Model

- The activity coefficient vs. composition relationship is a AB-CD-G matrix composite system is generated by using the TCC database of the Thermo-Calc (b) Figure of the diagram giving the compositions of the coexisting liquid (a) Fe-C binary phase diagram and solid Fe-Mn-C systems in the current work.

Procedure & Results

- The criteria of carbon equilibrium is term of partial molar free energy (G) i.e., \( \gamma_i(\text{solid}) = \gamma_i(\text{liquid}) \). By solving the standard molar free energy, \( \Delta G_{\text{mol}}(i) \), of solid carbon (graphite) from either side of the above equation, substituting \( \Delta G_i = RT \ln C_i \) and writing as the product \( x_iC_i \), one gets:

\[
\ln C_i \gamma_i(\text{solid}) - \ln C_i \gamma_i(\text{liquid}) = \ln(\frac{C_i(\text{liquid})}{C_i(\text{solid})})
\]

- Applying the quadratic activity coefficient vs. composition relation (Eq.(4)) for solute (carbon, here) in both solid and liquid solutions:

\[
\ln(\frac{C_i(\text{liquid})}{C_i(\text{solid})}) = \frac{1}{2} \left[ \ln(\frac{C_i(\text{liquid})}{C_i(\text{solid})}) + \ln(\frac{C_i(\text{solid})}{C_i(\text{liquid})}) \right] = \ln(\frac{C_i(\text{liquid})}{C_i(\text{solid})}) + \ln(\frac{C_i(\text{solid})}{C_i(\text{liquid})})
\]

- The reported values of \( \gamma_i(\text{solid}) \) at 1273 K is 8.75, \( \gamma_i(\text{liquid}) \) at 1273 K is 0.57, and \( \gamma_i(\text{liquid}) \) at 1273 K is 11 [4]. Applying the temperature corrections for molar, the following values are obtained at 1273 K:

\[
\gamma_i(\text{solid}) = -5.85, \quad \gamma_i(\text{liquid}) = 0.56265, \quad \gamma_i(\text{liquid}) = 0.04451.
\]

- Solving equations (4) and (7) for three more new data, which pertain to manganese, are generated:

\[
\gamma_i(\text{solid}) = 1.63, \quad \gamma_i(\text{liquid}) = -1.06, \quad \gamma_i(\text{liquid}) = -5.79.
\]