Fuels and Combustion

Any material that can be burned to release thermal energy is called a **fuel**. Most familiar fuels consist primarily of hydrogen and carbon. They are called **hydrocarbon fuels** and are denoted by the general formula C_nH_m. Hydrocarbon fuels exist in all phases, some examples being coal, gasoline, and natural gas. A chemical reaction during which a fuel is oxidized and a large quantity of energy is released is called **combustion**. The oxidizer most often used in combustion processes is air, for the obvious reasons that it is free and readily available. Pure oxygen O_2 is used as an oxidizer only in some specialized applications, such as cutting and welding, where air cannot be used. During a combustion process, the components that exist before the reaction are called **reactants** and the components that exist after the reaction are called **products**. Consider, for example, the combustion of 1 kmol of carbon with 1 kmol of pure oxygen, forming carbon dioxide as follows:

$$C + O_2 \rightarrow CO_2$$

Here C and O_2 are the reactants since they exist before combustion, and CO_2 is the product since it exists after combustion. Note that a reactant does not have to react chemically in the combustion chamber. For example, if carbon is burned with air instead of pure oxygen, both sides of the combustion equation will include N_2. That is, the N_2 will appear both as a reactant and as a product. We should also mention that bringing a fuel into intimate contact with oxygen is not sufficient to start a combustion process. The fuel must be brought above its **ignition temperature** to start the combustion.

Chemical equations are balanced on the basis of the **conservation of mass principle** (or the **mass balance**), which can be stated as follows: **The total mass of each element is conserved during a chemical reaction**. That is, the total mass of each element on the right-hand side of the reaction equation (the products) must be equal to the total mass of that element on the left-hand side (the reactants) even though the elements exist in different chemical compounds in the reactants and products. Also, the total number of atoms of each element is conserved during a chemical reaction since the total number of atoms is equal to the total mass of the element divided by its atomic mass.

A frequently used quantity in the analysis of combustion processes to quantify the amounts of fuel and air is the **air-fuel ratio (***AF*). It is usually expressed on a mass basis and is defined as the ratio of the mass of air to the mass of fuel for a combustion process. That is:

$$AF = \frac{m_{\text{air}}}{m_{\text{fuel}}} \qquad \dots\dots\dots\dots\dots\dots\dots (7.22)$$

The reciprocal of air–fuel ratio is called the **fuel-air ratio** (*FA*). The air-fuel ratio can also be expressed on a mole basis as the ratio of the mole numbers of air to the mole numbers of fuel:

$$AF = \frac{N_{\text{air}}}{N_{\text{fuel}}} \qquad \dots\dots\dots\dots\dots\dots\dots (7.23)$$

The dry air can be approximated as 21 percent oxygen and 79 percent nitrogen by mole numbers. Therefore, each mole of oxygen entering a combustion chamber is accompanied by 0.79/0.21 = 3.76 mole of nitrogen.

Example (7.5): Calculate the theoretical air-fuel ratio on mole basis for the combustion of octane, C_8H_{18}.

Solution:

The chemical reaction of methane with air is:

$$\mathrm{C_8H_{18}} + x\mathrm{O_2} + 3.76x\mathrm{N_2} \rightarrow y\mathrm{CO_2} + z\mathrm{H_2O} + 3.76x\mathrm{N_2}$$

Balancing the two sides of the equation:

Carbon (C): $8 = y$

Hydrogen (H_2): $18 = 2z \rightarrow z = 9$

Oxygen (O_2): $2x = 2y + z \rightarrow 2x = 2 \times 8 + 9 \rightarrow x = 12.5$

Then, the reaction equation becomes:

$$\mathrm{C_8H_{18} + 12.5O_2 + 47N_2 \rightarrow 8CO_2 + 9H_2O + 47N_2}$$

The air-fuel ratio on a mole basis is:

$$AF = \frac{N_{\text{air}}}{N_{\text{fuel}}} = \frac{12.5 + 47}{1} = 59.5 \text{ kmol air/kmol fuel}$$

Theoretical and Actual Combustion Processes

A combustion process is **complete** if all the carbon in the fuel burns to CO_2 and all the hydrogen burns to H_2O. That is, all the combustible components of a fuel are burned to completion during a complete combustion process. Conversely, the combustion process is **incomplete** if the combustion products contain any unburned fuel or components such as C, H_2, CO or OH.

Insufficient oxygen is an obvious reason for incomplete combustion, but it is not the only one. Incomplete combustion occurs even when more oxygen is present in the combustion chamber than is needed for complete combustion. This may be attributed to insufficient mixing in the combustion chamber during the limited time that the fuel and the oxygen are in contact. Another cause of incomplete combustion is dissociation, which becomes important at high temperatures.

The minimum amount of air needed for the complete combustion of a fuel is called the **stoichiometric** or **theoretical air**. Thus, when a fuel is completely burned with theoretical air, no uncombined oxygen is present in the product gases. The theoretical air is also referred to as the chemically correct amount of air, or 100 percent theoretical air. A combustion process with less than the theoretical air is bound to be incomplete. The ideal combustion process during which a fuel is burned completely with theoretical air is called the **stoichiometric** or **theoretical combustion** of that fuel.

In actual combustion processes, it is common practice to use more air than the stoichiometric amount to increase the chances of complete combustion or to control the temperature of the combustion chamber. The amount of air in excess of the stoichiometric amount is called **excess air**. The amount of excess air is usually expressed in terms of the stoichiometric air as **percent excess air** or **percent theoretical air**. The amount of air used in combustion processes is also expressed in terms of the **equivalence ratio**, which is the ratio of the actual fuel-air ratio to the stoichiometric fuel-air ratio.

Example (7.6): Determine the air-fuel ratio, when ethane C_2H_6 is burned with 20 percent excess air during a combustion process. The molar masses of air and ethane are 29 and 30 kg/kmol, respectively.

Solution:

The chemical reaction of ethane with 20% excess air is:

$$\mathrm{C_2H_6} + 1.2x\mathrm{O_2} + 1.2 \times 3.76x\mathrm{N_2} \rightarrow y\mathrm{CO_2} + z\mathrm{H_2O} + 0.2x\mathrm{O_2} + 1.2 \times 3.76x\mathrm{N_2}$$

Balancing the two sides of the equation:

Carbon (C): $2 = y$

Hydrogen (H_2): $6 = 2z \rightarrow z = 3$

Oxygen (O_2): $2 \times 1.2x = 2y + z + 2 \times 0.2x \rightarrow 2.4x = 2 \times 2 + 3 + 0.4x \rightarrow x = 3.5$

Then, the reaction equation becomes:

$$\mathrm{C_2H_6} + 4.2\mathrm{O_2} + 15.79\mathrm{N_2} \rightarrow 2\mathrm{CO_2} + 3\mathrm{H_2O} + 0.7\mathrm{O_2} + 15.79\mathrm{N_2}$$

The air-fuel ratio on mass basis is:

$$AF = \frac{m_{\text{air}}}{m_{\text{fuel}}} = \frac{N_{\text{air}}M_{\text{air}}}{N_{\text{fuel}}M_{\text{fuel}}} = \frac{(4.2 + 15.79) \times 29}{1 \times 30} = 19.93\ \text{kg air/kg fuel}$$

Example (7.7): Methane CH_4 is burned with atmospheric air. The analysis of the products on a dry basis is as follows: 10% CO_2, 0.53% CO, 2.37% O_2 and 87.1% N_2. Determine the combustion equation then find the percent theoretical air.

Solution:

The chemical reaction is:

$$a\mathrm{CH_4} + b\mathrm{O_2} + c\mathrm{N_2} \rightarrow 10\mathrm{CO_2} + 0.53\mathrm{CO} + 2.37\mathrm{O_2} + d\mathrm{H_2O} + 87.1\mathrm{N_2}$$

Balancing the two sides of the equation:

Nitrogen (N_2): $c = 87.1$

Since the nitrogen comes from the air:

$$c = b \times 3.76 \rightarrow b = \frac{c}{3.76} = \frac{87.1}{3.76} = 23.16$$

Carbon (C): $a = 10 + 0.53 \rightarrow a = 10.53$

Hydrogen (H_2): $4a = 2d \rightarrow d = 2 \times 10.53 = 21.06$

Then, the reaction equation becomes:

$$10.53CH_4 + 23.16O_2 + 87.1N_2 \rightarrow 10CO_2 + 0.53CO + 2.37O_2 + 21.06H_2O + 87.1N_2$$

Dividing by 10.53 yields the combustion equation per kmol of fuel:

$$CH_4 + 2.2O_2 + 8.27N_2 \rightarrow 0.95CO_2 + 0.05CO + 0.225O_2 + 2H_2O + 8.27N_2$$

To find the percentage of theoretical air used, we need to know the theoretical amount of air, which is determined from the theoretical combustion equation of the fuel as follows:

$$CH_4 + xO_2 + 3.76xN_2 \rightarrow yCO_2 + zH_2O + 3.76xN_2$$

Balancing the two sides of the equation:

Carbon (C): $1 = y$

Hydrogen (H_2): $4 = 2z \rightarrow z = 2$

Oxygen (O_2): $2x = 2y + z \rightarrow 2x = 2 \times 1 + 2 \rightarrow x = 2$

Then, the reaction equation becomes:

$$CH_4 + 2O_2 + 7.52N_2 \rightarrow CO_2 + 2H_2O + 7.52N_2$$

Then:

$$\text{Percentage of theoretical air} = \frac{m_{\text{air,act}}}{m_{\text{air,th}}} = \frac{N_{\text{air,act}}}{N_{\text{air,th}}} = \frac{2.2 + 8.27}{2 + 7.52} \times 100\% = 110\%$$

Exercises

Problem (1): Determine the mole fractions of a gas mixture that consists of 75% CH_4 and 25% CO_2 by mass. Also, determine the gas constant of the mixture. The molar masses of CH_4 and CO_2 are 16 and 44 kg/kmol, respectively.

Ans. (89.2%, 10.8%, 0.437 kJ/kg.K)

Problem (2): A gas mixture consists of 8 kmol of H_2 and 2 kmol of N_2. Determine the mass of each gas and the apparent gas constant of the mixture. The molar masses of H_2 and N_2 are 2 and 28 kg/kmol, respectively.

Ans. (16 kg, 56 kg, 1.155 kJ/kg.K)

Problem (3): A gas mixture at 350 K and 300 kPa has the following volumetric analysis: 65% N_2, 20% O_2 and 15% CO_2. Determine the mass fraction and partial pressure of each gas. The molar masses of N_2, O_2 and CO_2 are 28, 32 and 44 kg/kmol, respectively.

Ans. (58.3%, 20.5%, 21.2%, 195 kPa, 60 kPa, 45 kPa)

Problem (4): A rigid tank contains 0.5 kmol of Ar and 2 kmol of N_2 at 250 kPa and 280 K. The mixture is now heated to 400 K. Determine the volume of the tank and the final pressure of the mixture.

Ans. (23.3 m^3, 357.1 kPa)

Problem (5): A gas mixture at 300 K and 200 kPa consists of 1 kg of CO_2 and 3 kg of CH_4. Determine the partial pressure of each gas and the apparent molar mass of the gas mixture. The molar masses of CO_2 and CH_4 are 44 and 16 kg/kmol, respectively.

Ans. (21.6 kPa, 178.4 kPa, 19.03 kg/kmol)

Problem (6): Propane C_3H_8 is burned with 75 percent excess air during a combustion process. Assuming complete combustion, determine the air-fuel ratio. The molar masses of air and propane are 29 and 44 kg/kmol, respectively.

Ans. (27.5 kg air/kg fuel)

Problem (7): Acetylene C_2H_2 is burned with the stoichiometric amount of air during a combustion process. Assuming complete combustion, determine the air-fuel ratio on a mass and on a mole basis. The molar masses of air and acetylene are 29 and 26 kg/kmol, respectively.

Ans. (13.3 kg air/kg fuel, 11.9 kmol air/kmol fuel)

Problem (8): One kmol of ethane C_2H_6 is burned with an unknown amount of air during a combustion process. An analysis of the combustion products reveals that the combustion is complete, and there are 3 kmol of free O_2 in the products. Determine (a) the air-fuel ratio (b) the percentage of theoretical air used during this process. The molar masses of air and ethane are 29 and 30 kg/kmol, respectively.

Ans. (29.9 kg air/kg fuel, 186%)

Problem (9) A certain natural gas has the following volumetric analysis: 65% CH_4, 8% H_2, 18% N_2, 3% O_2 and 6% CO_2. This gas is now burned completely with the stoichiometric amount of dry air. What is the air-fuel ratio for this combustion process? The molecular weights are as follows: CH_4 (16), H_2 (2), N_2 (28), O_2 (32) and CO_2 (44).

Ans. (9.42 kg air/kg fuel)

Problem (10): A gaseous fuel with a volumetric analysis of 60% CH_4, 30% H_2 and 10% N_2 is burned to completion with 130 percent theoretical air. What is the air-fuel ratio for this combustion process? The molecular weights are as follows: CH_4 (16), H_2 (2) and N_2 (28).

Ans. (18.6 kg air/kg fuel)