4. Reaction Equilibrium for Multiple Gas Phase Reactions

4.1 Numerical Methods

Solution of systems of nonlinear algebraic equations.

4.2 Concepts Utilized

Complex chemical equilibrium calculations involving multiple reactions.

4.3 Course Useage

Thermodynamics or Reaction Engineering.

4.4 Problem Statement

The following reactions are taking place in a constant volume, gas-phase batch reactor.

$$A + B \leftrightarrow C + D$$
$$B + C \leftrightarrow X + Y$$
$$A + X \leftrightarrow Z$$

A system of algebraic equations describes the equilibrium of the above reactions. The nonlinear equilibrium relationships utilize the thermodynamic equilibrium expressions, and the linear relationships have been obtained from the stoichiometry of the reactions.

$$\begin{aligned} &K_{C1} = \frac{C_C C_D}{C_A C_B} \qquad K_{C2} = \frac{C_X C_Y}{C_B C_C} \qquad K_{C3} = \frac{C_Z}{C_A C_X} \\ &C_A = C_{A0} - C_D - C_Z \qquad C_B = C_{B0} - C_D - C_Y \\ &C_C = C_D - C_Y \qquad C_Y = C_X + C_Z \end{aligned} \tag{12}$$

In this equation set C_A, C_B, C_C, C_D, C_X, C_Y and C_Z are concentrations of the various species at equilibrium resulting from initial concentrations of only C_{A0} and C_{B0}. The equilibrium constants K_{C1}, K_{C2} and K_{C3} have known values.

Solve this system of equations when $C_{A0} = C_{B0} = 1.5$, $K_{C1} = 1.06$, $K_{C2} = 2.63$ and $K_{C3} = 5$ starting from four sets of initial estimates.

(a) $C_D = C_X = C_Z = 0$

(b) $C_D = C_X = C_Z = 1$

(c) $C_D = C_X = C_Z = 10$