## 4.3 MATERIAL BALANCES INVOLVING CHEMICAL REACTIONS

The law of conservation of mass stated in Chapter 3 holds good for the material balances involving chemical reactions also.

The general mathematical statement can be written as:

Total mass entering the chemical reactor = total mass of products leaving the chemical reactor.

Very often, it is convenient to work with moles rather than with mass, particularly in gaseous systems. It should be noted that in chemical reactions, the total mass of the input remains constant, but the total moles may or may not remain constant. This fact can be understood by studying the following two reactions. Consider the shift reaction:

$$\underset{1\text{ mole}}{CO} + \underset{1\text{ mole}}{H_2O} = \underset{1\text{ mole}}{CO_2} + \underset{1\text{ mole}}{H_2} \qquad (4.5)$$

In this, it can be observed that two moles react with each other and produce also two moles. Thus, the number of moles of the reactants entering the reactor equals the number of moles of the products leaving the reactor. The ammonia synthesis reaction can be written as

$$\underset{1\text{ mole}}{N_2} + \underset{3\text{ moles}}{3H_2} \rightleftharpoons \underset{2\text{ moles}}{2NH_3} \qquad (4.6)$$

It can be observed that four moles (of reactants) produce two moles of ammonia in forward direction. Thus, the number of moles have been reduced, although the total mass of the reactants entering and of the products leaving the reactor are equal. For reaction (4.5), one can write

$$1\text{ mole } CO \equiv 1\text{ mole } H_2O \equiv 1\text{ mole } H_2 \equiv 1\text{ mole } CO_2$$

Similarly, for reaction (4.6), 1 mole $N_2 \equiv 3$ moles $H_2 \equiv 2$ moles $NH_3$

The above equalities decide the stoichiometric requirements of the components. (The sign $\equiv$ represents *equivalent to* from the point of view of the chemical equilibrium, and not *equal to* from the mathematical point of view.)

## 4.4 DEFINITION OF TERMS

Some of the terms used in chemical reaction engineering will now be defined.

In most chemical reactions, two or more components reacting together are not in stoichiometric proportions due to technical, economic or safety considerations. In such cases, a *limiting component* is defined as one which decides the conversion in the reactions. An *excess reactant* is the one which is in excess amount over the stoichiometric requirement of the reactant as determined by the desired chemical reaction.

Consider the reforming reactions between methane and steam.

$$CH_4 + H_2O \longrightarrow CO + 3H_2 \qquad (4.7)$$

$$CH_4 + 2H_2O \longrightarrow CO_2 + 4H_2 \qquad (4.8)$$