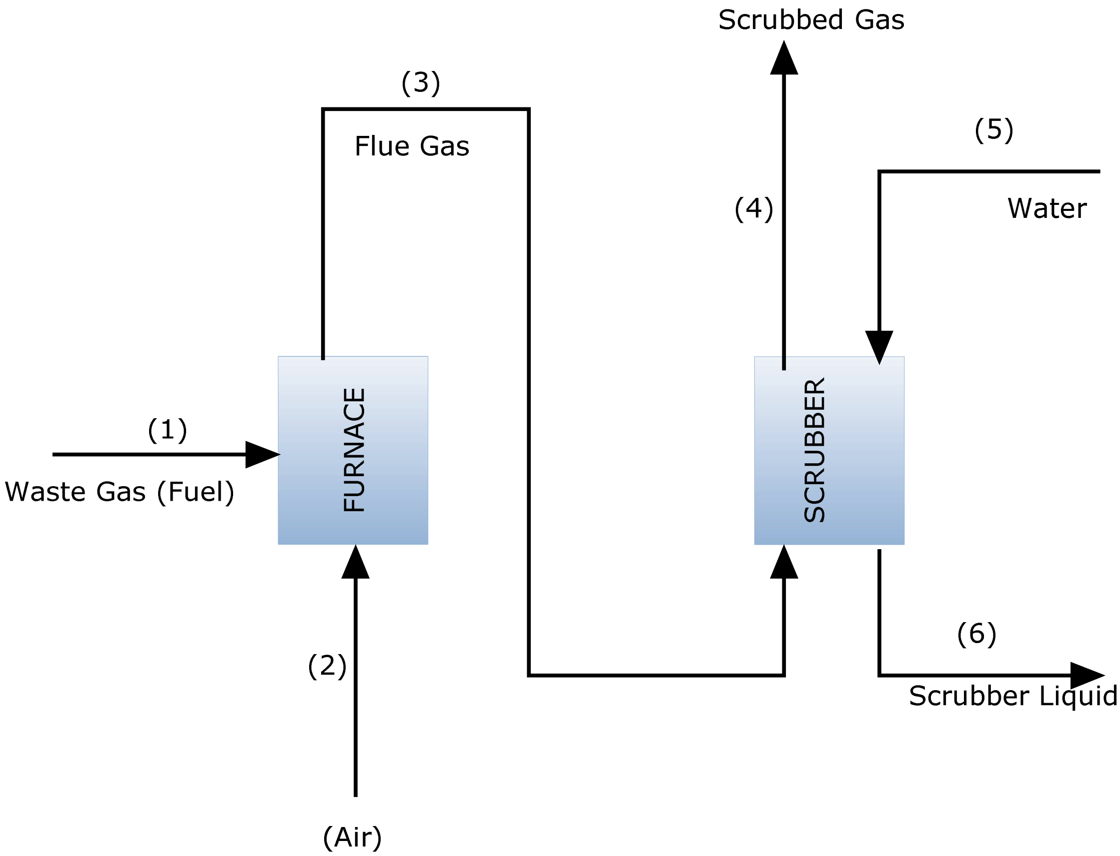
CHE 302 Computerized Material and Energy Balances
Solution to Tutorial (10)

Problem Statement
(Reklaitis G.V.,"Introduction to Material and Energy Balances", Problem 4.21, page 257)

A process waste gas containing H_2S is burned with air (see diagram below). A sample of 1.285 mol gas leaving the furnace is analyzed and found to contain 0.1 mol CO_2 and 0.08 mol SO_2. Because of this high SO_2 content, the flue gas is scrubbed with H_2O. The resulting scrubbed gas has a dry-basis analysis of 1.0% CO, 7.5% CO_2, 2.6% O_2, and 88.9% N_2 and a water mole fraction of 1/11. The scrubber liquid consists of 1.5% CO_2, 8% SO_2, and the rest H_2O. If 10% excess air was used, calculate the fuel consumption. All compositions are in mole fractions or percent.



SOLUTION

Basis: 1.285 mol gas leaving the furnace

Solution strategy:

1. Check process degree of freedom on the basis of element balances. If the problem is correctly specified, then use element balances to solve the problem.
2. If the problem is underspecified on the basis of element balances, then construct a set of independent chemical reactions to represent the system and solve the problem using species balances.

First construct the atom matrix and then reduce it using the **array reduction procedure** operations.

The atom matrix is:

	CO	CO2	SO2	H2O	O2	CH4	H2S
C	1	1	0	0	0	1	0
O	1	2	2	1	2	0	0
S	0	0	1	0	0	0	1
H	0	0	0	2	0	4	2

→

	CO	CO2	SO2	H2O	O2	CH4	H2S
C	1	1	0	0	0	1	0
O	0	1	2	1	2	-1	0
S	0	0	1	0	0	0	1
H	0	0	0	1	0	2	1

→

	CO	CO2	SO2	H2O	O2	CH4	H2S
C	1	0	0	-1	-2	2	2
O	0	1	0	1	2	-1	-2
S	0	0	1	0	0	0	1
H	0	0	0	1	0	2	1

	CO	CO2	SO2	H2O	O2	CH4	H2S
C	1	0	0	0	-2	4	3
O	0	1	0	0	2	-3	-3
S	0	0	1	0	0	0	1
H	0	0	0	1	0	2	1

Therefore the elements C, O, S, H have independent balances.
Number of independent reactions = Number of species – Number of independent element balances
Number of species = 7
Number of independent element balances = 4
Number of independent reactions = 7 – 4 = 3 reactions.
Now we check the process degree of freedom on the basis of element balances:

	Process
Number of stream variables	22
Number of element balances	10
Number of compositions	3
Dry air relations (in stream 4)	3
Water mole fraction (in stream 4)	1
Percent excess air relation	1
Flows in stream 3	2
Basis	1
Degree of freedom = 22 – 21 =	1

The problem is underspecified on the basis of element balances because the degree of freedom is greater than zero. We need to consider the species balances. We first have to construct a set of 3 independent chemical reactions. This set of reactions will be used to determine the degree of freedom on the basis of species balances. If the degree of freedom is zero, we then proceed to solve the problem using these three reactions in the material balances.

From the last reduced atom matrix the block of nonreduced columns (**C**) is:

-2	4	3
2	-3	-3
0	0	1
0	2	1

Therefore the array $\begin{pmatrix} -C \\ I \end{pmatrix}$, where (I) is an identity matrix of size equal to the number of columns of **C,** is:

CO	2	-4	-3
CO2	-2	3	3
SO2	0	0	-1
H2O	0	-2	-1
O2	1	0	0
CH4	0	1	0
H2S	0	0	1

Therefore the set of the 3 independent chemical reactions which represent the system are:

$$2CO + O_2 \longrightarrow 2CO_2 \quad R_1$$
$$CH_4 + 3CO_2 \longrightarrow 4CO + 2H_2O \quad R_2$$
$$H_2S + 3CO_2 \longrightarrow 3CO + H_2O + SO_2 \quad R_3$$

Degree of freedom on the basis of species balances:

	Process
Number of stream variables	22+3
Number of species balances	14
Number of compositions	3
Dry air relations (in stream 4)	3
Water mole fraction (in stream 4)	1
Percent excess air relation	1
Flows in stream 3	2
Basis	1
Degree of freedom = 25 – 25 =	ZERO

Variables Table:

Stream Number	1	2	3	4	5	6	Total
Number of Independent Unknown variables	5	1	5	2	1	1	15+3♣ = 18
Selected Unknown Variables	CH_4, CO, H_2S O_2, N_2	O_2	CO, CO_2, SO_2 O_2, N_2	H_2O, CO	H_2O	H_2O	

♣ Number of independent reactions = 3

Number of independent unknowns = 18 variables

Number of independent equations:

Species material balances = 14

Relations in stream 3 = 2

Water mole fraction relation in stream 4 = 1

Percent excess air relation = 1

Total = 18 equations

EZ Solve Computer Code:

/* Symbols: Water = W, Oxygen = O, Nitrogen = N, Hydrogen = H, Hydrogen disulfide = HS, Methane = CH, Sulfur dioxide = S, Carbon monoxide = C

Basis: 1.285 mol gas leaving the furnace*/

//Furnace Material Balances:
0.0 = CH1 – R2 // CH_4 balance
C3 = C1 - 2* R1 + 4*R2 + 3*R3 // CO balance
1.285 – (C3 + S3 + O3 + N3 + W3) = 2* R1- 3* R2 - 3* R3 // CO_2 balance
S3 = 3*R3 // SO_2 balance
O3 = O1 + O2 – R1 // O_2 balance
N3 = N1 + (79/21)*O2 // N_2
0.0 = HS1 – R3 // H_2S balance
W3 = 2*R2 + R3 // H_2O balance

//Scrubber Material Balances:
W4 + W6 = W5 + W3
C4 = C3
(7.5/1.0)*C4 + (2.5/89.5)*W6 = 1.285 – (C3 + S3 + O3 + N3 + W3)
(2.6/1.0)*C4 = O3
(88.9/1.0)*C4 = N3
(8.0/89.5)*W6 = S3

//Stream 3 relations:
1.285 – (C3 + S3 + O3 + N3 + W3) = 0.1 // CO_2 relation in stream 3
S3 = 0.08 // SO_2 relation in stream 3

//Stream 4 relation (the water mole fraction)
W4 = (1.0/11.0)*((100.0/1.0)*C4 + W4)

//Percent excess relation
O2 = 1.1*(0.5*C1)

//Fuel consumption

Fuel_consumption = CH1 + C1 + HS1 + O1 + N1

Solution:

Fuel_consumption = 1.16937 moles