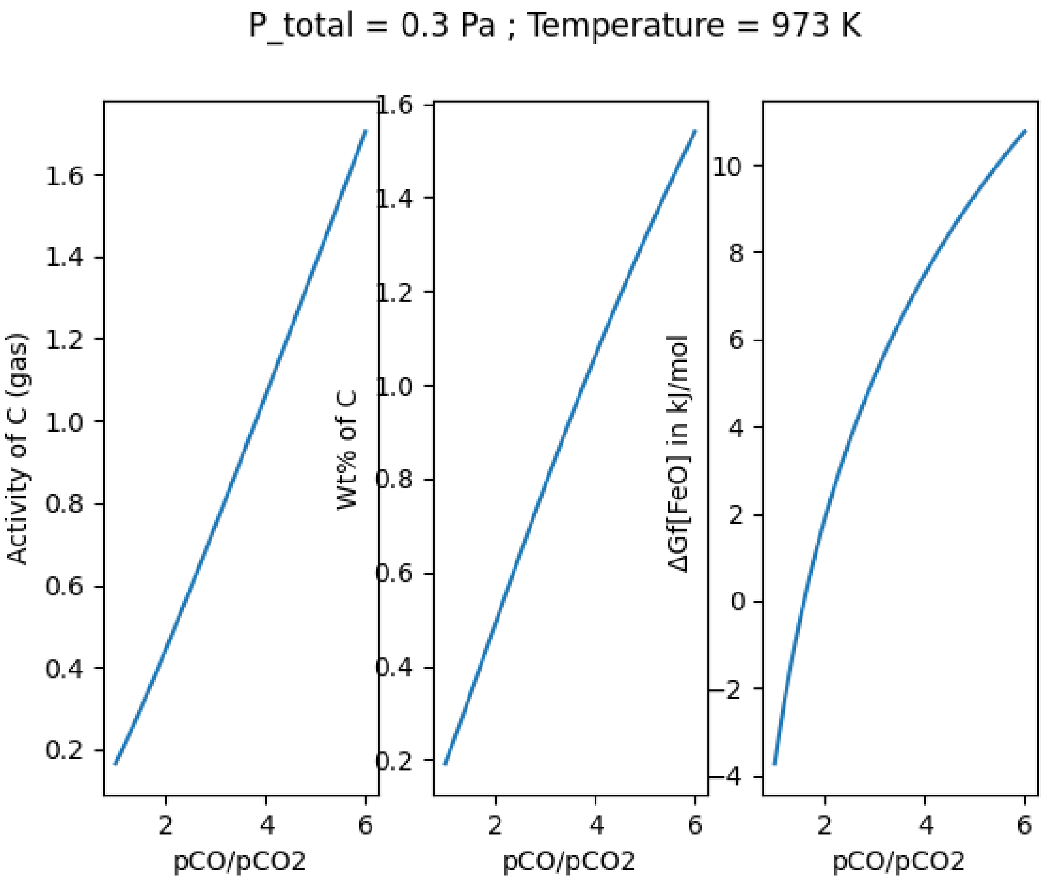


3. For Total pressure of 0.3 pascals

The lower limit of desired Wt% of Carbon 0.2

The upper limit of desired Wt% of Carbon 0.4

Allowed values of CO/CO_2 composition ratio are from1.612 to 1.612

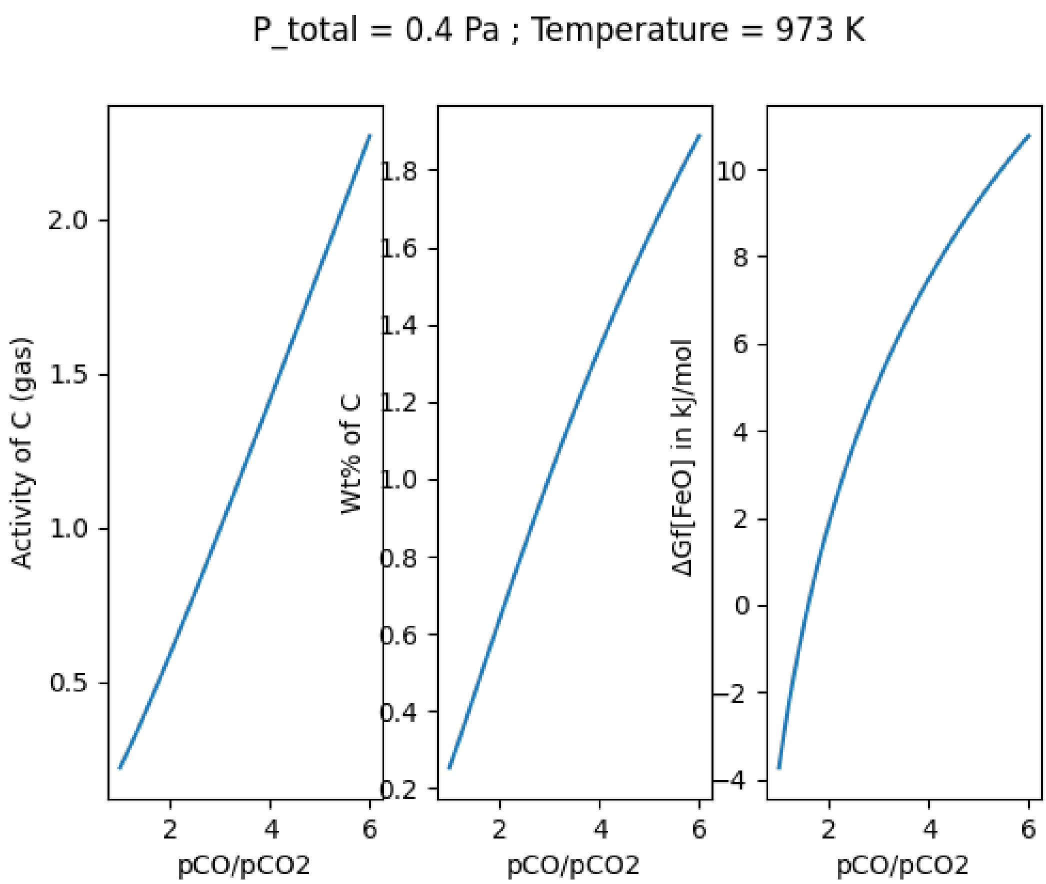


4. For Total pressure of 0.4 pascals

The lower limit of desired Wt% of Carbon 0.2

The upper limit of desired Wt% of Carbon 0.4

No suitable P_{CO}/P_{CO2} values are possible to deposit desired Wt% of C.



5. For Total pressure of 0.5 pascals
The lower limit of desired Wt% of Carbon 0.2
The upper limit of desired Wt% of Carbon 0.4
No suitable P_{CO}/P_{CO2} values are possible to deposit desired Wt% of C

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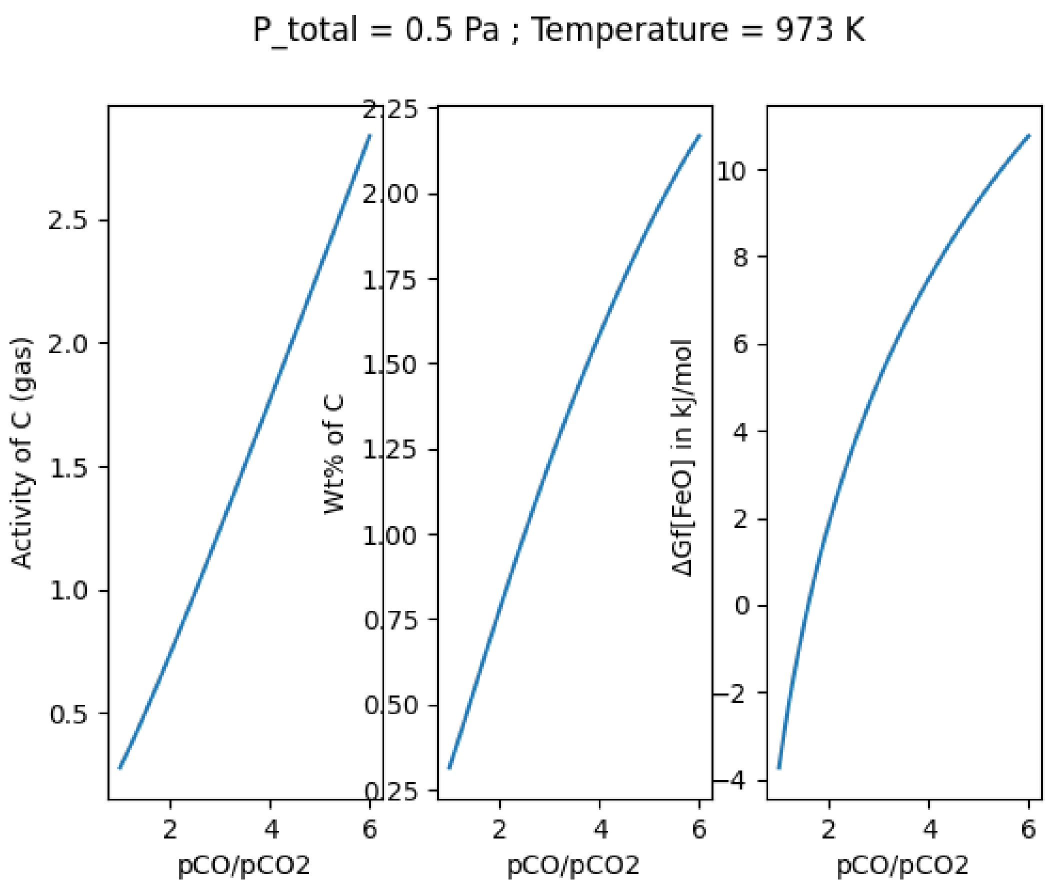

Contribution by Each Member:

Jagruti Lahamge(200110060) -
Contributed to Coding the framed solution using Python
Contributed to documenting the solved problem
Generated plots and interpreted data for different test cases in python

Sakshi Agarwal(20D110022) -
Contributed to Coding the framed solution using Python
Contributed to documenting the solved problem
Collected the necessary data for solving the problem

Komalika Shirud(200110058) -
Contributed to Coding the framed solution using Python
Contributed to documenting the solved problem
Prepared test cases for different variables in the problem and created Readme file