Lecture Eleven

(MATERIAL BALANCES FOR PROCESSES INVOLVING REACTION BY ELEMENT MATERIAL BALANCES)

This Lecture discusses material balances for reacting systems. We begin by discussing material balances based on chemical elements.

11.1 Element Material Balances

10.1.1 Processes Involving Multiple Reactions

Your Objectives in Studying this Lecture are :

- Carry out a degree of freedom analysis for processes involving chemical reaction(s).
- Formulate and solve material balances using species balances.

11.1 Element Material Balances

As you know, elements in a process are conserved, and consequently you can apply Equation (1) to the elements in a process. Because elements are *not generated or consumed*, the generation and consumption terms in Equation (1) can be ignored. **Why not use element balances to solve material balance problems rather than species balances?**

You can, but you must first make sure that the element balances are independent. Species balances are always independent.

EXAMPLE 11.1: ***Here is an illustration of the issue. Carbon dioxide is absorbed in water in the process shown in Figure11.1. The reaction is;***

$$CO_2(g) + H_2O(\ell) \rightarrow H_2CO_3(\ell)$$

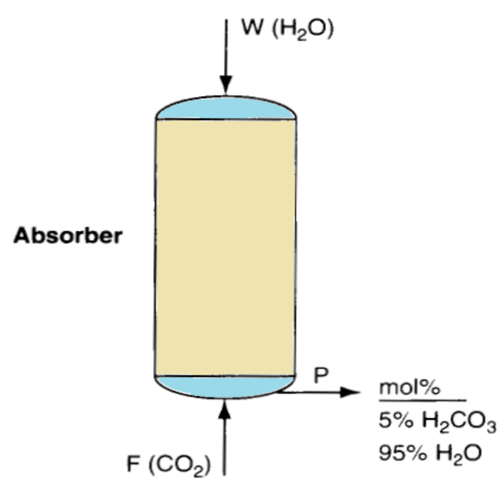

Figure E11.1: Schematic of the CO_2 absorber.

Solution:

Three unknowns exist: *W, F, and P*, and the process involves three elements: C, H, and O. It would appear that you can use the three element balances (in moles)

C: W(0) + F(l) = 0.05P(1)

H: W(2) + F(0) = [0.05(2) + 0.95(2)] P = 2P

O: W(1) + F(2) = [0.05(3) + 0.95(l)] P = 1.10P

EXAMPLE 11.2: ***Use of Element Balances to Solve a Hydrocracking Problem***

Hydrocracking is an important refinery process for converting low-valued heavy hydrocarbons into more valuable lower molecular weight hydrocarbons by exposing the feed to a zeolite catalyst at high temperature and pressure in the presence of hydrogen. Researchers in this field study the hydrocracking of pure components, such as octane (C_8H_{18}), to understand the behavior of cracking reactions. In one such experiment for the hydrocracking of octane, the cracked products had the following composition in mole percent: 19.5% C_3H_8, 59.4% C_4H_{10}, and 21.1% C_5H_{12}. You are asked to determine the molar ratio of hydrogen consumed to octane reacted for this process.

Solution

We will use element balances to solve this problem because the reactions involved in the process are not specified.

Steps 1, 2, 3, and 4

Figure E11.2 is a sketch of the laboratory hydrocracker reactor together with the data for the streams.

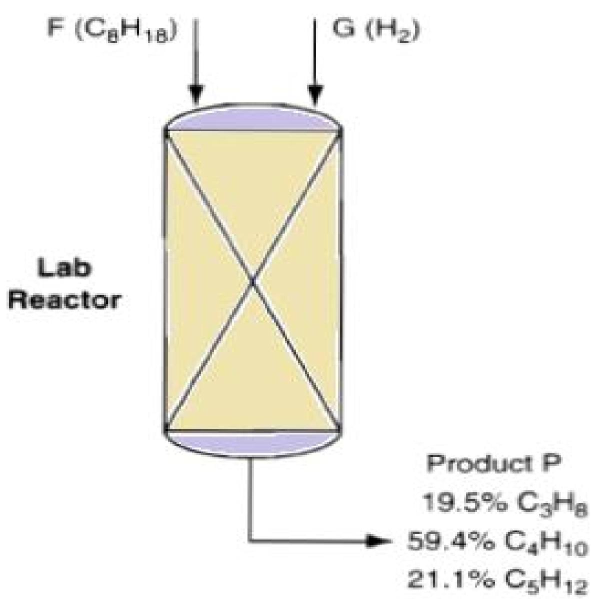

Figure E11.2: Laboratory hydrocracker reactor.

Step 5 Basis: $P = 100$ g mol

Steps 6 and 7

The degree-of-freedom analysis is

Variables: 3

F, G, P

Equations: 3

Element balances: 2

H, C

Basis: $P = 100$

If you calculate the degrees of freedom based on species balances, you have as unknowns five species molar flows, P, and R (the number of independent reaction equations which equals the number of unknown extents of reaction), and as equations five species balances, one specification (the basis), and one implicit equation so that

$$\text{degrees of freedom} = (6 + R) - (5 + 2) = R - 1$$

Thus, although you do not know what R is from the problem statement, for zero degrees of freedom to occur, $R = 1$, that is, one independent reaction equation exists. You can be assuaged that if you do not know R and a minimum reaction set, and thus you do not know how to involve the respective ξ in the species equations, you can fall back on element balances.

Step 8

The element balances after introducing the specification and basis are:

$$\text{C: } F(8) + G(0) = 100[(0.195)(3) + (0.594)(4) + (0.211)(5)]$$

$$\text{H: } F(18) + G(2) = 100[(0.195)(8) + (0.594)(10) + (0.211)(12)]$$

and the solution is

$$F = 50.2 \text{ g mol} \qquad G = 49.8 \text{ g mol}$$

The ratio

$$\frac{H_2 \text{ consumed}}{C_8H_{18} \text{ reacted}} = \frac{49.8 \text{ g mol}}{50.2 \text{ g mol}} = 0.992$$

You will find that employing element material balances can be simpler than employing the extent of reaction for problems in which the reaction equations are not specifically known or must be inferred, as shown in the examples in the next section.

Lecture Eleven / Tutorials

(MATERIAL BALANCES FOR PROCESSES INVOLVING REACTION by Element MATERIAL BALANCES)

PROBLEM: ***Solution EXAMPLE 10.2 by Using Element Balances***

P.11.1 ***Reaction in Which the Fraction Conversion is Specified***

The chlorination of methane occurs by the following reaction

$$CH_4 + Cl_2 \longrightarrow CH_3Cl + HCl$$

You are asked to determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH_4, 50 % Cl_2, and 10 % N_2.

Solution:

Instead of the degree-of-freedom analysis in Steps 6 and 7 of Example **Ex.10.2** the following applies when element balances are used:

Number of variables: 10 (ξ is not involved)

Number of equations: 10

Basis: $F = 100$

Element material balances: 4 (independent)

C, H, Cl, N

Specifications: 3 as in Example **Ex.10.2**

Implicit equations: 2 as in Example **Ex.10.2**

The degrees of freedom are zero.

In Steps 8 and 9 the element material balances are:

$$\text{C:} \quad 100\,(0.40) = n^{out}_{CH_4}(1) + n^{out}_{CH_3Cl}(1)$$

$$\text{H:} \quad 100\,(0.40)(4) = n^{out}_{CH_4}(4) + n^{out}_{HCl}(1) + n^{out}_{CH_3Cl}(3)$$

$$\text{Cl:} \quad 100\,(0.50)(2) = n^{out}_{Cl_2}(2) + n^{out}_{HCl}(1) + n^{out}_{CH_3Cl}(1)$$

$$\text{2N:} \quad 100\,(0.10)(1) = n^{out}_{N_2}(1)$$

Substitute these equations for the species balances used in Example **Ex.10.2** . As expected, the solution of the problem will be the same as found in Example **Ex.10.2**

PROBLEM: ***Solution EXAMPLE 10.3 by Using Element Balances***

P.11.2 ***Reaction Material Balances for a Process in Which Two Simultaneous Reaction Occur***

Formaldehyde (CH_2O) is produced industrially by the catalytic oxidation of methanol (CH_3OH) according to the following reaction:

$$CH_3OH + 1/2O_2 \rightarrow CH_2O + H_2O \qquad (1)$$

Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is,

$$CH_2O + 1/2O_2 \rightarrow CO + H_2O \qquad (2)$$

Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) are fed to the reactor. Also assume that 90% conversion of the methanol results, and that a 75% yield of formaldehyde occurs based on the theoretical production of CH_2O by Reaction 1. Determine the composition of the product gas leaving the reactor.

Solution:

The degree-of-freedom analysis in Steps 6 and 7 is:

Variables: 9 (ξ_1 and ξ_2 are not involved)

Equations: 9
Basis: $F = 1$
Element balances: 4 (independent)
C, H, O, N
Specifications: 3 (the same as in Example 10.3)
Implicit equations: 1 (the same as in Example 10.3)

The degrees of freedom are zero.

In Steps 8 and 9 the element balances are:

$$C: \quad 1(1) + 4.76(0) = P[y^P_{CH_3OH}(1) + y^P_{CH_2O}(1) + y^P_{CO}(1)]$$

$$H: \quad 1(4) + 4.76(0) = P[y^P_{CH_3OH}(4) + y^P_{CH_2O}(2) + y^P_{H_2O}(2)]$$

$$O: \quad 1(1) + 1.00 = P[y^P_{CH_3OH}(1) + y^P_{O_2}(2) + y^P_{CH_2O}(1) + y^P_{H_2O}(1) + y^P_{CO}(1)]$$

$$2N: \quad 1(0) + 3.76 = P[y^P_{N_2}(1)]$$

Substitute these equations for the species balances used in Example 10.3. The solution of the problem will not change.

It would be easier to use the term $y^P_i P = n^P_i$ in the equations above in place of the product of two variables, y^P_i and P.