3.6 ENERGY BALANCE FOR REACTING SYSTEMS

Multiple Reactions - Online supplement

When multiple reactions are present, a reaction coordinate is written for each reaction. When a species is present in multiple reactions, the material balance uses the reaction coordinate for each reaction along with the correct stoichiometric numbers.

Example 3.5 Solving multireaction equilibrium equations by EXCEL

Methanol has a lower vapor pressure than gasoline. That can make it difficult to start a car fueled by pure methanol. One solution is to convert some of the methanol to methyl ether *in situ* during the start-up phase of the process (i.e., automobile). At a given temperature, 1 mole of MeOH vapor is fed to a reactor at atmospheric pressure. It is assumed that only the two reactions given below take place.

$CH_3OH_{(g)} = CO_{(g)} + 2H_{2\,(g)}$ (1)

$2CH_3OH_{(g)} = CH_3OCH_{3(g)} + H_2O_{(g)}$ (2)

For an initial basis of 1 mol of methanol, determine the final concentrations if a sample of the outlet is $y_{methanol} = 0.004$ and $y_{ether} = 0.01$.

Solution:

Material Balances:

Specie	initial	final
1 MeOH	1	$1 - \xi_1 - 2\xi_2$
2 CO	0	ξ_1
3 H_2	0	$2\xi_1$
4 MeOMe	0	ξ_2
5 H_2O	0	ξ_2
Total	1	$1 + 2\xi_1$

$$y_{methanol} = 0.004 = (1 - \xi_1 - 2\xi_2)/(1 + 2\xi_1) \quad 3.1$$

$$y_{ether} = 0.01 = \xi_2/(1 + 2\xi_1) \quad 3.2$$

We will solve simultaneously using Excel. Excel is most successful if the objective functions do not use unknowns in ratios. Writing as objective functions that should go to zero,

$$OBJ1 = -0.996 + 0.992\xi_1 + 2\xi_2$$

$$OBJ2 = 0.01(1 + 2\xi_1) - \xi_2$$

Solving simultaneously as explained in Appendix A, $\xi_1 = 0.946$, $\xi_2 = 0.029$. The other mole fractions can be found immediately from the material balances above. For example,

$$y_{CO} = \xi_1/(1 + 2\xi_1) = 0.946/2.89 = 0.327$$