Lecture Twelve

(MATERIAL BALANCES FOR PROCESSES INVOLVING COMBUSTION)

In this Lecture, we discuss combustion as an extension of the previous discussion about chemical reactions. Combustion (عملية الاحتراق) is the reaction of a substance with oxygen with the associated release of energy and generation of product gases such as H_2O, CO_2, CO, and SO_2.

Typical examples of combustion are the combustion of coal, heating oil, and natural gas used to generate electricity in utility power stations, and engines that operate using the combustion of gasoline or diesel fuel.

Most combustion processes use air as the source of oxygen. For our purposes you can assume that air contains 79% N_2, and 21% O_2.

Your Objectives in Studying this Lecture are:

Understand the meanings of stack gas, flue gas, Orsat analysis, dry basis, wet basis, theoretical air (oxygen) and excess air (oxygen), and employ these concepts in combustion problems.

12.1 Terminology of Combustion

Combustion requires special attention because of some of the terminology involved. You should become acquainted with these special terms:

a. **Complete combustion**—the complete reaction of the hydrocarbon fuel producing CO_2, SO_2, and H_2O.

b. In Complete combustion (Partial combustion) —If parts of the fuel remain unburned, or if CO appears with produced gases, the combustion is termed in complete or partial combustion. Not that the reaction of S with O_2 yields SO_2 and SO_3. Conversion of S to SO_3 requires specific conditions. Hence, it is customary to requires the conversion of all S to SO_2 as a complete union for stoichiometric calculation.

The quantity of heat produced from complete combustion of any fuel is higher than that produced from incomplete combustion. Theoretical quantity of oxygen required for any combustion process is computed on the assumption of complete combustion.

The three general constituents of any combustion process are:

Fuels

The fuel used in power plant combustion furnaces may be *solids, liquids, or gases*.

a. Solid fuels: principally *coal* is the most important classical and natural fuel. It consists of:

- Elemental carbon.
- Complex hydrocarbons of unknown structures consist of C, H, O, N, and S.
- Noncombustible Matter that form the ash.

b. Liquid fuels: principally hydrocarbons obtained from distillation of crude oil such as *gasoline, kerosene, diesel oil, and fuel oil*. However, there is a growing interest to use alcohols obtained by fermentation of grains as liquid fuel.

c. Gas fuels: Principally natural gas is an important gaseous fuel it consists of:

- 90-95% CH_4.
- The remainder being ethane, propane, and small quantity of other gases.
- Light hydrocarbons obtained from petroleum or coal treatment are examples of synthetic gaseous fuels.
- Acetylene and hydrogen can be also used as fuel but their productions are relatively expensive.

Air

Air is the source of oxygen in most of combustion processes for obvious economic reasons. Air has the following composition:

- N_2 78.03 mol%.
- O_2 20.99 mole% .
- Ar 0.94 mole% .
- CO_2 0.03 mole% .
- H_2, He, Ne, Kr, Xe 0.01 mole% .

However, combustion calculations are usually carried out with composition of 79%N_2 and 21%O_2 to simplify such calculations.

a. **Theoretical air (or theoretical oxygen):** the minimum amount of air (or oxygen) required to be brought into the process for complete combustion. Sometimes this quantity is called the required air (or oxygen). So that all C, H, and S are converted to CO_2, H_2O, and SO_2 respectively.

b. **Excess air (or excess oxygen):** in line with the definition of excess reactant, excess air (or oxygen) is the amount of air (or oxygen) in excess of that required for complete combustion as defined in (a).

In actual practice, theoretical air is not sufficient to get complete combustion.

The calculated amount of *excess air does not depend on how much material is actually burned* but what is possible to be burned. Even if only partial combustion takes place, as, for example, C burning to both CO and CO_2, the excess air (or oxygen) is computed as if the process of combustion went to completion and produced only CO_2. Do not ever forget this basic assumption!

$$\%excess air = 100\frac{excess air}{required air} = 100\frac{excess O_2/0.21}{required\ O_2/0,21} \qquad (12.1)$$

Note that the ratio 1/0.21 of air to O_2 cancels out in Equation (1). Percent excess air may also be computed as

$$\%excess air = 100\frac{O_2 entering process - O_2 required}{O_2 required} \qquad (12.2)$$

$$\%excess air = 100\frac{excess O_2}{O_2 entering - excess O_2} \qquad (12.3)$$

Flue or stack gas

a. **Wet basis** : All the gases resulting from combustion process including the water vapor, sometimes known as a *wet basis*.

b. **Dry basis or Orsat analysis**: all the gases resulting from combustion process *not including the water vapor*. (Orsat analysis refers to a type of gas analysis apparatus in which the volumes of the respective gases are measured over and in equilibrium with water; hence each component is saturated with water vapor. The net result of the analysis is to eliminate water as a component that is measured.) Look at **Figure (12.1)**. To convert from one analysis to another, you have to adjust the percentages of the components to the desired basis.

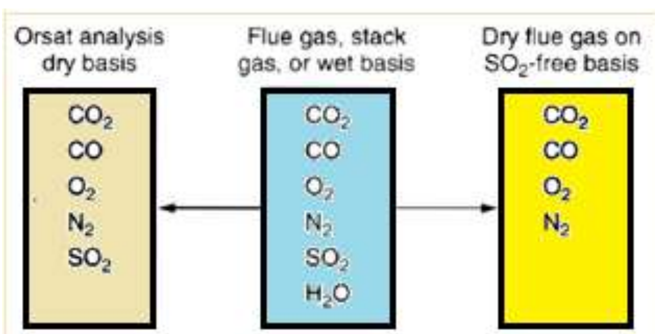

Figure 12.1: Comparison of a gas analysis on different bases .

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 (10.1) 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 -12.1: ***Excess Air***

Fuels other than gasoline are being \ for motor vehicles because they generate lower levels of pollutants than does gasoline. Compressed propane is one such proposed fuel. Suppose that in a test 20 kg of C_3H_8 is burned with 400 kg of air to produce 44 kg of CO_2 and 12 kg of CO. What was the percent excess air?

Solution:

This is a problem involving the following reaction (is the reaction equation correctly balanced?)

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

Basis: 20 kg of C_3H_8

Since the percentage of excess air is based on the *complete combustion* of C_3H_8 to CO_2 and H_2O, the fact that combustion is not complete has no influence on the calculation of "excess air." The required O_2 is

$$\frac{20 \text{ kg } C_3H_8}{} \left| \frac{1 \text{ kg mol } C_3H_8}{44.09 \text{ kg } C_3H_8} \right| \frac{5 \text{ kg mol } O_2}{1 \text{ kg mol } C_3H_8} = 2.27 \text{ kg mol } O_2$$

The entering O_2 is

$$\frac{400 \text{ kg air}}{} \left| \frac{1 \text{ kg mol air}}{29 \text{ kg air}} \right| \frac{21 \text{ kg mol } O_2}{100 \text{ kg mol air}} = 2.90 \text{ kg mol } O_2$$

The percentage of excess air is

$$100 \times \frac{\text{excess } O_2}{\text{required } O_2} = 100 \times \frac{\text{entering } O_2 - \text{required } O_2}{\text{required } O_2}$$

$$\% \text{ excess air} = \frac{2.90 \text{ lb mol } O_2 - 2.27 \text{ lb mol } O_2}{2.27 \text{ lb mol } O_2} \left| \frac{100}{} \right. = 28\%$$

EXAMPLE -12.2: ***A Fuel Cell to Generate Electricity From Methane***

"A Fuel Cell in Every Car" is the headline of an article in *Chemical and Engineering News*, March 5, 2001, p.19. In essence, a fuel cell is an open system into which fuel and air are fed, and out of which comes electricity and waste products. Figure (2) is a sketch of a fuel cell in which a continuous flow of methane **(CH_4)** and air **(O_2 plus N_2)** produce electricity plus **CO_2 and H_2O**. Special membranes and catalysts are needed to promote the reaction of **CH_4.**

Based on the data given in **Figure 2**, you are asked to ***calculate the composition of the products in P.***

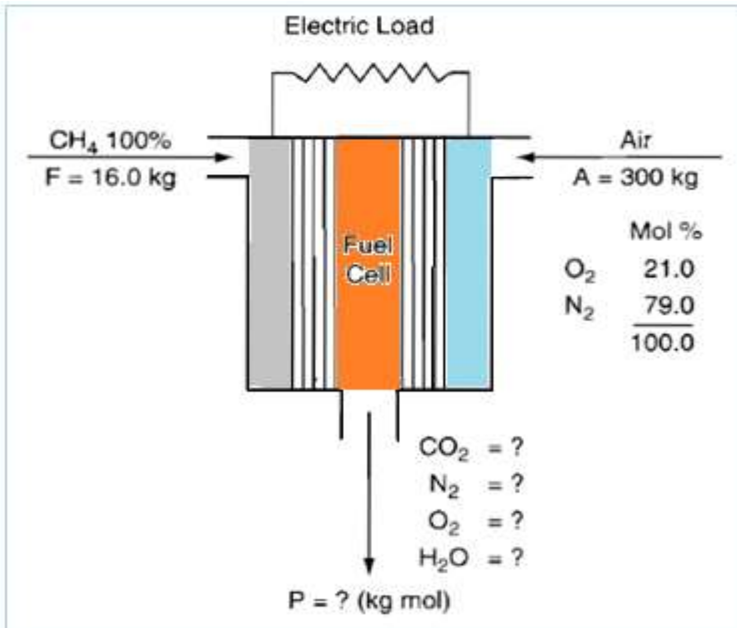

Figure -2 A Fuel cell.

Solution:

Steps 1, 2, 3, and **4** This is a steady-state process with reaction. Can you assume a complete reaction occurs? Yes. No CH_4 appears in *P*. The system is the fuel cell (open, steady state). Because the process output is a gas, the composition will be mole fractions or moles, hence it is more convenient to use moles rather than mass in this problem even though the quantities of CH_4 and air are stated in kg. You can carry out the necessary preliminary conversions as follows:

$$\frac{300 \text{ kg A}}{} \left| \frac{1 \text{ kg mol A}}{29.0 \text{ kg A}} \right. = 10.35 \text{ kg mol A in}$$

$$\frac{16.0 \text{ kg } CH_4}{} \left| \frac{1 \text{ kg mol } CH_4}{16.0 \text{ kg } CH_4} \right. = 1.00 \text{ kg mol } CH_4 \text{ in}$$

$$\frac{10.35 \text{ kg mol A}}{} \left| \frac{0.21 \text{ kg mol } O_2}{1 \text{ kg mol A}} \right. = 2.17 \text{ kg mol } O_2 \text{ in}$$

$$\frac{10.35 \text{ kg mol A}}{} \left| \frac{0.79 \text{ kg mol } N_2}{1 \text{ kg mol A}} \right. = 8.18 \text{ kg mol } N_2 \text{ in}$$

Step 5 Since no particular basis is designated we will pick a convenient basis

Basis: 16.0 kg CH_4 entering = 1 kg mol CH_4

Steps 6 and 7

The degree-of-freedom analysis is (*A* has been calculated):

Variables: 8

$$F, P, n^P_{CO_2}, n^P_{N_2}, n^P_{O_2}, n^P_{H_2O}, n^A_{O_2}, n^A_{N_2},$$

Equations: 8

Basis: $F = 1$ kg mol

Element material balances: 4 (independent)

C, H, O, N

Specifications and calculated quantities: 2

$$n^A_{O_2} = 2.17, \; n^A_{N_2} = 8.18$$

Implicit equation: 1

$$\Sigma n^P_i = P$$

The degrees of freedom are zero.

If you use species balances in solving the problem, you have to involve the reaction: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$: Then (*A* has been calculated)

Variables: 10

$$F, P, n^A_{O_2}, n^A_{N_2}, n^P_{CH_4}, n^P_{CO_2}, n^P_{N_2}, n^P_{O_2}, n^P_{H_2O}, \xi$$

Equations: 10

Basis: F = 1

Species balances: 5

Calculated quantities: 2 (as above)

Specifications: 1

$\xi = 1$ (because the reaction is complete)

Implicit equation: 1

$$\Sigma n^P_i = P$$

Step 8

After introduction of the specified and calculated quantities, the element material balances are (in moles):

	Out		In
C:	$n^P_{CO_2}(1)$	=	1(1)
H:	$n^P_{H_2O}(2)$	=	1(4)
O:	$n^P_{CO_2}(2) + n^P_{O_2}(2) + n^P_{H_2O}(1)$	=	2.17(2)
2N:	$n^P_{N_2}$	=	8.18

The species material balances are:

Compound	Out		In		$v_i\xi$		g mol
CH_4:	$n^P_{CH_4}$	=	1.0	−	1 × 1	=	0
O_2:	$n^P_{O_2}$	=	2.17	−	2 × 1	=	0.17
N_2:	$n^P_{N_2}$	=	8.18	−	0 × 1	=	8.18
CO_2:	$n^P_{CO_2}$	=	0	+	1 × 1	=	1.0
H_2O:	$n^P_{H_2O}$	=	0	+	2 × 1	=	2.0

Step 9

The solution of either set of equations gives

$$n^P_{CH_4} = 0,\ n^P_{O_2} = 0.17,\ n^P_{N_2} = 8.18,\ n^P_{CO_2} = 1.0,\ n^P_{H_2O} = 2.0,\ P = 11.35$$

and the mole percentage composition of P is

$$y_{O_2} = 1.5\%,\ y_{N_2} = 72.1\%,\ y_{CO_2} = 8.8\%,\ \text{and}\ y_{H_2O} = 17.6\%$$

Step 10

You can check the answer by determining the total mass of the exit gas and comparing it to total mass entering (316 kg), but we will omit this step here to save space.

Lecture Twelve / Tutorials

(MATERIAL BALANCES FOR PROCESSES INVOLVING COMBUSTION)

P.12.1 Explain the difference between a flue gas analysis and an Orsat analysis; wet basis and dry basis.

P.12.2 What does an SO_2-free basis mean?

P.12.3 Write down the equation relating percent excess air to the required air and entering air.

P.12.4 Will the percent excess air always be the same as the percent excess oxygen in combustion (by oxygen)?

P.12.5 In a combustion process in which a specified percentage of excess air is used, and in which CO is one of the products of combustion, will the analysis of the resulting exit gases contain more or less oxygen than if all the carbon had burned to CO_2?

P.12.6 Answer the following questions true or false.

a. Excess air for combustion is calculated using the assumption of complete reaction whether or not a reaction takes place.
b. For the typical combustion process the products are CO_2 gas and H_2O vapor.
c. In combustion processes, since any oxygen in the coal or fuel oil is inert, it can be ignored in the combustion calculations.
d. The concentration of N_2 in a flue gas is usually obtained by direct measurement.

P.12.7 *Methane is Completely Burned*

Methane is completely burned with 26% excess air. Calculate (a) the orsat analysis of flue gas, (b) the molal ratio of water vapor to dry flue gas, and (c) the molal ratio of air to methane.

P.12.8 CH_2 *Burned*

A furnace used to provide heat to anneal steel burns a fuel oil whose composition can be represented as $(CH_2)_n$. It is planned to burn this fuel with stoichiometric air.

a. Assume complete combustion and calculate the Orsat analysis of the flue gas.
b. Recalculate the Orsat analysis assuming that 5 % of the carbon in the fuel burns to CO only.

P.12.9

Your assistant reports the following experimental data for the exit Orsat gas analysis from the combustion of a hydrocarbon oil in a furnace: CO_2 11.8 %; CO 5.0 %; H_2 1.5 %; O_2 1.0 % and N_2 by difference. The oil is being burned with 10 % excess air. Would you compliment him on his work ?

P.12.10

Moist hydrogen containing 4 mole percent water is burnt completely in a furnace with 32 % excess air. Calculate the Orsat analysis of the resulting flue gas.