

A First Course on Kinetics and Reaction Engineering

How To Calculate an Equilibrium Constant

1. Determine the stoichiometric coefficient, including sign, of every species that participates in the reaction.
2. For every species that participates in the reaction, find values for the standard Gibbs free energy of formation at 298 K.
 - a. Take note of the standard states used for all species (that is those that participate in the reaction being analyzed as well as the elements appearing in the formation reactions).
3. Calculate the standard Gibbs free energy change of reaction at 298 K from the standard Gibbs free energies of formation of the reagents at 298 K
 - a. See equation (2.7) from Unit 2.
4. If any species in the equation being analyzed are in a state different from the standard state used in the formation reactions, find the Gibbs free energy change associated with converting that species to its standard state, multiply that value by the stoichiometric coefficient of the species and add it to the standard Gibbs free energy change at 298 K from step 4.
5. Use the standard Gibbs free energy change at 298 K from step 4 to calculate the equilibrium constant at 298 K.
 - a. See equation (3.1) from Unit 3
6. Generate an expression for the standard heat of the reaction as a function of temperature
 - a. See "How to Calculate a Standard Heat of Reaction" from Unit 2.
7. Use the equilibrium constant at 298 K from step 5 and the expression for the heat of reaction as a function of temperature from step 6 to generate an expression for the equilibrium constant as a function of T.
 - a. See equation (3.6) from Unit 3.
8. Use the equation from step 7 to calculate the equilibrium constant at any desired temperature.