

Combustion is the oldest technology of mankind; it has been used for more than one million years. At present, about 90% of our worldwide energy support (e. g., in traffic, electrical power generation, heating) is provided by combustion; therefore it is really worthwhile studying this process.

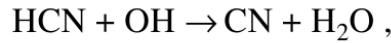
Combustion research in the past was directed to fluid mechanics that included global heat release by chemical reaction. This heat release was often described simply with the help of thermodynamics, which assumes infinitely fast chemical reaction. This approach was useful to some extent for designing stationary combustion processes; it is not sufficient for treating transient processes like ignition and quenching or if pollutant formation shall be treated. However, pollutant formation during combustion of fossil fuels is, and will continue to be, a central topic in the future.

The focus of this book is therefore to treat the coupling of chemical reaction and fluid flow; in addition, combustion-specific topics of chemistry (hydrocarbon oxidation, large reaction mechanisms, simplification of reaction mechanisms) and combustion-specific topics of fluid mechanics (turbulent flow with density change by heat release, potential generation of turbulence by heat release) shall be considered.

Thus, this book will not consider in great detail the theory of chemical reaction rates and experimental methods for the determination of reaction rate coefficients (this is the task of reaction kinetics). Nor will this book discuss the details of turbulence theory and the handling of complex geometries (this is the task of fluid mechanics), although all of these topics are needed in understanding combustion.

The quantitative treatment of combustion processes requires some understanding of fundamental concepts and definitions, which shall be described in this section.

A *chemical reaction* is the exchange and/or rearrangement of atoms between colliding molecules. In the course of a chemical reaction, e. g.,



the atoms (relevant in combustion: C, H, O, and N) are conserved; i. e., they are not created or destroyed. On the other hand, molecules (e. g., HCN, OH, CN, and H₂O) are not conserved. A partial list of molecules relevant in combustion is given in Table 1.1. Reactant molecules are rearranged to become product molecules, with simultaneous release of heat. A primary interest in the heat of reaction sets combustion engineering apart from chemical engineering.

Atoms and molecules are conveniently counted in terms of *amount of substance* or (worse, but used everywhere) *mole numbers* (unit: mol). 1 mol of a compound corresponds to $6.023 \cdot 10^{23}$ particles (atoms, molecules, etc.). Accordingly, the *Avogadro constant* (also called *Avogadro's constant*) is $N_A = 6.023 \cdot 10^{23} \text{ mol}^{-1}$. The *mole fraction* x_i of the species i denotes the ratio of the *mole number* n_i of species i to the total *mole number* $n = \sum n_i$ of the mixture ($x_i = n_i / n$).

The *mass* m is a fundamental property of matter (units of kg in the SI system). The *mass fraction* w_i is the ratio of the mass m_i of the species i and the total mass $m = \sum m_i$ of the mixture ($w_i = m_i / m$).

The *molar mass* (obsolete: *molecular weight*) M_i (units of, e. g., g/mol) of species i is the mass of 1 mol of this species. Some examples (for atomic carbon, molecular hydrogen, molecular oxygen, and methane) are $M_C = 12 \text{ g/mol}$, $M_{\text{H}_2} = 2 \text{ g/mol}$, $M_{\text{O}_2} = 32 \text{ g/mol}$, $M_{\text{CH}_4} = 16 \text{ g/mol}$. The mixture *mean molar mass* \bar{M} (in g/mol, e. g.) denotes an average molar mass, using the mole fractions as weighting ($\bar{M} = \sum x_i M_i$).

Frequently mass fractions w_i and mole fractions x_i are expressed in terms of percentages (*mole-%* or *mass-%*). The following relations hold, which can be verified by simple calculations (S denotes the number of different compounds):

$$w_i = \frac{M_i n_i}{\sum_{j=1}^S M_j n_j} = \frac{M_i x_i}{\sum_{j=1}^S M_j x_j}, \quad (1.1)$$

$$x_i = \frac{w_i \bar{M}}{M_i} = \frac{w_i / M_i}{\sum_{j=1}^S w_j / M_j}. \quad (1.2)$$

Densities do not depend on the size (extent) of a system. Such variables are called *intensive* properties, and are defined as the ratio of the corresponding *extensive* properties (which depend on the extent of the system) and the system volume V . Examples of intensive properties are

$$\begin{array}{lll} \text{mass density (density)} & \rho = m/V & (\text{in, e. g., kg/m}^3), \\ \text{molar density (called concentration)} & c = n/V & (\text{in, e. g., mol/m}^3). \end{array}$$

It follows (very easy to verify) that the mean molar mass is given by the expression

$$\frac{\rho}{c} = \frac{m}{n} = \overline{M}. \quad (1.3)$$

In chemistry, concentrations c of chemical species defined in this way are usually denoted by species symbols in square brackets (e. g., $c_{\text{H}_2\text{O}} = [\text{H}_2\text{O}]$).

For the gases and gas mixtures in combustion processes, an equation of state relates temperature, pressure, and density of the gas. For many conditions it is satisfactory to use the *ideal gas equation of state*,

$$pV = nRT, \quad (1.4)$$

where p denotes the pressure (in units of Pa), V the volume (in m^3), n the mole number (in mol), T the absolute temperature (in K), and R the *universal gas constant* ($R = 8.314 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$). It follows that

$$c = \frac{p}{RT} \quad \text{and} \quad \rho = \frac{p\overline{M}}{RT} = \frac{p}{RT} \sum_{i=1}^s \frac{w_i}{M_i}. \quad (1.5)$$

When temperatures are near or less than the critical temperature, or when pressures are near or above the critical pressures, the concentration or density is inadequately predicted using the ideal gas equation of state, i. e., (1.5). The system is better approximated as a *real gas*. One example of a real gas equation of state is that of *van der Waals*. Details of this and other equations of state for real gas conditions can be found in textbooks on physical chemistry (e. g., Atkins 1990).