**Methodology/Principle behind the problem**

The main principle involved in predicting the stability of iron and its oxide in an environment of Hydrogen () and Water () is based on **Gibb’s Free Energy** and the **spontaneity** of the reaction.

At constant **temperature** and **pressure**, the change in Gibbs free energy is defined as .

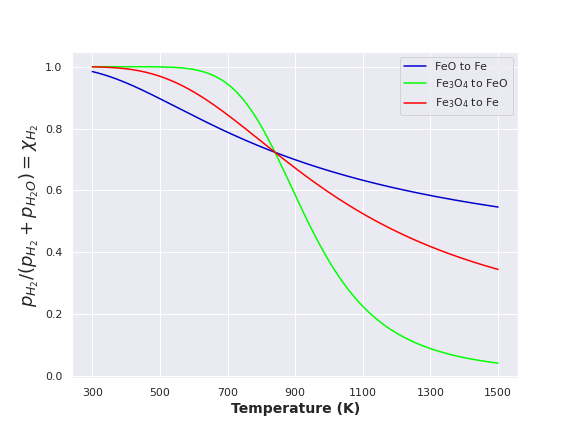
When , the reaction is spontaneous in the **forward** reaction and when , the reaction is spontaneous in the **backward** direction.

Our calculations were based on these expressions,

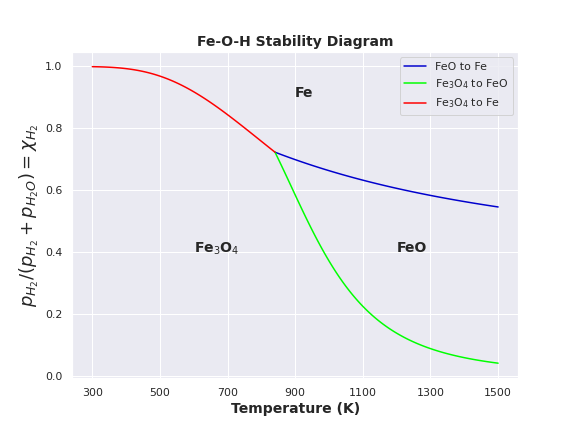
**Plots and explanation**

The above expression was used to plot the graphs at various temperatures for all the three reactions. (Please refer to the pdf submitted for more detailed working.)

|  |  |
| --- | --- |
|  |  |
|  | ΔG° = *259600 - 62.55T* *J/mol* |
|  | ΔG° = *1091000 - 312.80T* *J/mol* |
|  | ΔG° = *312200 – 125.15T* *J/mol* |
|  | ΔG°=-52600+62.6T J/mol |



**Stability regions\***

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The above plot removes some of the lines from the previous plot. The point of intersection comes out to be 840.25K (52600/62.6) with =0.7233, the intersection represents the **triple point** and the point where are in **equilibrium** with one another and hence so ΔG°=0 as Keq = 1 as all reactants are solid, so T\_eqm = 52600/62.6 = 840.25 K

Above 840.25K, according to the Gibb’s Free energy equation, the reaction

will be spontaneous in the backward direction as ΔG>0. Hence, whenever are present together, they’ll combine together to form . Therefore, the line corresponding to equilibrium will be absent after 840.25K.

Below 840.25K, according to Gibb’s Free energy equation, the reaction

will be spontaneous in the forward direction as ΔG<0. Hence, always decomposes to form . Thus, the lines containing will be absent below 840.25K.

**Source**

All Thermodynamic Data was taken from MM209 Assignment 4 Question numbers 2 and 3 (Autumn 2020). (The base data used is given in the pdf file submitted)

**Contribution**

The problem was discussed among us and solved cumulatively. The report was prepared and drafted equally by us three.

**Kunind Sahu (190110039)**: - The python Code for FeO-Fe and the calculation of thermodynamic data related to it.

**Gunin Gupta (190110024)**: - The python Code for Fe3O4-Fe and the calculation of thermodynamic data related to it.

**Mohit Chhaparwal (190110047)**: - The python Code for Fe3O4-FeO and the calculation of thermodynamic data related to it.

**\***We’ve **submitted two files for our code**, a **.py** file and a **.ipynb** file, the .py file can be run in any Python environment (preferably PyCharm), the .ipynb file is an **Interactive Python Notebook** which shows the code in a report format. It can be viewed by uploading it to [www.colab.research.google.com](http://www.colab.research.google.com)

You can also click [here](https://colab.research.google.com/drive/1vWhRqo39OMg-xnRDZ-GWeCPgHYXj86cX?usp=sharing) to directly check our pre-hosted .ipynb file on google colab (same as the one submitted for grading)!