A First Course on Kinetics and Reaction Engineering

How To Calculate the Equilibrium Composition of a Reacting Mixture*

1. Find a set mathematically independent reactions from among all the reactions taking place in the system, and generate a mole table for the system
   a. See Unit 1 and Supplemental Unit S1.
2. Calculate the value of the equilibrium constant for each of the independent reactions at the desired reaction temperature.
   a. See "How to Calculate an Equilibrium Constant" from Unit 3.
3. Write an equilibrium expression for each of the independent reactions, substituting the equilibrium constants from step 2.
   a. See equation (3.7) from Unit 3
4. Express the thermodynamic activities appearing in the equilibrium expressions in terms of composition variables.
   a. See, for example, equations (3.11) through (3.16) from Unit 3.
5. Express the composition variables appearing in the equilibrium expressions after step 4 in terms of the extents of the independent reactions using the mole table from step 1.
6. Solve the set of equilibrium expressions resulting from step 5 to obtain values for the equilibrium extents of the independent reactions.
7. Substitute the equilibrium extents of the independent reactions into the mole table to compute the equilibrium composition.

* There are several ways to calculate equilibrium composition; only one of those ways is presented here.