Gasification

Exercise 2b

29 padziernika 2013

Consider water gas shift reaction:

$$CO + H_2O \Leftrightarrow CO_2 + H2$$

Calculate equlibrium composition in this process, knowing inlet streams: $CO = 2kmol/h$, $H_2O = 1kmol/h$ and temperature in the reactor $T = 700K$.

To calculate the equilibrium solve the system of equation consisting of mass balance (or mole balance) for every element in the system and use the equation for equilibrium constant:

$$K_{reac} = exp(\frac{-\Delta G_r}{RT})$$

Free Gibbs energy is calculated as follows:

1. heat capacity is given by the polynomial:

$$Cp(T) = a + b * 10^{-3}T + c * 10^{-6}T^2 + d * 10^{-9}T^3$$

2. enthalpy

$$\Delta H(T) = H^0 + \frac{1}{Tx - T0}\int_{298}^{Tx} Cp(T)dT * (T - 298)$$

3. entropy

$$\Delta S(T) = \frac{1}{Tx - T0}\int_{298}^{Tx} \frac{Cp(T)}{T}dT$$

4. Gibbs free energy

$$\Delta G(T) = \Delta H(T) - T * \Delta S(T)$$

Create a plot of equilibrium constant versus temperature.
How does temperature affect equlibrium compostion. Try to create the plot of yields of products vs. temperature.