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1 Fundamentals and Challenges

By N. Swaminathan and K. N. C. Bray

1.1 Aims and Coverage

Currently the energy required for domestic and industrial use and for transportation is predominantly met by burning fossil fuels. Although alternative sources are evolving, for example, by harvesting wind and solar energies, energy production by means of combustion is expected to remain dominant for many decades to come, especially for high-power density applications. Thus pollutant emission regulations for power-producing devices are set with the aim of reducing the impact of combustion on the environment, both by curtailing pollutant emissions and by increasing the efficiency of combustion equipment. Conventional combustion technologies are unable to achieve these two demands simultaneously but *fuel-lean* combustion, in which the fuel–air mixture contains a controlled excess of air, has the potential to fulfil both requirements.

The aim of this book is to bring together a review of the physics of lean combustion and its current modelling practices, together with a description of scientific challenges to be faced and ways to achieve stable lean combustion in practical devices. Additional material on non-reacting turbulent flows may be found in [1–5], and basic theories of combustion and turbulent reacting flows and their governing equations are presented in [6–9].

The present chapter sets the scene for the remainder of this volume. It has three main aims: (1) to provide a brief review of the governing equations and auxiliary relations that are required for the description of turbulent premixed combustion, (2) to review the present status of the analysis of turbulent premixed combustion, and (3) to identify flame data that can be employed to verify modelling assumptions and to propose experiments that could usefully add to such data. Different levels of detail in numerical simulations are identified, and various regimes of combustion are defined. The important concept of a *turbulent flame speed* is also introduced. Although this quantity is central to some modelling methods, it can be defined in several different ways, and consequently comparisons between measurements and theoretical predictions are often a difficult task. The review provided here is not intended to be exhaustive but to be sufficiently detailed in providing background for later chapters. Earlier comprehensive treatments of turbulent premixed flames are provided in a number of references [e.g., 9–11].

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Various modelling approaches are described in Chapter 2. As a consequence of averaging, these models are required to provide statistical information related to the unresolved small-scale structure of a turbulent flame and the two-way interaction between heat release and turbulence. It is intended that this presentation will help the reader to appreciate the physics of lean premixed and partially premixed flames, its links to modelling, and the inter-relationship among the various modelling approaches.

As we shall see, lean premixed flames are inherently unstable, and thus the discussion would be incomplete without the description of various instability processes, presented in Chapter 3. As explained there, the instabilities can be broadly classified as thermodiffusive, hydrodynamic, and thermoacoustic, based on the physical processes involved. Thermodiffusive instabilities are related to differences in the diffusion rates of mass and heat to and from the flame front, respectively. If the mass diffusion rate of reactant to the flame front is larger than the rate of heat diffusion away from the front, then the flame becomes unstable. The strong density jump across a perturbed flame front and the corresponding induced velocity changes lead to an inherent thermal instability, called the Darrieus–Landau instability. When this is coupled with buoyancy or an imposed pressure gradient, another hydrodynamic instability, called Rayleigh–Taylor instability, results. Thermoacoustic oscillations result when heat release fluctuations are in phase with fluctuations in pressure. The thermodiffusive and Darrieus–Landau instabilities are important in premixed laminar flames but are usually overwhelmed by sufficiently intense turbulence. However, the Rayleigh–Taylor and thermoacoustic instabilities can play significant roles in turbulent flames. The physics of these instabilities and methods to capture their effects on turbulent premixed flames are described in Chapter 3. The effects of thermoacoustic instabilities are of vital importance in gas turbine engines, so the science behind them and various strategies adopted to control them are also fully discussed in Chapter 3.

In appropriate circumstances, lean flames emit a very low level of pollutants and thus provide an ideal candidate for environmentally friendly engines and power-generation devices. However, premixing of fuel and oxidiser must occur inside the combustion chamber for safety reasons, creating only *partially* premixed reactants because of the limited space and time available for mixing. Nevertheless, depending on the level of partial premixing, it is still possible for a significant proportion of the combustion to occur in the premixed mode [12]. The scientific challenges involved in achieving stable lean combustion in practical devices, the physical processes involved, their interactions, and their modelling are all discussed in Chapter 4, in three different perspectives. The first section of Chapter 4 deals with the internal combustion (IC) engines employing intermittent combustion along with a detailed review of emissions legislation for automotive engines; the second and third sections consider continuous combustion systems, but differentiate the requirements for and challenges in aero gas turbines and their counterparts for power generation. This chapter also identifies some major challenges to be faced in future developments together with the factors driving them.

Chapter 5 discusses possible methods and technologies to meet the demands of the next and future generations of combustion devices. Scientific and technological challenges are also identified, and these challenges are discussed in three different

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perspectives: The concepts, specifically of combustion with high-temperature air and exhaust recirculation, are discussed in a broad sense in the first section of this chapter. The second section discusses the scientific aspects of partially premixed flames that will form the central element of future combustors and also identifies challenges for experimental investigation of lean combustion. The future modelling challenges are discussed in the third section.

Section 1.2 sets out to explain more fully what is meant by lean combustion, why it can be advantageous, what problems it introduces, and how these various topics are addressed in this book.

1.2 Background

It is convenient to identify two different modes for the combustion of a gaseous fuel: If the fuel and air are fully premixed before they enter the combustion zone, the flame is said to be *premixed*. On the other hand, when the fuel is kept separate until it burns, so that the reactants must diffuse towards each other before they react, a *diffusion* flame results. Combustion in a diffusion flame is centred on the stoichiometric or chemically balanced mixture of fuel and air, resulting in high temperatures and pollutant concentrations in combustion products. A difference between these two types of burning, leading to a burning-mode criterion known as the flame index [13, 14], is that fuel and air enter a premixed flame from the same side, whereas they go in from opposite sides of a diffusion flame. Fuel–air mixing is incomplete in many practical systems, leading to *partially* premixed combustion.

The term *lean* implies that the fuel–air mixture contains air in excess of that required by stoichiometry for a given amount of fuel, an amount that is determined by the overall energy output of the system and its thermal efficiency. The equivalence ratio, often denoted by ϕ, is defined as the ratio of the actual fuel-to-air mass proportion to its stoichiometric value and is typically small in most practical systems other than spark-ignited IC engines. At present, these are usually required to operate under stoichiometric conditions because of the requirements of the catalytic convertor. Future spark-ignition engines are expected to burn fuel lean, leading to a significant improvement in thermal efficiency, together with a significant reduction in emissions of oxides of nitrogen and carbon. However, careful design is required because of the inherent difficulty of achieving stable lean combustion, as explained in Chapters 4 and 5. Even when the *overall* equivalence ratio of the combustion system is very lean, some arrangements, such as exhaust gas recirculation (EGR for diesel engines), or flue gas recirculation (FGR for furnaces and boilers), or rich burn–quench–lean burn (RQL for gas turbines), are required for controlling nitric oxide emissions. This is because *local* combustion occurs mostly at the stoichiometric condition, resulting in a high flame temperature, which increases nitric oxide formation. The special arrangements such as the EGR just noted dilute the local combustible mixture with cooled combustion products and limit the peak flame temperature.

Figure 1.1 shows typical variations of flame temperature T_f and concentrations of oxides of nitrogen and carbon with equivalence ratio. The peak flame temperature and concentrations of pollutants decrease sharply as the equivalence ratio is reduced below unity, irrespective of operating pressure and reactant temperature.

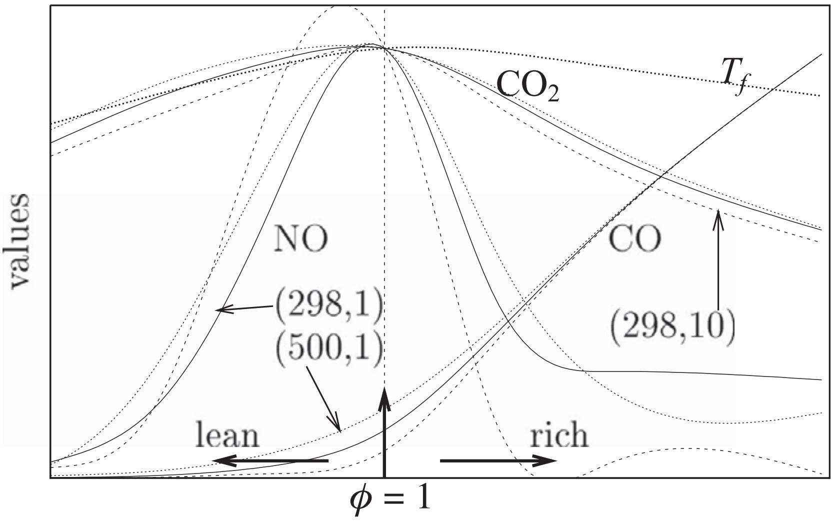

Figure 1.1. Typical variation of NO, CO, CO$_2$, and T_f with equivalence ratio. Effects of reactant temperature and operating pressure are also shown. (298.1) implies 298 K and 1 atm.

It is clear that locally lean combustion, which requires some degree of premixing, offers low levels of emission. Although this is very desirable, Fig. 1.2 shows that the laminar flame speed varies sharply with the equivalence ratio on the lean side. Thus a small change in local equivalence ratio, which may be caused by variations in local fluid dynamics induced by a number of factors in a practical situation, can lead to a substantial change in the local heat release rate. The sensitivity of the flame speed to the equivalence ratio ϕ is expressed by $\mathrm{d}\ln \hat{S}_L/\mathrm{d}\phi = m\phi/\hat{S}_L$, where $\hat{S}_L$ is the normalised flame speed and $m = \mathrm{d}\hat{S}_L/\mathrm{d}\phi$, as shown in Fig. 1.2. The following observations can be made from this figure, which is constructed with the available experimental data [15–18]: (1) The sensitivity does not depend on the fuel, but it depends on the reactant temperature, and (2) the hydrocarbons are more sensitive to local-equivalence-ratio oscillation than hydrogen and acetylene (compare the values for $T = 298$ K). These are purely thermochemical effects, which are compounded by effects of fluid dynamics and its interaction with thermochemistry in practical systems.

If the change in the local heat release rate is highly intermittent or if it is in phase with pressure oscillations, then the combustion process can become very rough, which is highly undesirable. Combustion instabilities are discussed in Chapter 3. Achieving smooth, stable lean combustion in practical devices is difficult because of the strong coupling between heat release from chemical reactions, diffusion, and fluid dynamics; see Chapter 4. The requirement to ensure thorough mixing between the fuel and air, often at significantly raised values of temperature and pressure, poses additional problems, because of the danger of the mixture auto-igniting upstream of the location where a flame is to be stabilised. In the purely chemical ignition or auto-ignition process [6], the temperature initially rises only slowly during an *ignition delay* stage in which a pool of reaction intermediates is formed before increasing more steeply in a second, heat release stage. Auto-ignitive burning and ignition delay times are discussed in Section 3.1.

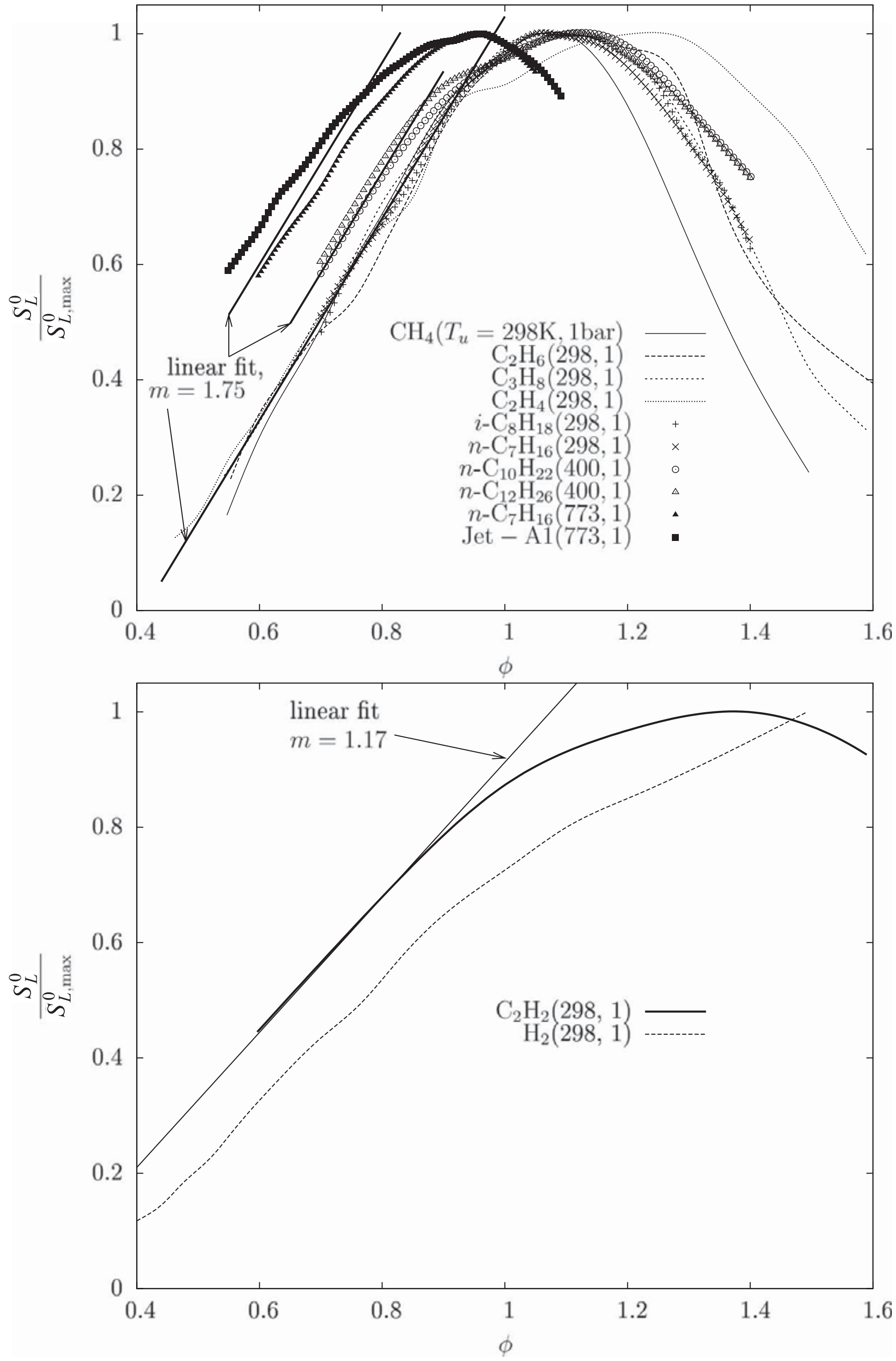

Figure 1.2. Variation of laminar flame speed with equivalence ratio for commonly used hydrocarbon–air mixtures. The flame speed is normalised by its maximum value $S^0_{L,\max}$, which is 0.416, 0.433, 0.449, and 0.722 m/s [15], 0.352 and 0.405 m/s [16], 0.658 and 0.682 m/s [17], and 2.312 and 2.023 m/s [18] in the same order as in the legend. For acetylene – and hydrogen–air mixtures [15] it is 1.559 and 2.856 m/s, respectively.

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To avoid auto-ignition, many practical systems feed the fuel and air into the combustion zone while it is only *partially* premixed, and then the potential benefits of premixing are only partially achieved. All of these processes are invariably turbulent, which greatly compounds the complexity level. As explained in Section 1.4, turbulent flow and combustion involve a very wide range of length and time scales that cannot all be resolved in numerical simulations of practical systems. This difficulty is overcome by the introduction of some form of *averaging* into the governing differential equations. Averaging involves a loss of information, with the result that the number of unknowns always exceeds the number of equations, and an appropriate number of *model* expressions must be devised from an understanding of the controlling physics; see Chapter 2. Thus designing and constructing successful lean combustion systems are major challenges [19] that require a close and thorough understanding of all the relevant physical processes and their interactions.

1.3 Governing Equations

This section provides a brief summary of the equations governing the flow of a chemically reacting gas mixture; their derivation is described in detail elsewhere, for example by Williams [7] and Law [6]. These equations consist of conservation laws of mass, momentum, and energy and concentrations of reacting chemical species, together with equations specifying molecular transport and thermodynamic properties of the mixture and the rates of chemical conversion. Mass, momentum, and species conservation equations are

$$\begin{aligned}\frac{\mathrm{D}\rho}{\mathrm{D}t} + \rho\frac{\partial u_k}{\partial x_k} &= 0,\\ \rho\frac{\mathrm{D}u_\ell}{\mathrm{D}t} &= -\frac{\partial p}{\partial x_\ell} + \frac{\partial \tau_{\ell k}}{\partial x_k} + \rho\sum_{i=1}^{N} Y_i f_{i\ell},\\ \rho\frac{\mathrm{D}Y_i}{\mathrm{D}t} &= -\frac{\partial J_{ik}}{\partial x_k} + \dot{\omega}_i. \qquad (1.1)\end{aligned}$$

Here and in the following chapters, Cartesian tensor notations are used with the indices k, ℓ, and m. These indices imply summation when they are repeated in the same term. In Eqs. (1.1), the substantial derivative is $\mathrm{D}/\mathrm{D}t \equiv \partial/\partial t + u_k\partial/\partial x_k$ and the symbols x_k, u_k, ρ, p, and Y_i represent, respectively, the spatial coordinate in direction k, velocity component in that direction, gas density, pressure, and the mass fraction of a chemical species i, where $i = 1 \ldots N$. The quantity $f_{i\ell}$ is a body force per unit volume acting on species i in direction ℓ; if this body force is due to a gravitational acceleration g, the body-force term becomes $\overline{\rho} g_\ell$. Subscripts i and j are consistently used for chemical species; when their summation is required, it is shown explicitly. Also, $\dot{\omega}_i$ is the mass rate of production or destruction of species i that is due to chemical reactions. Finally, $\tau_{\ell k}$ is a shear-stress component in the ℓth direction on a surface whose outward normal is in the kth direction, which may be represented by

$$\tau_{\ell k} = \mu\left(\frac{\partial u_\ell}{\partial x_k} + \frac{\partial u_k}{\partial x_\ell} - \frac{2}{3}\frac{\partial u_m}{\partial x_m}\delta_{\ell k}\right), \qquad (1.2)$$

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where μ is viscosity coefficient of the mixture and $\delta_{\ell k}$ is the Kronecker delta. For present purposes the molecular diffusion flux J_{ik}, which is the mass molecular flux of species i in direction k, can be approximated by Fick's law:

$$J_{ik} = -\rho \mathcal{D}_i \frac{\partial Y_i}{\partial x_k}, \tag{1.3}$$

where $\mathcal{D}_i$ is a diffusion coefficient.

The thermodynamic properties of a mixture of ideal gases may be described by the equation of state,

$$p = \rho \mathcal{R} T \sum_{i=1}^{N} \frac{Y_i}{W_i}, \tag{1.4}$$

where W_i is the molecular weight of species i and $\mathcal{R}$ is the universal gas constant, 8.314 kJ kmol^{-1} K^{-1}. The specific enthalpy of the mixture is

$$h = \sum_{i=1}^{N} Y_i h_i, \tag{1.5}$$

and the specific enthalpy of a species i is

$$h_i = h_i^0 + h_i^s(T; T^0), \tag{1.6}$$

where h_i^0 is the standard specific heat of formation of species i at temperature T^0 and

$$h_i^s(T; T^0) = \int_{T^0}^{T} c_{p,i}\, \mathrm{d}T, \tag{1.7}$$

is the specific sensible enthalpy of the species i relative to T^0. This can sometimes be approximated by treating $c_{p,i}$ as an appropriately chosen constant.

The energy equation can be written in several alternative forms [6, 9], one of which is

$$\rho \frac{\mathrm{D}h}{\mathrm{D}t} = \frac{\mathrm{D}p}{\mathrm{D}t} + \tau_{\ell k} \frac{\partial u_\ell}{\partial x_k} - \frac{\partial q_k}{\partial x_k} - \rho \sum_{i=1}^{N} \mathcal{D}_i f_{ik} \frac{\partial Y_i}{\partial x_k} + \dot{Q}_{\mathrm{rad}}. \tag{1.8}$$

In this equation q_k is the molecular flux of enthalpy, given by

$$q_k = -\hat{\lambda} \frac{\partial T}{\partial x_k} - \rho \sum_{i=1}^{N} h_i \mathcal{D}_i \frac{\partial Y_i}{\partial x_k}, \tag{1.9}$$

where $\hat{\lambda}$ is the thermal conductivity of the mixture and $\dot{Q}_{\mathrm{rad}}$ is the energy exchange per unit volume due to radiation.

Three dimensionless parameters are conventionally introduced to characterise molecular transport. The *Prandtl* number of the mixture is defined as $\mathrm{Pr} = \mu c_p / \hat{\lambda}$, where $c_p = \sum_{i=1}^{N} Y_i c_{p,i}$ is the specific heat at constant pressure of the mixture. The *Schmidt* number of species i is $\mathrm{Sc}_i = \mu / \rho \mathcal{D}_i$, and the *Lewis* number of species i is $\mathrm{Le}_i = \hat{\lambda} / c_p \rho \mathcal{D}_i = \mathrm{Sc}_i / \mathrm{Pr}$.

Equation (1.8) may be greatly simplified if certain restrictive conditions are met; see for example Libby and Williams [10]: (1) It is assumed that the flow Mach

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number is sufficiently low for compressibility effects to be neglected, allowing the first two terms on the right-hand side of Eq. (1.8) to be set to zero. (2) Radiative heat transfer and energy changes arising from body forces are assumed to be negligible. (3) It is also assumed that $\mathrm{Sc}_i = \mathrm{Pr}$ for all species; this requires both that $\mathcal{D}_i$ can be approximated by a common value $\mathcal{D}$ for all species and also that $\mathrm{Sc} = \mathrm{Pr}$, implying that the Lewis number is unity. Then the molecular-diffusion terms arising when Eq. (1.9) is substituted into Eq. (1.8) cancel, with molecular heat flux terms generated if Eqs. (1.5) and (1.6) are used to replace $\partial h_i/\partial x_k$ with $c_{p,i}\partial T/\partial x_k$. The molecular flux of enthalpy becomes $q_k = -\rho\mathcal{D}\partial h/\partial x_k$, and Eq. (1.8) can be written as

$$\rho\frac{\mathrm{D}h}{\mathrm{D}t} = \frac{\partial}{\partial x_k}\left(\rho\mathcal{D}\frac{\partial h}{\partial x_k}\right). \tag{1.10}$$

Subject to appropriate initial and boundary conditions, Eq. (1.10) is satisfied by $h =$ constant, i.e., an *isenthalpic* flow. This simplified form of the energy equation is often used in turbulent combustion models, and it is applicable for different situations of lean premixed combustion noted in the previous section as long as restrictive conditions (2) and (3) are met. However, the prediction of lean premixed combustion and flow in IC engines will involve $\partial p/\partial t$ because of a cyclic variation of pressure inside the cylinder. Situations in which the preceding restrictive conditions are to be relaxed are noted appropriately in the following chapters.

1.3.1 Chemical Reaction Rate

Two different types of information are required for specifying the chemical-reaction-rate term $\dot{\omega}_i$ appearing in the last of Eqs. (1.1): a reaction *mechanism* and a set of reaction *rates*. The first of these consists of a set of n elementary reactions, the rth of which is written as

$$\sum_{i=1}^{N} \nu'_{ri} M_i \underset{k_{br}}{\overset{k_{fr}}{\rightleftharpoons}} \sum_{i=1}^{N} \nu''_{ri} M_i, \tag{1.11}$$

where M_i is the chemical symbol for species i involved in the rth reaction and ν' and ν'' are the *stoichiometric coefficients* for species i in the forward and backward steps of the reaction, respectively. If reaction (1.11) describes the actual elementary process by which these species are created and destroyed, then the stoichiometric coefficients will be integers. If the reaction is a purely phenomenological description of the effects of several elementary reactions, then it is called a *global* reaction, which can have non-integer stoichiometric coefficients. As shown, the reaction is *reversible*, i.e., it proceeds in both directions. A reaction mechanism can be of any length, and detailed mechanisms consisting of some hundreds of elementary reactions are not uncommon (see for example [20, 21]).

The quantity $\dot{\omega}_i$ is the net result of all n chemical reactions, and thus

$$\dot{\omega}_i = \sum_{r=1}^{n} (\nu''_{ir} - \nu'_{ir})\varpi_r W_i, \tag{1.12}$$

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where ϖ_r is the molar rate of reaction r, which can be expressed in the form

$$\varpi_r = k_{\mathrm{fr}} \prod_{j=1}^{N} \left(\frac{\rho Y_j}{W_j} \right)^{\nu'_{jr}} - k_{\mathrm{br}} \prod_{j=1}^{N} \left(\frac{\rho Y_j}{W_j} \right)^{\nu''_{jr}}, \tag{1.13}$$

where k_{fr} and k_{br} are the forward- and backward-rate coefficients, respectively, of reaction r, which are conventionally written in the form

$$k_{\mathrm{fr}}(T) = A_{\mathrm{fr}} T^{\alpha_{\mathrm{fr}}} \exp\left(\frac{-E^a_{\mathrm{fr}}}{\mathcal{R}T} \right). \tag{1.14}$$

A similar expression can be written for the specific rate constant k_{br} of the backward step of the elementary reaction r. The ratio of the forward-rate to the backward-rate constants is given by the equilibrium constant. The pre-exponential factor A_{fr}, the temperature exponent α_{fr}, and the activation energy E^a_{fr} are constants, which are often obtained from shock-tube experiments [22–24] and are of an empirical nature.

1.3.2 Mixture Fraction

If partially premixed combustion occurs, that is, if fuel and air are not fully mixed when they enter the combustion zone, then some means must be found to track variations in their ratio. This may be done by the introduction of so-called *conserved scalar* variables, which remain unaffected by the progress of chemical reactions. The mass fractions of chemical elements, the pth of which is denoted by ξ_p, where $p = 1, \ldots, q$, are conserved scalars and are related to the species mass fractions by

$$\xi_p = \sum_{i=1}^{N} \mu_{pi} Y_i,$$

in which μ_{pi} represents the number of kilograms of element p in 1 kg of species i. Because elements are conserved in chemical reactions, we have

$$\sum_{i=1}^{N} \mu_{pi} \dot{\omega}_i = 0.$$

It follows [10] from this expression, together with the third of Eqs. (1.1) and the simple Fick's law of diffusion expression of Eq. (1.3), that the element mass fraction ξ_p is governed by

$$\rho \frac{\mathrm{D}\xi_p}{\mathrm{D}t} = \frac{\partial}{\partial x_k} \sum_{i=1}^{N} \rho \mu_{pi} \mathcal{D}_i \frac{\partial Y_i}{\partial x_k}. \tag{1.15}$$

If the approximation $\mathcal{D}_i \approx \mathcal{D}$ can be justified, where $\mathcal{D}$ is a single molecular-diffusion coefficient applicable to all chemical species, then Eq. (1.15) may be seen to have the same form as simplified energy equation (1.10), namely,

$$\rho \frac{\mathrm{D}\xi_p}{\mathrm{D}t} = \frac{\partial}{\partial x_k} \rho \mathcal{D} \frac{\partial \xi_p}{\partial x_k}, \tag{1.16}$$

from which it follows that ξ_p and the specific enthalpy h are linearly related, provided they have the same boundary conditions. This can be achieved by the introduction

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of a normalised conserved scalar Z, the *mixture fraction*, based either on h or on an element mass fraction so

$$Z = \frac{h - h_0}{h_1 - h_0} = \frac{\xi_p - \xi_{p,0}}{\xi_{p,1} - \xi_{p,0}},$$

where the subscripts 0 and 1 respectively represent conditions in pure air and pure fuel, and

$$\rho \frac{\mathrm{D}Z}{\mathrm{D}t} = \frac{\partial}{\partial x_k} \rho \mathcal{D} \frac{\partial Z}{\partial x_k}. \tag{1.17}$$

However, it must be kept in mind that this formulation involves significant simplifications of molecular-transport processes. Such simplifications are known to lead to large errors in predicting laminar flame properties in some circumstances and, as we shall see, structures resembling laminar flames are often found to occur in premixed turbulent combustion.

1.3.3 Spray Combustion

Liquid fuel must be *atomised* into a fine spray that is either mixed with air before it enters the combustion chamber or is fed directly into the combustion zone. The physics of spray formation, evaporation, and combustion is described in detail elsewhere [25–32]. Our aim here is simply to identify the most important processes controlling this type of combustion. An isolated liquid drop, at rest in a stationary medium, evaporates in a time proportional to the square of its initial diameter. However, the process is more complex in the presence of relative motion, in which details of the flow fields and heat and mass transfer rates both inside and outside the drop must be taken into account [32]. The vapour evaporating from an isolated drop in a stagnant environment can burn in a laminar diffusion flame, forming an envelope surrounding the drop, and, once again, relative motion can complicate the picture, with burning sometime occurring in the wake behind the drop. Liquid sprays can burn in a variety of arrangements [33, 34]: in envelopes diffusion flames surrounding either single drops or groups of drops, in wakes behind drops, in flames that are distinct from the evaporating liquid drops, or in a combination of ways. Turbulence adds further complexity, but this categorisation can still be applied.

If fuel-lean combustion is to be achieved, the diffusion-flame mode of burning, which takes place under stoichiometric conditions, must always be minimised, if it cannot be eliminated. This means that burning in envelope or wake flames must be avoided to the extent possible; droplets need to evaporate as quickly as possible and their vapour thoroughly mixed with air before burning takes place. Efficient atomisation into a fine mist of droplets aids this process. Nevertheless, the need to avoid the possibility of auto-ignition or flashback limits the time available for evaporation and mixing, and spray combustion will generally be only partially premixed. The twin annular premixed system (TAPS), discussed in Sections 4.2 and 5.2, is a good example for a practical arrangment to minimise, if not to completely avoid, stoichiometric combustion.