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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).

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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

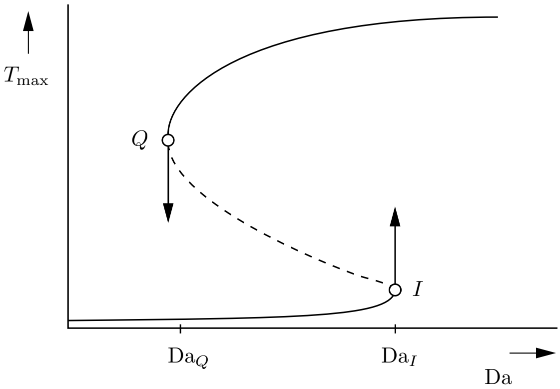

Figure 1.1. The S-shaped curve showing the maximum temperature in a well-stirred reactor as a function of the Damköhler number.

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

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

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 $\bar{u}$ and $\bar{v}$ 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

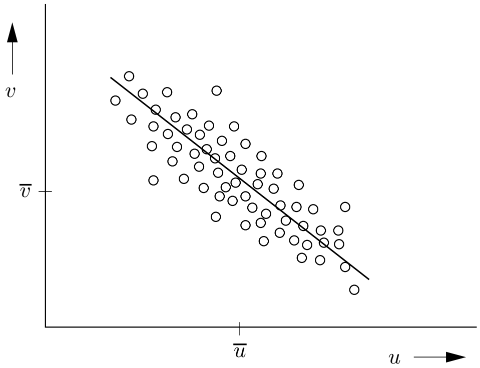

Figure 1.2. A scatter plot of two velocity components u and v illustrating the correlation coefficient.

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

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

Multiplying both sides with u and integrating yields

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

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

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