TURBULENT COMBUSTION

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Turbulent combustion: The state of the art

1.1 What Is Specific about Turbulence with Combustion?

In recent years, nothing seems to have inspired researchers in the combustion community so much as the unresolved problems in turbulent combustion. Turbulence in itself is far from being fully understood; it is probably the most significant unresolved problem in classical physics. Since the flow is turbulent in nearly all engineering applications, the urgent need to resolve engineering problems has led to preliminary solutions called turbulence models. These models use systematic mathematical derivations based on the Navier–Stokes equations up to a certain point, but then they introduce closure hypotheses that rely on dimensional arguments and require empirical input. This semiempirical nature of turbulence models puts them into the category of an art rather than a science.

For high Reynolds number flows the so-called eddy cascade hypothesis forms the basis for closure of turbulence models. Large eddies break up into smaller eddies, which in turn break up into even smaller ones, until the smallest eddies disappear due to viscous forces. This leads to scale invariance of energy transfer in the inertial subrange of turbulence. We will denote this as *inertial range invariance* in this book. It is the most important hypothesis for large Reynolds number turbulent flows and has been built into all classical turbulence models, which thereby satisfy the requirement of Reynolds number independence in the large Reynolds number limit. Viscous effects are of importance in the vicinity of solid walls only, a region of minor importance for combustion.

The apparent success of turbulence models in solving engineering problems has encouraged similar approaches for turbulent combustion, which consequently led to the formulation of turbulent combustion models. This is, however, where problems arise.

Combustion requires that fuel and oxidizer be mixed at the molecular level. How this takes place in turbulent combustion depends on the turbulent mixing process. The general view is that once a range of different size eddies has developed, strain and shear at the interface between the eddies enhance the mixing. During the eddy break-up process and the formation of smaller eddies, strain and shear will increase and thereby steepen the concentration gradients at the interface between reactants, which in turn enhances their molecular interdiffusion. Molecular mixing of fuel and oxidizer, as a prerequisite of combustion, therefore takes place at the interface between small eddies. Similar considerations apply, once a flame has developed, to the conduction of heat and the diffusion of radicals out of the reaction zone at the interface.

While this picture follows standard ideas about turbulent mixing, it is less clear how combustion modifies these processes. Chemical reactions consume the fuel and the oxidizer at the interface and will thereby steepen their gradients even further. To what extent this will modify the interfacial diffusion process still needs to be understood.

This could lead to the conclusion that the interaction between turbulence and combustion invalidates classical scaling laws known from nonreacting turbulent flows, such as the Reynolds number independence of free shear flows in the large Reynolds number limit. To complicate the picture further, one has to realize that combustion involves a large number of elementary chemical reactions that occur on different time scales. If all these scales would interact with all the time scales within the inertial range, no simple scaling laws could be found. Important empirical evidence, however, does not confirm such pessimism:

- The difference between the turbulent and the laminar burning velocity, normalized by the turbulence intensity, is independent of the Reynolds number. It is Damköhler number independent for large scale turbulence, but it becomes proportional to the square root of the Damköhler number for small scale turbulence (cf. Section 2.10).
- The flame length of a nonbuoyant turbulent jet diffusion flame, for instance, is Reynolds number and Damköhler number independent (cf. Section 3.9).
- The NO emission index of hydrogen–air diffusion flames is independent of the Reynolds number but proportional to the square root of the Damköhler number (cf. Section 3.14).
- The lift-off height in lifted jet diffusion flames is independent of the nozzle diameter and increases nearly linearly with the jet exit velocity (cf. Section 4.6).

Power law Damköhler number scaling laws may be the exception rather than the rule, but they indicate that there are circumstances where only a few chemical and turbulent time scales are involved. As far as Reynolds number independence is concerned, it should be noted that the Reynolds number in many laboratory experiments is not large enough to approach the large Reynolds number limit. A remaining Reynolds number dependence of the turbulent mixing process would then show up in the combustion data. Apart from these experimental limitations (which become more serious owing to the increase of viscosity with temperature) it is not plausible that there would be a Reynolds number dependence introduced by combustion, because chemical reactions introduce additional time scales but no viscous effects. Even if chemical time scales interact with turbulent time scales in the inertial subrange of turbulence, these interactions cannot introduce the viscosity as a parameter for dimensional scaling, because it has disappeared as a parameter in that range. This does not preclude that ratios of molecular transport properties, Prandtl or Lewis numbers, for instance, would not appear in scaling laws in combustion. As we have restricted the content of this book to low speed combustion, the Mach number will not appear in the analysis.

There remains, however, the issue of to what extent we can expect an interaction between chemical and turbulent scales in the inertial subrange. Here, we must realize that combustion differs from isothermal mixing in chemically reacting flows by two specific features:

- heat release by combustion induces an increase of temperature, which in turn
- accelerates combustion chemistry. Because of the competition between chain branching and chain breaking reactions this process is very sensitive to temperature changes.

Heat release combined with temperature sensitive chemistry leads to typical combustion phenomena, such as ignition and extinction. This is illustrated in Figure 1.1 where the maximum temperature in a homogeneous flow combustor is plotted as a function of the Damköhler number, which here represents the ratio of the residence time to the chemical time. This is called the S-shaped curve in the combustion literature. The lower branch of this curve corresponds to a slowly reacting state of the combustor prior to ignition, where the short residence times prevent a thermal runaway. If the residence time is increased by lowering the flow velocity, for example, the Damköhler number increases until the ignition point I is reached. For values larger than Da_I thermal runaway

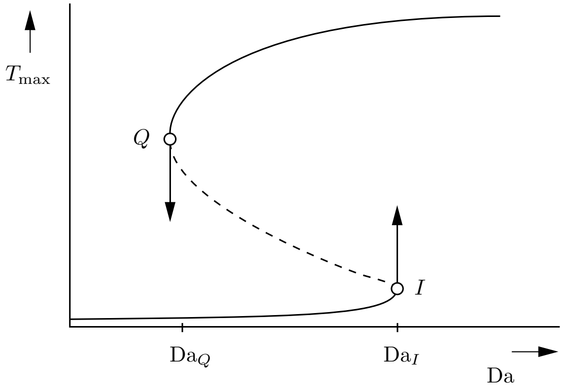

Figure 1.1. The S-shaped curve showing the maximum temperature in a well-stirred reactor as a function of the Damköhler number.

leads to a rapid unsteady transition to the upper close-to-equilibrium branch. If one starts on that branch and decreases the Damköhler number, thereby moving to the left in Figure 1.1, one reaches the point Q where extinction occurs. This is equivalent to a rapid transition to the lower branch. The middle branch between the point I and Q is unstable.

In the range of Damköhler numbers between Da_Q and Da_I, where two stable branches exist, any initial state with a temperature in the range between the lower and the upper branch is rapidly driven to either one of them. Owing to the temperature sensitivity of combustion reactions the two stable branches represent strong attractors. Therefore, only regions close to chemical equilibrium or close to the nonreacting state are frequently accessed. In an analytic study of stochastic Damköhler number variations Oberlack et al. (2000) have recently shown that the probability of finding realizations apart from these two steady state solutions is indeed very small.

Chemical reactions that take place at the high temperatures on the upper branch of Figure 1.1 are nearly always fast compared to all turbulent time scales and, with the support of molecular diffusion, they concentrate in thin layers of a width that is typically smaller than the Kolmogorov scale. Except for density changes these layers cannot exert a feedback on the flow. Therefore they cannot influence the inertial range scaling. If these layers extinguish as the result of excessive heat loss, the temperature decreases such that chemistry becomes very slow and mixing can also be described by classical inertial range scaling.

In both situations, fast and slow chemistry, time and length scales of combustion are separated from those of turbulence in the inertial subrange. This *scale separation* is a specific feature of most practical applications of turbulent combustion.[†] It makes the mixing process in the inertial range independent of chemistry and simplifies modeling significantly. Almost all turbulent combustion models explicitly or implicitly assume scale separation.

As a general theme of this chapter, we will investigate whether the turbulence models to be discussed are based on the postulate of scale separation between turbulent and chemical time scales. In addition, it will be pointed out if a combustion model does not satisfy the postulate of Reynolds number independence in the large Reynolds number limit.

1.2 Statistical Description of Turbulent Flows

The aim of stochastic methods in turbulence is to describe the fluctuating velocity and scalar fields in terms of their statistical distributions. A convenient starting point for this description is the distribution function of a single variable, the velocity component u, for instance. The distribution function $F_u(U)$ of u is defined by the probability p of finding a value of $u < U$:

$$F_u(U) = p(u < U), \tag{1.1}$$

where U is the so-called sample space variable associated with the random stochastic variable u. The sample space of the random stochastic variable u consists of all possible realizations of u. The probability of finding a value of u in a certain interval $U_- \leq u < U_+$ is given by

$$p(U_- \leq u < U_+) = F_u(U_+) - F_u(U_-). \tag{1.2}$$

The probability density function (pdf) of u is now defined as

$$P_u(U) = \frac{dF_u(U)}{dU}. \tag{1.3}$$

It follows that $P_u(U)dU$ is the probability of finding u in the range $U \leq u < U + dU$. If the possible realizations of u range from $-\infty$ to $+\infty$, it follows that

$$\int_{-\infty}^{+\infty} P_u(U)\, dU = 1, \tag{1.4}$$

which states that the probability of finding the value u between $-\infty$ and $+\infty$ is certain (i.e., it has the probability unity). It also serves as a normalizing condition for P_u.

[†] A potential exception is the situation prior to ignition, where chemistry is neither slow enough nor fast enough to be separated from the turbulent time scales. We will discuss this situation in detail in Chapter 3, Section 3.12.

In turbulent flows the pdf of any stochastic variable depends, in principle, on the position $\boldsymbol{x}$ and on time t. These functional dependencies are expressed by the following notation:

$$P_u(U;\boldsymbol{x},t). \tag{1.5}$$

The semicolon used here indicates that P_u is a probability density in U-space and is a function of $\boldsymbol{x}$ and t. In stationary turbulent flows it does not depend on t and in homogeneous turbulent fields it does not depend on $\boldsymbol{x}$. In the following, for simplicity of notation, we will not distinguish between the random stochastic variable u and the sample space variable U, dropping the index and writing the pdf as

$$P(u;\boldsymbol{x},t). \tag{1.6}$$

Once the pdf of a variable is known one may define its moments by

$$\overline{u(\boldsymbol{x},t)^n} = \int_{-\infty}^{+\infty} u^n P(u;\boldsymbol{x},t)\,du. \tag{1.7}$$

Here the overbar denotes the average or mean value, sometimes also called expectation, of u^n. The first moment ($n = 1$) is called the mean of u:

$$\bar{u}(\boldsymbol{x},t) = \int_{-\infty}^{+\infty} u\; P(u;\boldsymbol{x},t)\,du. \tag{1.8}$$

Similarly, the mean value of a function $g(u)$ can be calculated from

$$\bar{g}(\boldsymbol{x},t) = \int_{-\infty}^{+\infty} g(u)P(u;\boldsymbol{x},t)\,du. \tag{1.9}$$

Central moments are defined by

$$\overline{[u(\boldsymbol{x},t) - \overline{u(\boldsymbol{x},t)}]^n} = \int_{-\infty}^{+\infty} (u-\bar{u})^n P(u;\boldsymbol{x},t)\,du, \tag{1.10}$$

where the second central moment

$$\overline{[u(\boldsymbol{x},t) - \overline{u(\boldsymbol{x},t)}]^2} = \int_{-\infty}^{+\infty} (u-\bar{u})^2 P(u;\boldsymbol{x},t)\,du \tag{1.11}$$

is called the variance. If we split the random variable u into its mean and the fluctuations u' as

$$u(\boldsymbol{x},t) = \bar{u}(\boldsymbol{x},t) + u'(\boldsymbol{x},t), \tag{1.12}$$

where $\overline{u'} = 0$ by definition, the variance is found to be related to the first and second moment by

$$\overline{u'^2} = \overline{(u-\bar{u})^2} = \overline{u^2 - 2u\bar{u} + \bar{u}^2} = \overline{u^2} - \bar{u}^2. \tag{1.13}$$

Models for turbulent flows traditionally start from the Navier–Stokes equations to derive equations for the first and the second moments of the flow variables using (1.12). Since the three velocity components and the pressure depend on each other through the solutions of the Navier–Stokes equations they are correlated. To quantify these correlations it is convenient to introduce the joint probability density function of the random variables. For instance, the joint pdf of the velocity components u and v is written as

$$P(u, v; \boldsymbol{x}, t).$$

The pdf of u, for instance, may be obtained from the joint pdf by integration over all possible realizations of v,

$$P(u) = \int_{-\infty}^{+\infty} P(u, v)\, dv, \tag{1.14}$$

and is called the marginal pdf of u in this context. The correlation between u and v is given by

$$\overline{u'v'} = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} (u - \overline{u})(v - \overline{v}) P(u, v)\, du dv. \tag{1.15}$$

This can be illustrated by a so-called scatter plot (cf. Figure 1.2). If a series of instantaneous realizations of u and v are plotted as points in a graph of u and v, these points will scatter within a certain range. The means $\overline{u}$ and $\overline{v}$ are the average positions of the points in u and v directions, respectively. The correlation $\overline{u'v'}/(\overline{u'^2}\,\overline{v'^2})^{1/2}$ is proportional to the slope of the average straight line through the data points.

A joint pdf of two variables can always be written as a product of a conditional pdf of one variable times the marginal pdf of the other, for

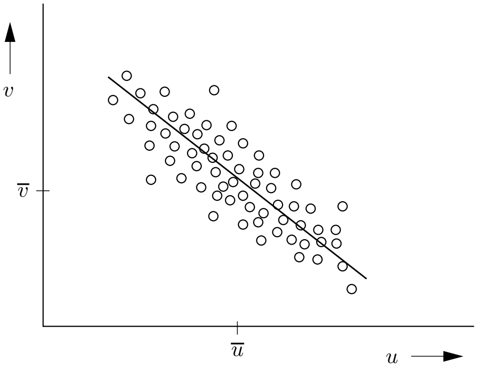

Figure 1.2. A scatter plot of two velocity components u and v illustrating the correlation coefficient.

example

$$P(u, v; \boldsymbol{x}, t) = P(u \mid v; \boldsymbol{x}, t) P(v; \boldsymbol{x}, t). \tag{1.16}$$

This is called Bayes' theorem. In this example the conditional pdf $P(u \mid v; \boldsymbol{x}, t)$ describes the probability density of u, conditioned at a fixed value of v. If u and v are not correlated they are called statistically independent. In that case the joint pdf is equal to the product of the marginal pdfs:

$$P(u, v; \boldsymbol{x}, t) = P(u; \boldsymbol{x}, t) P(v; \boldsymbol{x}, t). \tag{1.17}$$

By using this in (1.15) and integrating, we easily see that $\overline{u'v'}$ vanishes, if u and v are statistically independent. In turbulent shear flows $\overline{u'v'}$ is interpreted as a Reynolds shear stress, which is nonzero in general. The conditional pdf $P(u \mid v; \boldsymbol{x}, t)$ can be used to define conditional moments. For example, the conditional mean of u, conditioned at a fixed value of v, is given by

$$\langle u \mid v \rangle = \int_{-\infty}^{+\infty} u P(u \mid v)\, du. \tag{1.18}$$

In the following we will use angular brackets for conditional means only.

As a consequence of the nonlinearity of the Navier–Stokes equations several closure problems arise. These are not only related to correlations between velocity components among each other and the pressure, but also to correlations between velocity gradients and correlations between velocity gradients and pressure fluctuations. These appear in the equations for the second moments as dissipation terms and pressure–strain correlations, respectively. The statistical description of gradients requires information from adjacent points in physical space. Very important aspects in the statistical description of turbulent flows are therefore related to two-point correlations, which we will introduce in Section 1.4.

For flows with large density changes as occur in combustion, it is often convenient to introduce a density-weighted average $\tilde{u}$, called the Favre average, by splitting $u(\boldsymbol{x}, t)$ into $\tilde{u}(\boldsymbol{x}, t)$ and $u''(\boldsymbol{x}, t)$ as

$$u(\boldsymbol{x}, t) = \tilde{u}(\boldsymbol{x}, t) + u''(\boldsymbol{x}, t). \tag{1.19}$$

This averaging procedure is defined by requiring that the average of the product of u'' with the density ρ (rather than u'' itself) vanishes:

$$\overline{\rho u''} = 0. \tag{1.20}$$

The definition for $\tilde{u}$ may then be derived by multiplying (1.19) by the density ρ and averaging:

$$\overline{\rho u} = \overline{\rho \tilde{u}} + \overline{\rho u''} = \bar{\rho} \tilde{u}. \tag{1.21}$$

Here the average of the product $\rho\tilde{u}$ is equal to the product of the averages $\bar{\rho}$ and $\tilde{u}$, since $\tilde{u}$ is already an average defined by

$$\tilde{u} = \overline{\rho u}/\bar{\rho}. \tag{1.22}$$

This density-weighted average can be calculated, if simultaneous measurements of ρ and u are available. Then, by taking the average of the product ρu and dividing it by the average of ρ one obtains $\tilde{u}$. While such measurements are often difficult to obtain, Favre averaging has considerable advantages in simplifying the formulation of the averaged Navier–Stokes equations in variable density flows. In the momentum equations, but also in the balance equations for the temperature and the chemical species, the convective terms are dominant in high Reynolds number flows. Since these contain products of the dependent variables and the density, Favre averaging is the method of choice. For instance, the average of the product of the density ρ with the velocity components u and v would lead with conventional averages to four terms,

$$\overline{\rho u v} = \bar{\rho}\,\bar{u}\,\bar{v} + \bar{\rho}\overline{u'v'} + \overline{\rho'u'}\bar{v} + \overline{\rho'v'}\bar{u} + \overline{\rho'u'v'}. \tag{1.23}$$

Using Favre averages one writes

$$\begin{aligned} \rho u v &= \rho(\tilde{u} + u'')(\tilde{v} + v'') \\ &= \rho\tilde{u}\tilde{v} + \rho u''\tilde{v} + \rho v''\tilde{u} + \rho u''v''. \end{aligned} \tag{1.24}$$

Here fluctuations of the density do not appear. Taking the average leads to two terms only,

$$\overline{\rho u v} = \bar{\rho}\tilde{u}\tilde{v} + \bar{\rho}\widetilde{u''v''}. \tag{1.25}$$

This expression is much simpler than (1.23) and has formally the same structure as the conventional average of uv for constant density flows:

$$\overline{uv} = \bar{u}\bar{v} + \overline{u'v'}. \tag{1.26}$$

Difficulties arising with Favre averaging in the viscous and diffusive transport terms are of less importance since these terms are usually neglected in high Reynolds number turbulence.

The introduction of density-weighted averages requires the knowledge of the correlation between the density and the other variable of interest. A Favre pdf of u can be derived from the joint pdf $P(\rho, u)$ as

$$\bar{\rho}\tilde{P}(u) = \int_{\rho_{\min}}^{\rho_{\max}} \rho P(\rho, u)\, d\rho = \int_{\rho_{\min}}^{\rho_{\max}} \rho P(\rho \mid u) P(u)\, d\rho = \langle \rho \mid u \rangle P(u). \tag{1.27}$$

Multiplying both sides with u and integrating yields

$$\bar{\rho}\int_{-\infty}^{+\infty} u\tilde{P}(u)\,du = \int_{-\infty}^{+\infty} \langle\rho\,|\,u\rangle u P(u)\,du, \tag{1.28}$$

which is equivalent to $\bar{\rho}\tilde{u} = \overline{\rho u}$. The Favre mean value of u therefore is defined as

$$\tilde{u} = \int_{-\infty}^{+\infty} u\tilde{P}(u)\,du. \tag{1.29}$$

1.3 Navier–Stokes Equations and Turbulence Models

In the following we will first describe the classical approach to model turbulent flows. It is based on single point averages of the Navier–Stokes equations. These are commonly called Reynolds averaged Navier–Stokes equations (RANS). We will formally extend this formulation to nonconstant density by introducing Favre averages. In addition we will present the most simple model for turbulent flows, the k–ε model. Even though it certainly is the best compromise for engineering design using RANS, the predictive power of the k–ε model is, except for simple shear flows, often found to be disappointing. We will present it here, mainly to help us define turbulent length and time scales.

For nonconstant density flows the Navier–Stokes equations are written in conservative form:

Continuity

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}) = 0, \tag{1.30}$$

Momentum

$$\frac{\partial\rho\boldsymbol{v}}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla\cdot\boldsymbol{\tau} + \rho\boldsymbol{g}. \tag{1.31}$$

In (1.31) the two terms on the left-hand side (l.h.s.) represent the local rate of change and convection of momentum, respectively, while the first term on the right-hand side (r.h.s.) is the pressure gradient and the second term on the r.h.s. represents molecular transport due to viscosity. Here $\boldsymbol{\tau}$ is the viscous stress tensor

$$\boldsymbol{\tau} = \mu\left[2\,\boldsymbol{S} - \frac{2}{3}\boldsymbol{\delta}\nabla\cdot\boldsymbol{v}\right] \tag{1.32}$$

and

$$\boldsymbol{S} = \frac{1}{2}(\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^T) \tag{1.33}$$

is the rate of strain tensor, where $\nabla\boldsymbol{v}^T$ is the transpose of the velocity gradient and μ is the dynamic viscosity. It is related to the kinematic viscosity ν as $\mu = \rho\nu$. The last term in (1.31) represents forces due to buoyancy.

Using Favre averaging on (1.30) and (1.31) one obtains

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{v}}) = 0, \tag{1.34}$$

$$\frac{\partial \bar{\rho}\tilde{\boldsymbol{v}}}{\partial t} + \nabla\cdot(\bar{\rho}\tilde{\boldsymbol{v}}\tilde{\boldsymbol{v}}) = -\nabla\bar{p} + \nabla\cdot\bar{\boldsymbol{\tau}} - \nabla\cdot(\bar{\rho}\widetilde{\boldsymbol{v}''\boldsymbol{v}''}) + \bar{\rho}\boldsymbol{g}. \tag{1.35}$$

This equation is similar to (1.31) except for the third term on the l.h.s. containing the correlation $-\bar{\rho}\widetilde{\boldsymbol{v}''\boldsymbol{v}''}$, which is called the Reynolds stress tensor.

The Reynolds stress tensor is unknown and represents the first closure problem for turbulence modeling. It is possible to derive equations for the six components of the Reynolds stress tensor. In these equations several terms appear that again are unclosed. Those so-called Reynolds stress models have been presented for nonconstant density flows, for example, by Jones (1994) and Jones and Kakhi (1996).

Although Reynolds stress models contain a more complete description of the physics, they are not yet widely used in turbulent combustion. Many industrial codes still rely on the k–ε model, which, by using an eddy viscosity, introduces the assumption of isotropy. It is known that turbulence becomes isotropic at the small scales, but this does not necessarily apply to the large scales at which the averaged quantities are defined. The k–ε model is based on equations where the turbulent transport is diffusive and therefore is more easily handled by numerical methods than the Reynolds stress equations. This is probably the most important reason for its wide use in many industrial codes.

An important simplification is obtained by introducing the eddy viscosity ν_t, which leads to the following expression for the Reynolds stress tensor:

$$-\bar{\rho}\widetilde{\boldsymbol{v}''\boldsymbol{v}''} = \bar{\rho}\nu_t\left[2\tilde{S} - \frac{2}{3}\boldsymbol{\delta}\nabla\cdot\tilde{\boldsymbol{v}}\right] - \frac{2}{3}\boldsymbol{\delta}\bar{\rho}\tilde{k}. \tag{1.36}$$

Here $\boldsymbol{\delta}$ is the tensorial Kronecker symbol δ_{ij} ($\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq j$) and ν_t is the kinematic eddy viscosity, which is related to the Favre average turbulent kinetic energy

$$\tilde{k} = \frac{1}{2}\widetilde{\boldsymbol{v}''\cdot\boldsymbol{v}''} \tag{1.37}$$

and its dissipation $\tilde{\varepsilon}$ by

$$\nu_t = c_\mu\frac{\tilde{k}^2}{\tilde{\varepsilon}}, \qquad c_\mu = 0.09. \tag{1.38}$$

The introduction of the Favre averaged variables $\tilde{k}$ and $\tilde{\varepsilon}$ requires that modeled equations are available for these quantities. These equations are given here in their most simple form:

Turbulent kinetic energy

$$\bar{\rho}\frac{\partial \tilde{k}}{\partial t} + \bar{\rho}\tilde{\boldsymbol{v}} \cdot \nabla \tilde{k} = \nabla \cdot \left(\frac{\bar{\rho}\nu_t}{\sigma_k} \nabla \tilde{k} \right) - \bar{\rho}\widetilde{\boldsymbol{v}''\boldsymbol{v}''} : \nabla \tilde{\boldsymbol{v}} - \bar{\rho}\tilde{\varepsilon}, \qquad (1.39)$$

Turbulent dissipation

$$\bar{\rho}\frac{\partial \tilde{\varepsilon}}{\partial t} + \bar{\rho}\tilde{\boldsymbol{v}} \cdot \nabla \tilde{\varepsilon} = \nabla \cdot \left(\bar{\rho}\frac{\nu_t}{\sigma_\varepsilon} \nabla \tilde{\varepsilon} \right) - c_{\varepsilon 1}\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{\boldsymbol{v}''\boldsymbol{v}''} : \nabla \tilde{\boldsymbol{v}} - c_{\varepsilon 2}\bar{\rho}\frac{\tilde{\varepsilon}^2}{\tilde{k}}. \qquad (1.40)$$

In these equations the two terms on the l.h.s. represent the local rate of change and convection, respectively. The first term on the r.h.s. represents the turbulent transport, the second one turbulent production, and the third one turbulent dissipation. As in the standard k–ε model, the constants $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$, $c_{\varepsilon 1} = 1.44$, and $c_{\varepsilon 2} = 1.92$ are generally used. A more detailed discussion concerning additional terms in the Favre averaged turbulent kinetic energy equation may be found in Libby and Williams (1994).

It should be noted that for constant density flows the k-equation can be derived with few modeling assumptions quite systematically from the Navier–Stokes equations. From this derivation follows the definition of the viscous dissipation as

$$\varepsilon = \nu\overline{[\nabla\boldsymbol{v}' + \nabla\boldsymbol{v}'^T] : \nabla\boldsymbol{v}'}. \qquad (1.41)$$

The ε-equation, however, cannot be derived in a systematic manner. The basis for the modeling of that equation are the equations for two-point correlations. Rotta (1972) has shown that by integrating the two-point correlation equations over the correlation coordinate r one can derive an equation for the integral length scale ℓ, which will be defined below. This leads to a k–ℓ-model. The ℓ-equation has been applied, for example, by Rodi and Spalding (1970) to turbulent jet flows. It is easily shown that from this model and from the algebraic relation between ℓ, k, and ε a balance equation for ε can be derived. A similar approach has recently been used by Oberlack (1997) to derive an equation for the dissipation tensor that is needed in Reynolds stress models.

The dissipation ε plays a fundamental role in turbulence theory, as will be shown in the next section. The eddy cascade hypothesis states that it is equal to the energy transfer rate from the large eddies to the smaller eddies and therefore is invariant within the inertial subrange of turbulence. By using this property for ε in the k-equation and by determining ε from an equation like (1.40) rather than from its definition (1.41) one obtains Reynolds number independent solutions for free shear flows where, owing to the absence of walls, the viscous stress tensor can be neglected compared to the Reynolds stress tensor. This is how inertial range invariance is built into turbulence models.

It may be counterintuitive to model dissipation, which is active at the small scales, by an equation that contains only quantities that are defined at the large integral scales (cf. Figure 1.5 below). However, it is only because inertial range invariance has been built into turbulence models that they reproduce the scaling laws that are experimentally observed. Based on the postulate formulated at the end of Section 1.1 the same must be claimed for turbulent combustion models in the large Reynolds number limit. Since combustion takes place at the small scales, inertial range invariant quantities must relate properties defined at the small scales to those defined at the large scales, at which the models are formulated.

1.4 Two-Point Velocity Correlations and Turbulent Scales

A characteristic feature of turbulent flows is the occurrence of eddies of different length scales. If a turbulent jet shown in Figure 1.3 enters with a high velocity into initially quiescent surroundings, the large velocity difference between the jet and the surroundings generates a shear layer instability, which, after a transition, becomes turbulent further downstream from the nozzle exit. The two shear layers merge into a fully developed turbulent jet. In order to characterize the distribution of eddy length scales at any position within the jet, one measures at point $\boldsymbol{x}$ and time t the axial velocity $u(\boldsymbol{x}, t)$, and simultaneously at a second point $(\boldsymbol{x}+\boldsymbol{r}, t)$ with distance $\boldsymbol{r}$ apart from the first one, the velocity $u(\boldsymbol{x}+\boldsymbol{r}, t)$. Then the correlation between these two velocities is defined by the

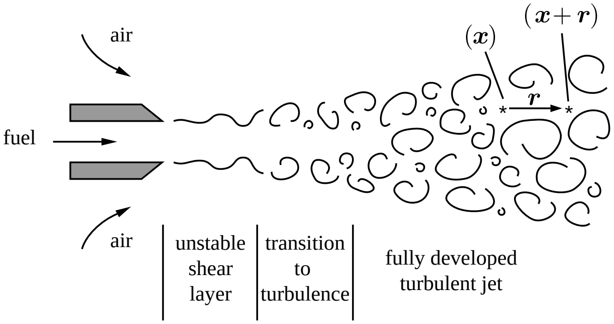

Figure 1.3. Schematic presentation of two-point correlation measurements in a turbulent jet.

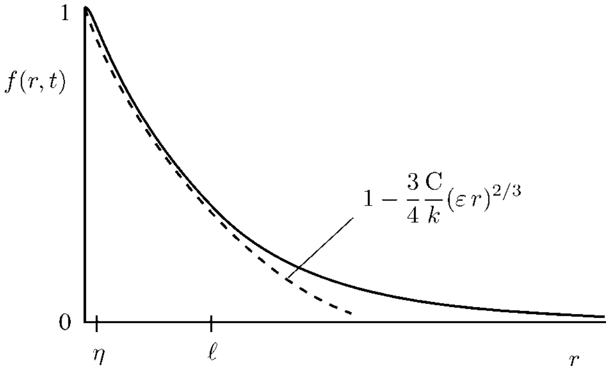

Figure 1.4. The normalized two-point velocity correlation for homogeneous isotropic turbulence as a function of the distance r between the two points.

average

$$R(\boldsymbol{x}, \boldsymbol{r}, t) = \overline{u'(\boldsymbol{x}, t)u'(\boldsymbol{x} + \boldsymbol{r}, t)}. \tag{1.42}$$

For homogeneous isotropic turbulence the location $\boldsymbol{x}$ is arbitrary and $\boldsymbol{r}$ may be replaced by its absolute value $r = |\boldsymbol{r}|$. For this case the normalized correlation

$$f(r, t) = R(r, t)/\overline{u'^2(t)} \tag{1.43}$$

is plotted schematically in Figure 1.4. It approaches unity for $r \to 0$ and decays slowly when the two points are only a very small distance r apart. With increasing distance it decreases continuously and may even take negative values. Very large eddies corresponding to large distances between the two points are rather seldom and therefore do not contribute much to the correlation.

Kolmogorov's 1941 theory for homogeneous isotropic turbulence assumes that there is a steady transfer of kinetic energy from the large scales to the small scales and that this energy is being consumed at the small scales by viscous dissipation. This is the eddy cascade hypothesis. By equating the energy transfer rate (kinetic energy per eddy turnover time) with the dissipation ε it follows that this quantity is independent of the size of the eddies within the inertial range. For the inertial subrange, extending from the integral scale ℓ to the Kolmogorov scale η, ε is the only dimensional quantity apart from the correlation coordinate r that is available for the scaling of $f(r, t)$. Since ε has the dimension [$\mathrm{m}^2/\mathrm{s}^3$], the second-order structure function defined by

$$F_2(r, t) = \overline{(u'(\mathbf{x}, t) - u'(\mathbf{x} + \mathbf{r}, t))^2} = 2\,\overline{u'^2(t)}(1 - f(r, t)) \tag{1.44}$$

with the dimension [$\mathrm{m}^2/\mathrm{s}^2$] must therefore scale as

$$F_2(r, t) = \mathrm{C}(\varepsilon\, r)^{2/3}, \tag{1.45}$$

where C is a universal constant called the Kolmogorov constant. In the case of homogeneous isotropic turbulence the velocity fluctuations in the three coordinate directions are equal to each other. The turbulent kinetic energy

$$k = \frac{1}{2}\overline{\boldsymbol{v}' \cdot \boldsymbol{v}'} \tag{1.46}$$

is then equal to $k = 3\overline{u'^2}/2$. Using this one obtains from (1.44) and (1.45)

$$f(r,t) = 1 - \frac{3}{4}\frac{\mathrm{C}}{k}(\varepsilon\, r)^{2/3}, \tag{1.47}$$

which is also plotted in Figure 1.4.

There are eddies of a characteristic size containing most of the kinetic energy. At these eddies there remains a relatively large correlation $f(r,t)$ before it decays to zero. The length scale of these eddies is called the integral length scale ℓ and is defined by

$$\ell(t) = \int_0^\infty f(r,t)\, dr. \tag{1.48}$$

The integral length scale is also shown in Figure 1.4.

We denote the root-mean-square (r.m.s.) velocity fluctuation by

$$v' = \sqrt{2\,k/3}, \tag{1.49}$$

which represents the turnover velocity of integral scale eddies. The turnover time ℓ/v' of these eddies is then proportional to the integral time scale

$$\tau = \frac{k}{\varepsilon}. \tag{1.50}$$

For very small values of r only very small eddies fit into the distance between $\boldsymbol{x}$ and $\boldsymbol{x}+\boldsymbol{r}$. The motion of these small eddies is influenced by viscosity, which provides an additional dimensional quantity for scaling. Dimensional analysis then yields the Kolmogorov length scale

$$\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}, \tag{1.51}$$

which is also shown in Figure 1.4.

The range of length scales between the integral scale and the Kolmogorov scale is called the inertial range. In addition to η a Kolmogorov time and a velocity scale may be defined as

$$t_\eta = \left(\frac{\nu}{\varepsilon}\right)^{1/2}, \qquad v_\eta = (\nu\varepsilon)^{1/4}. \tag{1.52}$$

The Taylor length scale λ is an intermediate scale between the integral and the Kolmogorov scale. It is defined by replacing the average gradient in the definition of the dissipation (1.41) by v'/λ. This leads to the definition

$$\varepsilon = 15\nu \frac{v'^2}{\lambda^2}. \tag{1.53}$$

Here the factor 15 originates from considerations for isotropic homogeneous turbulence. Using (1.52) we see that λ is proportional to the product of the turnover velocity of the integral scale eddies and the Kolmogorov time:

$$\lambda = (15\nu\, v'^2/\varepsilon)^{1/2} \sim v' t_\eta. \tag{1.54}$$

Therefore λ may be interpreted as the distance that a large eddy convects a Kolmogorov eddy during its turnover time t_η. As a somewhat artificially defined intermediate scale it has no direct physical significance in turbulence or in turbulent combustion. We will see, however, that similar Taylor scales may be defined for nonreactive scalar fields, which are useful for the interpretation of mixing processes.

According to Kolmogorov's 1941 theory the energy transfer from the large eddies of size ℓ is equal to the dissipation of energy at the Kolmogorov scale η. Therefore we will relate ε directly to the turnover velocity and the length scale of the integral scale eddies,

$$\varepsilon \sim \frac{v'^3}{\ell}. \tag{1.55}$$

We now define a discrete sequence of eddies within the inertial subrange by

$$\ell_n = \frac{\ell}{2^n} \geq \eta, \qquad n = 1, 2, \ldots. \tag{1.56}$$

Since ε is constant within the inertial subrange, dimensional analysis relates the turnover time t_n and the velocity difference v_n across the eddy ℓ_n to ε in that range as

$$\varepsilon \sim \frac{v_n^2}{t_n} \sim \frac{v_n^3}{\ell_n} \sim \frac{\ell_n^2}{t_n^3}. \tag{1.57}$$

This relation includes the integral scales and also holds for the Kolmogorov scales as

$$\varepsilon = \frac{v_\eta^2}{t_\eta} = \frac{v_\eta^3}{\eta}. \tag{1.58}$$

A Fourier transform of the isotropic two-point correlation function leads to a definition of the kinetic energy spectrum $E(k)$, which is the density of kinetic energy per unit wavenumber k. Here, rather than presenting a formal derivation, we relate the wavenumber k to the inverse of the eddy size ℓ_n as

$$k = \ell_n^{-1}. \tag{1.59}$$

The kinetic energy v_n^2 at scale ℓ_n is then

$$v_n^2 \sim (\varepsilon\, \ell_n)^{2/3} = \varepsilon^{2/3} k^{-2/3} \tag{1.60}$$

and its density in wavenumber space is proportional to

$$E(k) = \frac{dv_n^2}{dk} \sim \varepsilon^{2/3} k^{-5/3}. \tag{1.61}$$

This is the well-known $k^{-5/3}$ law for the kinetic energy spectrum in the inertial subrange.

If the energy spectrum is measured in the entire wavenumber range one obtains the behavior shown schematically in a log–log plot in Figure 1.5. For small wavenumbers corresponding to large scale eddies the energy per unit wavenumber increases with a power law between k^2 and k^4. This range is not universal and is determined by large scale instabilities, which depend on the boundary conditions of the flow. The spectrum attains a maximum at a wavenumber that corresponds to the integral scale, since eddies of that scale contain most of the kinetic energy. For larger wavenumbers corresponding to the inertial subrange the energy spectrum decreases following the $k^{-5/3}$ law. There is a cutoff at the Kolmogorov scale η. Beyond this cutoff, in the range called

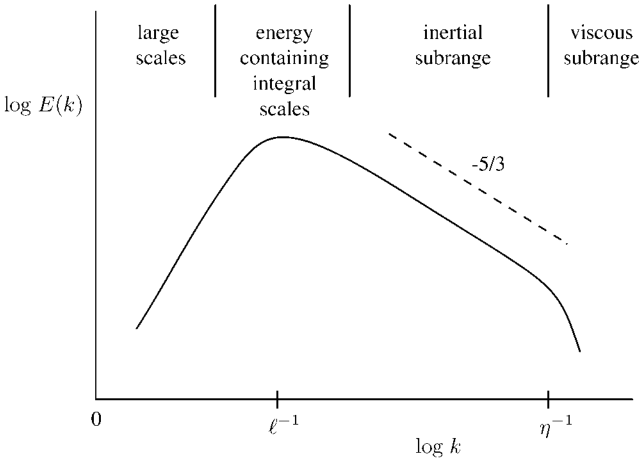

Figure 1.5. Schematic representation of the turbulent kinetic energy spectrum as a function of the wavenumber k.

the viscous subrange, the energy per unit wavenumber decreases exponentially owing to viscous effects.

In one-point averages the energy containing eddies at the integral length scale contribute the most to the kinetic energy. Therefore RANS averaged mean quantities essentially represent averages over regions in physical space that are of the order of the integral scale. This was meant by the statement at the end of Section 1.3 that RANS averages are defined at the large scales. In Large Eddy Simulations (LES), to be discussed in Section 1.14, filtering over smaller regions than the integral length scale leads to different mean values and, in particular, to smaller variances.

1.5 Balance Equations for Reactive Scalars

Combustion is the conversion of chemical bond energy contained in fossil fuels into heat by chemical reactions. The basis for any combustion model is the continuum formulation of the balance equations for energy and the chemical species. We will not derive these equations here but refer to Williams (1985a) for more details. We consider a mixture of n chemically reacting species and start with the balance equations for the mass fraction of species i,

$$\rho \frac{\partial Y_i}{\partial t} + \rho \boldsymbol{v} \cdot \nabla Y_i = -\nabla \cdot \boldsymbol{j}_i + \omega_i, \tag{1.62}$$

where $i = 1, 2, \ldots, n$. In these equations the terms on the l.h.s. represent the local rate of change and convection. The diffusive flux in the first term on the r.h.s. is denoted by $\boldsymbol{j}_i$ and the last term ω_i is the chemical source term.

The molecular transport processes that cause the diffusive fluxes are quite complicated. A full description may be found in Williams (1985a). Since in models of turbulent combustion molecular transport is less important than turbulent transport, it is useful to consider simplified versions of the diffusive fluxes; the most elementary is the binary flux approximation

$$\boldsymbol{j}_i = -\rho D_i \nabla Y_i, \tag{1.63}$$

where D_i is the binary diffusion coefficient, or mass diffusivity, of species i with respect to an abundant species, for instance N_2. It should be noted, however, that in a multicomponent system this approximation violates mass conservation, if nonequal diffusivities D_i are used, since the sum of all n fluxes has to vanish and the sum of all mass fractions is unity. Equation (1.63) is introduced here mainly for the ease of notation, but it must not be used in laminar flame calculations.

For simplicity it will also be assumed that all mass diffusivities D_i are proportional to the thermal diffusivity denoted by

$$D = \lambda/\rho\, c_p \tag{1.64}$$

such that the Lewis numbers

$$Le_i = \lambda/(\rho\, c_p D_i) = D/D_i \tag{1.65}$$

are constant. In these equations λ is the thermal conductivity and c_p is the heat capacity at constant pressure of the mixture.

Before going into the definition of the chemical source term ω_i to be presented in the next section, we want to consider the energy balance in a chemically reacting system. The enthalpy h is the mass-weighted sum of the specific enthalpies h_i of species i:

$$h = \sum_{i=1}^{n} Y_i h_i . \tag{1.66}$$

For an ideal gas h_i depends only on the temperature T:

$$h_i = h_{i,\mathrm{ref}} + \int_{T_{\mathrm{ref}}}^{T} c_{p_i}(T)\, dT . \tag{1.67}$$

Here c_{pi} is the specific heat capacity of species i at constant pressure and T is the temperature in Kelvins. The chemical bond energy is essentially contained in the reference enthalpies $h_{i,\mathrm{ref}}$. Reference enthalpies of H_2, O_2, N_2, and solid carbon are in general chosen as zero, while those of combustion products such as CO_2 and H_2O are negative. These values as well as polynomial fits for the temperature dependence of c_{p_i} are documented, for instance, for many species used in combustion calculations in Burcat (1984). Finally the specific heat capacity at constant pressure of the mixture is

$$c_p = \sum_{i=1}^{n} Y_i c_{p_i} . \tag{1.68}$$

A balance equation for the enthalpy can be derived from the first law of thermodynamics as (cf. Williams, 1985a)

$$\rho \frac{\partial h}{\partial t} + \rho \boldsymbol{v} \cdot \nabla h = \frac{\partial p}{\partial t} + \boldsymbol{v} \cdot \nabla p - \nabla \cdot \boldsymbol{j}_q + q_R . \tag{1.69}$$

Here the terms on the l.h.s. represent the local rate of change and convection of enthalpy. We have neglected the term that describes frictional heating because it is small for low speed flows. The local and convective change of pressure is important for acoustic interactions and pressure waves. We will not consider the term $\boldsymbol{v} \cdot \nabla p$ any further since we are interested in the small Mach number limit only. The transient pressure term $\partial p/\partial t$ must be retained in applications for reciprocating engines but can be neglected in open flames where the pressure is approximately constant and equal to the static pressure. The heat flux $\boldsymbol{j}_q$ includes the effect of enthalpy transport by the diffusive fluxes $\boldsymbol{j}_i$:

$$\boldsymbol{j}_q = -\lambda \nabla T + \sum_{i=1}^{n} h_i \boldsymbol{j}_i. \tag{1.70}$$

Finally, the last term in (1.69) represents heat transfer due to radiation and must be retained in furnace combustion and whenever strongly temperature dependent processes, such as NO_x formation, are to be considered.

The static pressure is obtained from the thermal equation of state for a mixture of ideal gases

$$p = \rho \frac{RT}{W}. \tag{1.71}$$

Here R is the universal gas constant and W is the mean molecular weight given by

$$W = \left(\sum_{i=1}^{n} \frac{Y_i}{W_i} \right)^{-1}. \tag{1.72}$$

The molecular weight of species i is denoted by W_i. For completeness we note that mole fractions X_i can be converted into mass fractions Y_i via

$$Y_i = \frac{W_i}{W} X_i. \tag{1.73}$$

We now want to simplify the enthalpy equation. Differentiating (1.66) one obtains

$$dh = c_p dT + \sum_{i=1}^{n} h_i dY_i, \tag{1.74}$$

where (1.67) and (1.68) have been used. If (1.70), (1.74), and (1.63) are inserted into the enthalpy equation (1.69) with the term $\boldsymbol{v} \cdot \nabla p$ removed, it takes the form

$$\begin{aligned} \rho \frac{\partial h}{\partial t} + \rho \boldsymbol{v} \cdot \nabla h = {} & \frac{\partial p}{\partial t} + \nabla \cdot \left(\frac{\lambda}{c_p} \nabla h \right) + q_R \\ & - \sum_{i=1}^{n} h_i \nabla \cdot \left[\left(\frac{\lambda}{c_p} - \rho D_i \right) \nabla Y_i \right]. \end{aligned} \tag{1.75}$$

It is immediately seen that the last term disappears, if all Lewis numbers are assumed equal to unity. If, in addition, unsteady pressure changes and radiation heat transfer can be neglected, the enthalpy equation contains no source terms.