EG3029 Chemical Thermodynamics

Tutorial 9

Problem 1:
For the ammonia synthesis reaction

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3$$

with 0.5 mol N_2 and 1.5 mol H_2 as the initial amounts of reactants and with the assumption that the equilibrium mixture is an ideal gas, show that

$$\varepsilon_e = 1 - \left(1 + 1.299K \cdot \frac{P}{P^\circ}\right)^{-1/2}$$

Problem 2:
Assuming that all species and their mixtures are ideal gases, derive an equation for the Gibbs energy *G* as a function of the reaction coordinate ε for the water-gas shift reaction at 1000 K.

$$H_2 + CO_2 \rightarrow H_2O + CO$$

Extra task: use Excel or Matlab to plot *G(ε)* and determine the equilibrium reaction coordinate as well as the composition at equilibrium.