

Laminar premixed flames on a flat burner constitute an instructive example for the mathematical treatment of combustion processes. As Fig. 3.1 illustrates, the burner is usually a porous disk, ~10 cm in diameter, through which premixed fuel and air

flow. The gases emerge from the disk and flow into the flame, which appears as a luminous disk levitating a few mm above the porous disk.

If one assumes that the burner diameter is sufficiently large, effects at the edge of the burner can be neglected as an approximation. Well within the edges, a flat flame front is observed. The properties in this flame (e. g., temperature and gas composition) depend only on the distance from the burner, i. e., only one spatial coordinate (z) is needed for the description. The conservation equations for this flame shall now be derived.

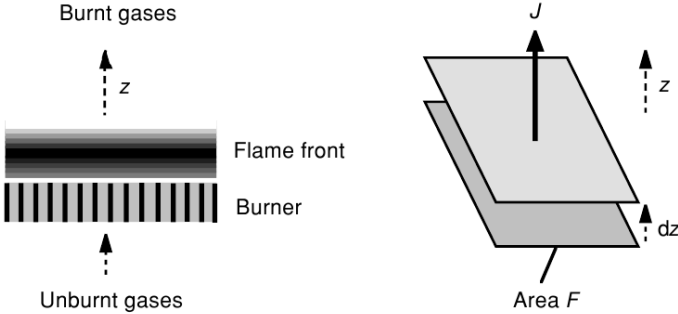


Fig. 3.1. Schematic illustration of a laminar premixed flat flame

The following assumptions will be made in order to simplify the treatment intended:

- The ideal gas law can be used ($p = c \cdot R \cdot T$; see Section 1.1).
- External forces (e. g., gravitation) are negligible.
- The system is continuous; the mean free path of the molecules is small compared to the flame thickness (a good assumption for most combustion problems).
- The pressure is constant (spatial or temporal pressure fluctuations are weak).
- The kinetic energy of the gas flow is negligible compared to other terms in the energy conservation equation (e. g., shock waves are not considered).
- The reciprocal thermal diffusion effect (*Dufour effect*) can be neglected (see below).
- Heat flux caused by radiation of gases and particles is negligible (this assumption is acceptable here when the flame is non-sooting).
- The system is in local thermal equilibrium.
- The flame is stationary, i. e., there are no temporal changes. (Formally, time-dependent equations are solved into stationarity (time-independence) in the following chapters for numerical reasons to be discussed.)

As will be seen below, these assumptions lead to reasonable predictions for laminar flat flames.

For any conserved variable E ($z =$ spatial coordinate, $t =$ time) in a one-dimensional system (see Fig. 3.1), the general relation

$$\frac{\partial W}{\partial t} + \frac{\partial J}{\partial z} = Q \quad (3.1)$$

holds, where W denotes the *density* of the conserved variable ($= E/\text{volume}$; in $[E]/\text{m}^3$), J a *flux* (more precisely *flux density*) of the conserved variable ($= E/(\text{surface}\cdot\text{time})$; in $[E]/(\text{m}^2\cdot\text{s})$), and Q a *source* (or *sink*) of the conserved variable ($= E/(\text{volume}\cdot\text{time})$; in $[E]/(\text{m}^3\cdot\text{s})$). (3.1) is a statement that accumulation can be accomplished by influx (or outflux) and by a source (or sink). It will be shown in the following how the general equation (3.1) appears in the specific cases of conservation of mass, species, and enthalpy.

Conservation of the overall mass m of the mixture: In the conservation of total mass, the density W in the conservation equation is given by the *total mass density* ρ (in kg/m^3). The flux J describes the movement of mass and is given as the product of density and the *mean mass velocity* (velocity of the center of mass, also called *flow velocity*), i. e., $J = \rho v$ (in $\text{kg}/(\text{m}^2\cdot\text{s})$). The source term in the mass conservation equation is zero, because chemical reactions neither create nor destroy mass ($Q = 0$). Substitution into (3.1) leads to

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v)}{\partial z} = 0 . \quad (3.2)$$

This equation is also called the *continuity equation* (here for one-dimensional systems).

Conservation of the mass m_i of species i : Here the density W is given by the *partial density* ρ_i of species i , which denotes the mass of species i per unit volume ($\rho_i = m_i/V = (m_i/m)(m/V) = w_i \rho$). The flux J is given by the product of the partial density and the mass velocity v_i of the species i ($J = \rho_i v_i = w_i \rho v_i$) and has units of $\text{kg}/(\text{m}^2\cdot\text{s})$.

In contrast to the conservation equation for the total mass (see above), this equation has a source term which describes the formation or consumption of species i in chemical reactions. This term is given by $Q = M_i (\partial c_i / \partial t)_{\text{chem}} = r_i$, where M_i denotes the molar mass of species i (in kg/mol), $(\partial c_i / \partial t)_{\text{chem}}$ the *chemical rate of production* of species i in chemical reactions (molar scale, units of $\text{mol}/(\text{m}^3\cdot\text{s})$), and r_i the chemical rate of production (mass scale, in $\text{kg}/(\text{m}^3\cdot\text{s})$). Together with (3.1) this leads to

$$\frac{\partial(\rho w_i)}{\partial t} + \frac{\partial(\rho w_i v_i)}{\partial z} = r_i . \quad (3.3)$$

The mass velocity v_i of the species i is composed of the mean mass velocity v of the center of mass of the mixture and a *diffusion velocity* V_i (relative to the center of mass), which is caused by molecular transport due to concentration gradients of the species i (discussed in Section 3.2 and Chapter 5),

$$v_i = v + V_i . \quad (3.4)$$

Simple transformations (product law for differentiation) of (3.3) lead then to

$$w_i \frac{\partial \rho}{\partial t} + \rho \frac{\partial w_i}{\partial t} + \rho v \frac{\partial w_i}{\partial z} + w_i \frac{\partial(\rho v)}{\partial z} + \frac{\partial j_i}{\partial z} = r_i ,$$

where the symbol j_i denotes the *diffusion flux* of species i (in the center of mass system),

$$j_i = \rho w_i V_i = \rho_i V_i .$$

Together with (3.2), this equation simplifies to the species mass conservation equation

$$\rho \frac{\partial w_i}{\partial t} + \rho v \frac{\partial w_i}{\partial z} + \frac{\partial j_i}{\partial z} = r_i . \quad (3.5)$$

Conservation of the enthalpy h of the mixture: In this case, the different terms in (3.1) are given by

$$\begin{aligned} W &= \sum_j \rho_j h_j &= \sum_j \rho w_j h_j & \text{J/m}^3 \\ J &= \sum_j \rho_j v_j h_j + j_q &= \sum_j \rho v_j w_j h_j + j_q & \text{J/(m}^2\text{s)} \\ Q &= 0 && \text{(energy conservation) .} \end{aligned}$$

Here h_j denotes the *specific enthalpy* of species j (in J/kg) and j_q a *heat flux*, which corresponds to the diffusion flux j_i introduced above and is caused by transport of energy due to temperature gradients (see below). The term $\sum \rho_j v_j h_j$ describes the change of enthalpy due to the flow of species (composed of the mean mass velocity v and the diffusion velocity V_j). Substitution into Eq. (3.1) using $v_j = v + V_j$ yields

$$\sum_j \frac{\partial}{\partial z}(\rho v w_j h_j) + \sum_j \frac{\partial}{\partial z}(\rho V_j w_j h_j) + \frac{\partial j_q}{\partial z} + \sum_j \frac{\partial}{\partial t}(\rho w_j h_j) = 0 .$$

Using (3.3) and (3.4) one obtains for the first and fourth summands (T_1, T_4) that

$$\begin{aligned} T_1 + T_4 &= \sum_j \left[\rho v w_j \frac{\partial h_j}{\partial z} + h_j \frac{\partial(\rho v w_j)}{\partial z} \right] + \sum_j \left[\rho w_j \frac{\partial h_j}{\partial t} + h_j \frac{\partial(\rho w_j)}{\partial t} \right] \\ &= \rho v \sum_j w_j \frac{\partial h_j}{\partial z} + \rho \sum_j w_j \frac{\partial h_j}{\partial t} + \sum_j h_j \left[\frac{\partial(\rho v w_j)}{\partial z} + \frac{\partial(\rho w_j)}{\partial t} \right] \\ &= \rho v \sum_j w_j \frac{\partial h_j}{\partial z} + \rho \sum_j w_j \frac{\partial h_j}{\partial t} + \sum_j h_j r_j - \sum_j h_j \frac{\partial j_j}{\partial z} . \end{aligned}$$

For the second term (T_2) in the equation above, simple transformations lead to

$$T_2 = \sum_j \rho w_j V_j \frac{\partial h_j}{\partial z} + \sum_j h_j \frac{\partial(\rho w_j V_j)}{\partial z} .$$

Summation over all terms using $j_j = \rho w_j V_j$ yields the relation

$$\rho v \sum_j w_j \frac{\partial h_j}{\partial z} + \rho \sum_j w_j \frac{\partial h_j}{\partial t} + \sum_j h_j r_j + \sum_j j_j \frac{\partial h_j}{\partial z} + \frac{\partial j_q}{\partial z} = 0 . \quad (3.6)$$

The values for j_i and j_q (diffusion and heat flux) still have to be specified with respect

to the properties of the mixture (pressure, temperature, composition). The empirical laws used to describe these relations are discussed in the next section.

Use of the conservation of momentum is not necessary here due to the assumption of constant pressure (see Chapter 12).

3.2 Heat and Mass Transport

Empirical observations have established that concentration gradients lead to mass transport called *diffusion* and temperature gradients lead to heat transport called *heat conduction*. These empirical observations were later explained by the theory of irreversible thermodynamics (Hirschfelder et al. 1964). For the sake of brevity only the empirical laws are discussed here.

For the heat flux j_q , numerous measurements support the empirical *law of Fourier* in the form

$$j_q = -\lambda \frac{\partial T}{\partial z} \quad \text{J/(m}^2\cdot\text{s)}, \quad (3.7)$$

where λ denotes the *heat conductivity* of the mixture (in J/(K·m·s)). For the mass flux j_i one obtains an extended form of the *law of Fick* (which includes the first term only)

$$j_i = \frac{c^2}{\rho} M_i \sum_j M_j D_{ij} \frac{\partial x_j}{\partial z} - \frac{D_i^T}{T} \frac{\partial T}{\partial z} \quad \text{kg/(m}^2\cdot\text{s)}, \quad (3.8)$$

where c denotes the molar concentration in mol/m³; D_{ij} (units of m²/s) are *multicomponent diffusion coefficients*, x_j mole fractions, and D_i^T the *thermal diffusion coefficient* (in kg/(m·s)) of the species i based on the temperature gradient. Species transport caused by a temperature gradient (*thermal diffusion*) is also called the *Soret effect*. For many practical applications the simplified formula

$$j_i = -D_i^M \rho \frac{w_i}{x_i} \frac{\partial x_i}{\partial z} - \frac{D_i^T}{T} \frac{\partial T}{\partial z} \quad (3.9)$$

is sufficiently accurate for the mass flux j_i . Here D_i^M denotes the diffusion coefficient for species i into the mixture of the other species (discussed in Chapter 5). For binary mixtures and for trace species ($w_i \rightarrow 0$) this simplified formulation is equivalent to (3.8). This assumption of strong dilution is reasonable if the oxidizer is air, because nitrogen is in excess in this case.