

Lecture 10

Turbulent Combustion: The State of the Art

Engineering applications are typically turbulent

→ turbulence models

These models use systematic mathematical derivations based on the Navier-Stokes equations

They introduce **closure hypotheses** that rely on dimensional arguments and require empirical input.

→ **semi-empirical nature** of turbulence models

The apparent success of turbulence models in solving engineering problems for non-reactive flows has encouraged similar approaches for turbulent combustion

→ turbulent combustion models

Problems:

Combustion requires that fuel and oxidizer are **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.

There remains, however, the question to what extent we can expect an [interaction between chemical and turbulent scales](#).

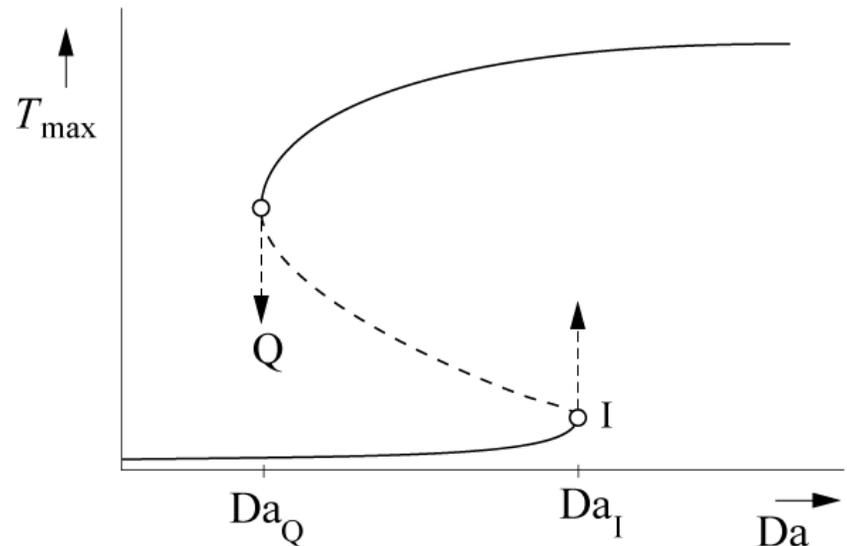
Combustion differs from isothermal mixing in chemically reacting flows by two specific features:

- heat release by combustion induces an increase of temperature
- increase of temperature accelerates combustion chemistry. Due to 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 like **ignition and extinction**.

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**.

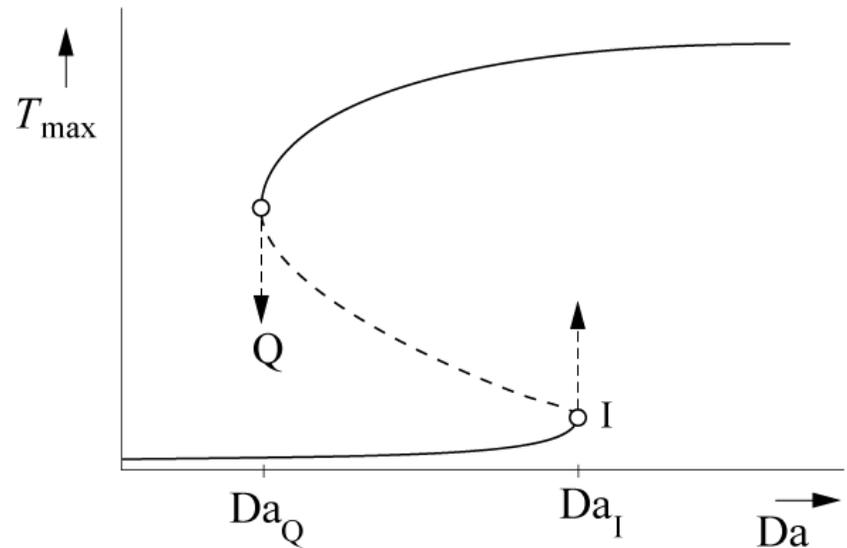
This is called the **S-shaped curve**.



The lower branch corresponds to a **slowly reacting** state of the combustor **prior to ignition**.

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 **ignition point I** is reached.

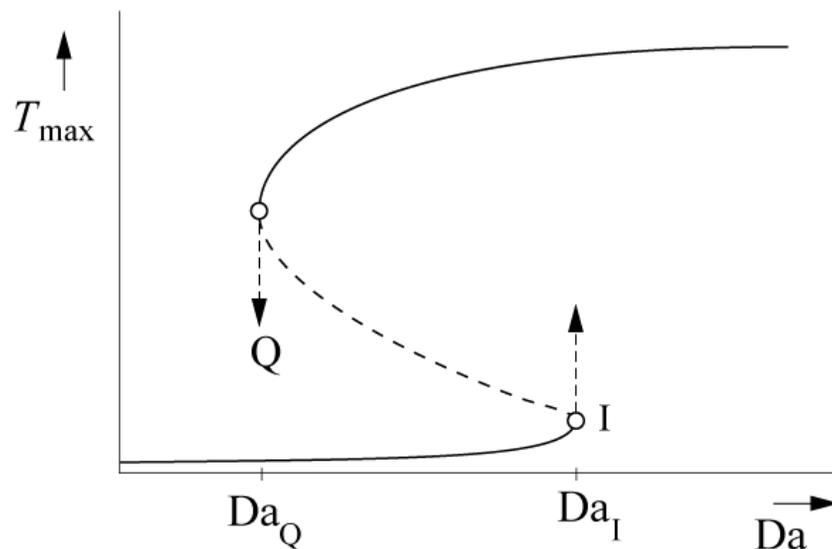


For values larger than Da_I thermal runaway leads to a rapid unsteady transition to the upper **close-to-equilibrium** branch.

If one starts on the upper branch and decreases the Damköhler number one reaches the point Q where **extinction** occurs.

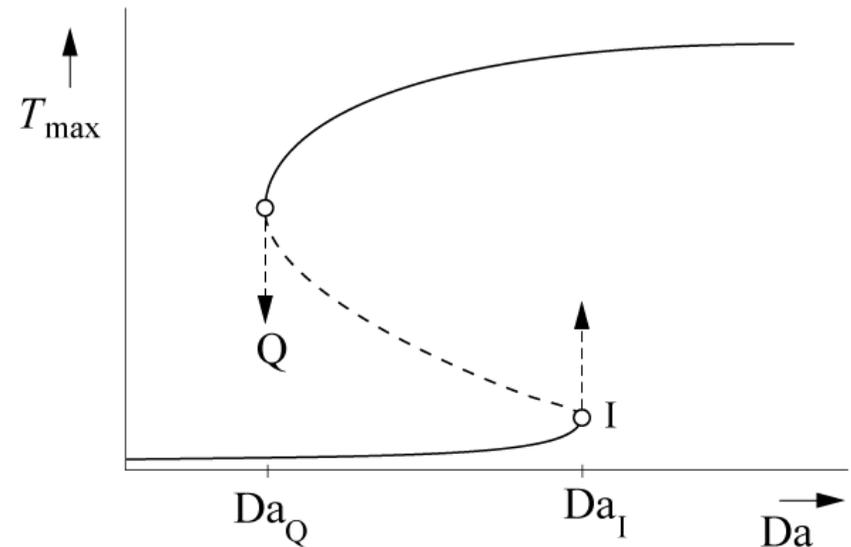
This is equivalent to a rapid transition to the lower branch. The middle branch between the point I and Q is unstable.

In the range of Damköhler numbers $Da_Q < Da < Da_I$, 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.



Due 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 non-reacting state are frequently accessed.



Statistical Description of Turbulent Flows

The aim of **stochastic methods** in turbulence is the description of the fluctuating velocity and scalar fields in terms of their **statistical distributions**.

Distribution function of a single variable of 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 $u < U$:

$$F_u(U) = p(u < U)$$

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 $U_- < u < U_+$ is given by

$$p(U_- < u < U_+) = F_u(U_+) - F_u(U_-)$$

The probability density function *pdf* of u is now defined as

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

It follows that $P_u(U)dU$ is the probability of finding u in the range $U \leq u \leq U+dU$.

If the possible realizations of u range from $-\infty \leq u \leq +\infty$, it follows that

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

which states that the probability of finding the value u in the range $-\infty \leq u \leq +\infty$ is certain, i.e. it has the probability unity.

It also serves as a normalizing condition for P_u .

In turbulent flows the *pdf* of any stochastic variable depends, in principle, on the position \mathbf{x} and on time t .

These functional dependencies are expressed by the following notation

$$P_u(U; \mathbf{x}, t)$$

The semicolon used in

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

indicates that P_u is a probability density in U -space and a function of \boldsymbol{x} and t .

In stationary turbulent flows it does not depend on t and in homogeneous turbulent fields not on \boldsymbol{x} .

In the following we will, for simplicity of notation, not distinguish between the random stochastic variable u and the sample space variable U , drop the index and write the *pdf* as

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

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

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

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

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

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

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

For flows with large density changes as they occur in combustion, it is often convenient to introduce a **density-weighted average** \tilde{u} , called the Favre average, by splitting $u(\mathbf{x}, t)$

$$u(\mathbf{x}, t) = \tilde{u}(\mathbf{x}, t) + u''(\mathbf{x}, t)$$

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

$$\overline{\rho u''} = 0$$

The definition for \tilde{u} may then be derived by multiplying $u(\mathbf{x}, t) = \tilde{u}(\mathbf{x}, t) + u''(\mathbf{x}, t)$ by the density ρ and averaging

$$\overline{\rho u} = \overline{\rho \tilde{u}} + \overline{\rho u''} = \overline{\rho \tilde{u}}$$

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

$$\tilde{u} = \overline{\rho u} / \bar{\rho}$$

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} .

$$\overline{\rho u''} = 0$$

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.

$$\tilde{u} = \overline{\rho u} / \bar{\rho}$$

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

$$\overline{\rho uv} = \bar{\rho} \bar{u} \bar{v} + \overline{\bar{\rho} u' v'} + \overline{\rho' u' \bar{v}} + \overline{\rho' v' \bar{u}} + \overline{\rho' u' v'}$$

Using Favre averages one writes

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

Here fluctuations of the density do not appear.

Taking the average leads to two terms only

$$\overline{\rho uv} = \bar{\rho} \tilde{u} \tilde{v} + \bar{\rho} \widetilde{u''v''}$$

This expression is much simpler than

$$\overline{\rho uv} = \bar{\rho} \bar{u} \bar{v} + \overline{\bar{\rho} u' v'} + \overline{\rho' u' \bar{v}} + \overline{\rho' v' \bar{u}} + \overline{\rho' u' v'}$$

and has formally the same structure as the conventional average of uv for constant density flows

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

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

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

Multiplying both sides with u and integrating yields

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

which is equivalent to

$$\bar{\rho}\tilde{u} = \overline{\rho u}$$

The Favre mean value of u therefore is defined as

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

Navier-Stokes Equations and Turbulence Models

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 **non-constant 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 be able to define **turbulent length and time scales**.

For non-constant density flows the Navier-Stokes equations are written in conservative form (cf. Lecture 3)

Continuity
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

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

The two terms on the left hand side (l.h.s.) of

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

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 τ is the viscous stress tensor (cf. Lecture 3)

$$\tau = -\mu \left[2S - \frac{2}{3} \nabla \cdot v \right]$$

with the rate of strain tensor

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

calculated from the velocity gradient and its transpose and the dynamic viscosity $\mu = \rho \nu$.

The last term in represents forces due to buoyancy.

Using Favre averaging and one obtains

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{\mathbf{v}}) = 0$$

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

This equation is similar to

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

except for the third term on the l.h.s. containing the correlation

$$-\bar{\rho} \widetilde{\mathbf{v}'' \mathbf{v}''}$$

which is called the **Reynolds stress tensor**.

An important simplification is obtained by introducing the

kinematic eddy viscosity ν_t

which leads to the following expression for the Reynolds stress tensor

$$-\bar{\rho} \widetilde{v''v''} = \bar{\rho} \nu_t \left[2\widetilde{S} - \frac{2}{3} \nabla \cdot \widetilde{v} \mathbf{I} \right] + \frac{2}{3} \bar{\rho} \widetilde{k} \mathbf{I}$$

Here \mathbf{I} is the unit tensor.

The kinematic eddy viscosity is related to the Favre average turbulent kinetic energy

$$\widetilde{k} = \frac{1}{2} \widetilde{v'' \cdot v''}$$

and its dissipation by

$$\nu_t = c_\mu \frac{\widetilde{k}^2}{\widetilde{\varepsilon}}, \quad c_\mu = 0.09$$

This requires that modeled equations are available for \tilde{k} , $\tilde{\varepsilon}$.

These equations are given here in their most simple form

Turbulent kinetic energy

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

Turbulent dissipation

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

In these equations the two terms on the l.h.s. represent the local rate of change and convection, respectively.

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

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

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

$$\sigma_k = 1.0, \quad \sigma_\varepsilon = 1.3, \quad c_{\varepsilon 1} = 1.44 \quad \text{and} \quad c_{\varepsilon 2} = 1.92$$

are generally used.

A more detailed discussion concerning additional terms in the Favre averaged turbulent kinetic equation may be found in Libby and Williams (1994) .

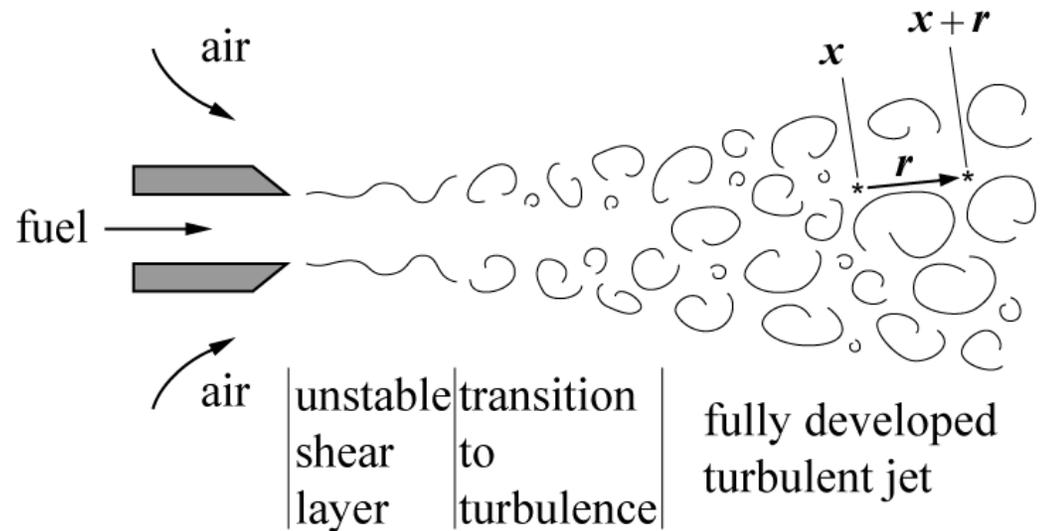
Two-Point Velocity Correlations and Turbulent Scales

A characteristic feature of turbulent flows is the occurrence of eddies of different length scales.

If a turbulent jet enters with a high velocity into initially quiescent surroundings, the large velocity difference between the jet and the surroundings generate a

shear layer instability which after

a **transition**, becomes turbulent further downstream from the nozzle exit.

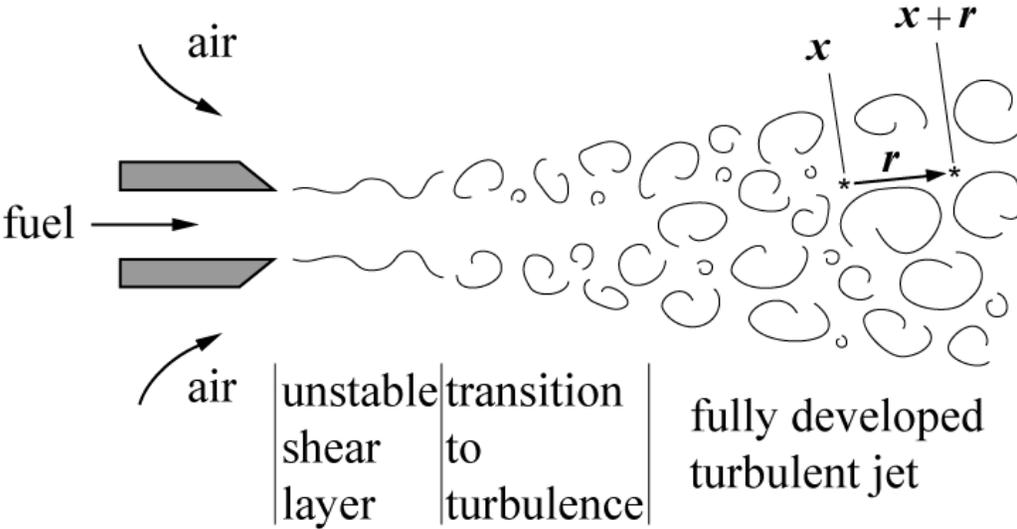


The two shear layers merge into a fully developed turbulent jet.

In order to characterize the distribution of eddy length scales at any position within the jet, one measures at point \mathbf{x} and time t the axial velocity $u(\mathbf{x},t)$, and simultaneously at a second point $(\mathbf{x}+\mathbf{r},t)$ with distance \mathbf{r} apart from the first one, the velocity $u(\mathbf{x}+\mathbf{r},t)$.

Then the correlation between these two velocities is defined by the average

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

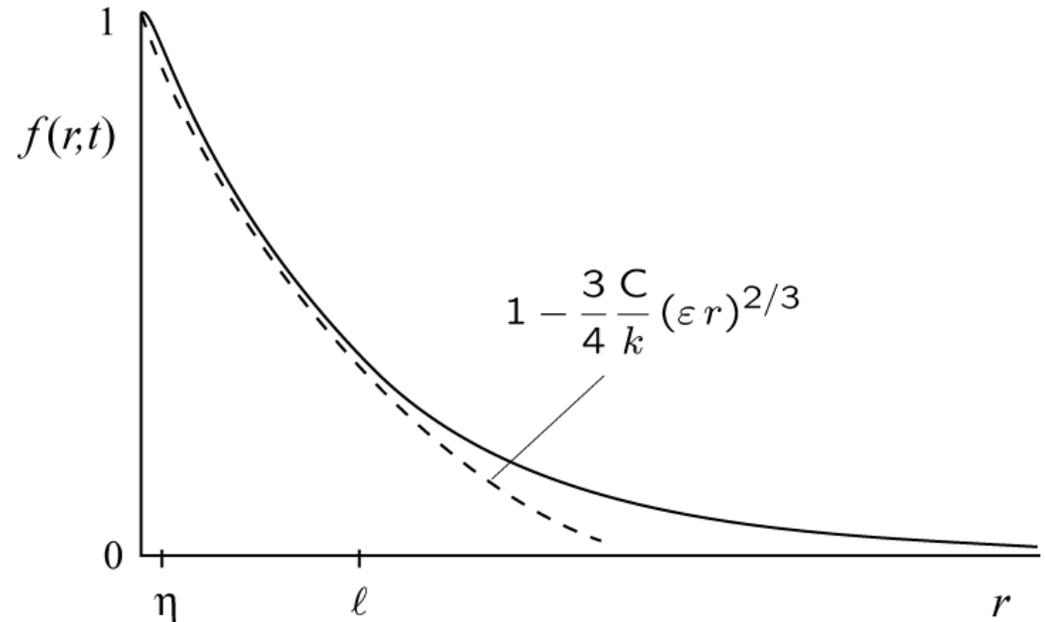


For **homogeneous isotropic turbulence** the location \mathbf{x} is arbitrary and \mathbf{r} may be replaced by its absolute value $r=|\mathbf{r}|$.

For this case the normalized correlation

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

is plotted schematically here.



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 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** to the Kolmogorov scale η , the dissipation ε is the only dimensional quantity apart from the correlation co-ordinate r that is available for the scaling of $f(r, t)$.

Since ε has the dimension m^2/s^3 , the second order structure function defined by

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

with the dimension m^2/s^2 must therefore scale as

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

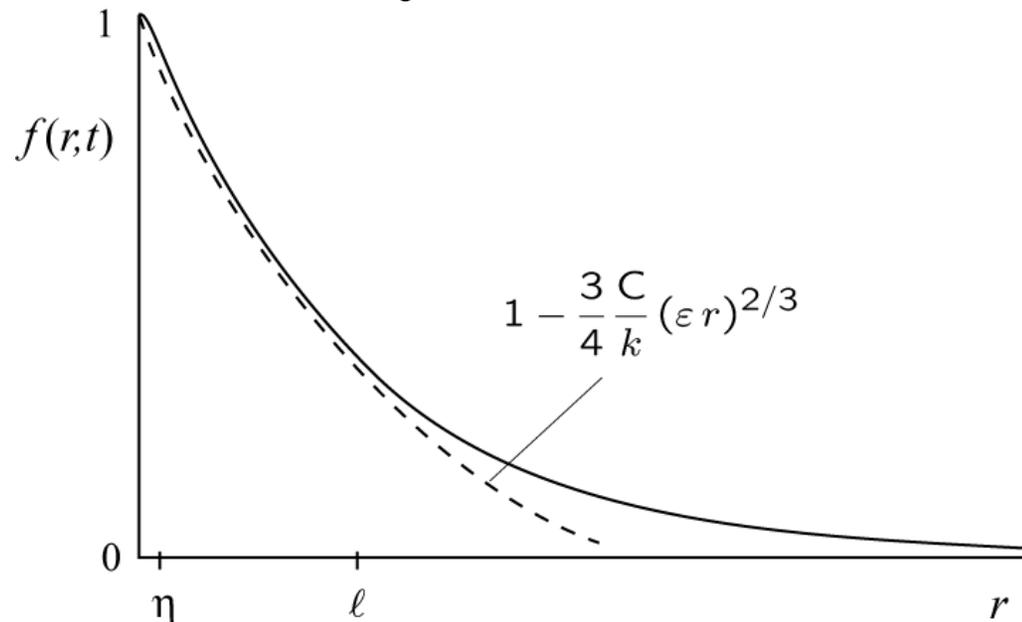
where C is a universal constant called the **Kolmogorov constant**.

There are eddies of a characteristic size which contain most of the kinetic energy.

At these eddies there still is a relatively large correlation $f(r, t)$ before it decays to zero.

The length scale of these eddies is called the **integral length scale** defined by

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



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

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

which represents the **turnover velocity** of integral scale eddies.

The turnover time

$$\ell/v'$$

of these eddies is then proportional to the **integral time scale**

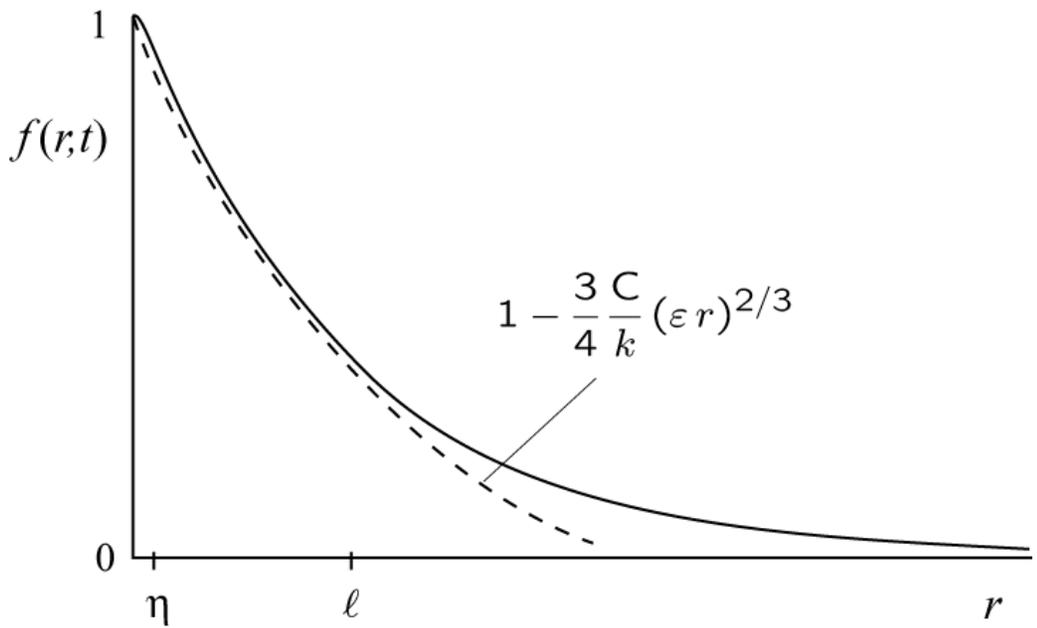
$$\tau = \frac{k}{\varepsilon}$$

For very small values of r only very small eddies fit into the distance between \mathbf{x} and $\mathbf{x}+r$.

The motion of these small eddies is influenced by viscosity which provides an additional dimensional quantity for scaling.

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

Dimensional analysis then yields the Kolmogorov length scale $\eta = \left(\frac{\nu^3}{\epsilon}\right)^{1/4}$



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

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

According to Kolmogorov's 1941 theory the energy transfer from the large eddies of the integral scale is equal to the dissipation of energy at the Kolmogorov scale.

Therefore we will relate ε directly to the turnover velocity and the length scale of the integral scale eddies

$$\varepsilon \sim \frac{v^3}{\ell}$$

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

$$l_n = \frac{\ell}{2^n} \geq \eta, \quad n = 1, 2, \dots$$

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

$$\varepsilon \sim \frac{v_n^2}{t_n} \sim \frac{v_n^3}{l_n} \sim \frac{l_n^2}{t_n^3}$$

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

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

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 wave number k .

Here, rather than to present a formal derivation, we relate the wave number k to the inverse of the eddy size as

$$k = \ell_n^{-1}$$

The kinetic energy v_n^2 is then

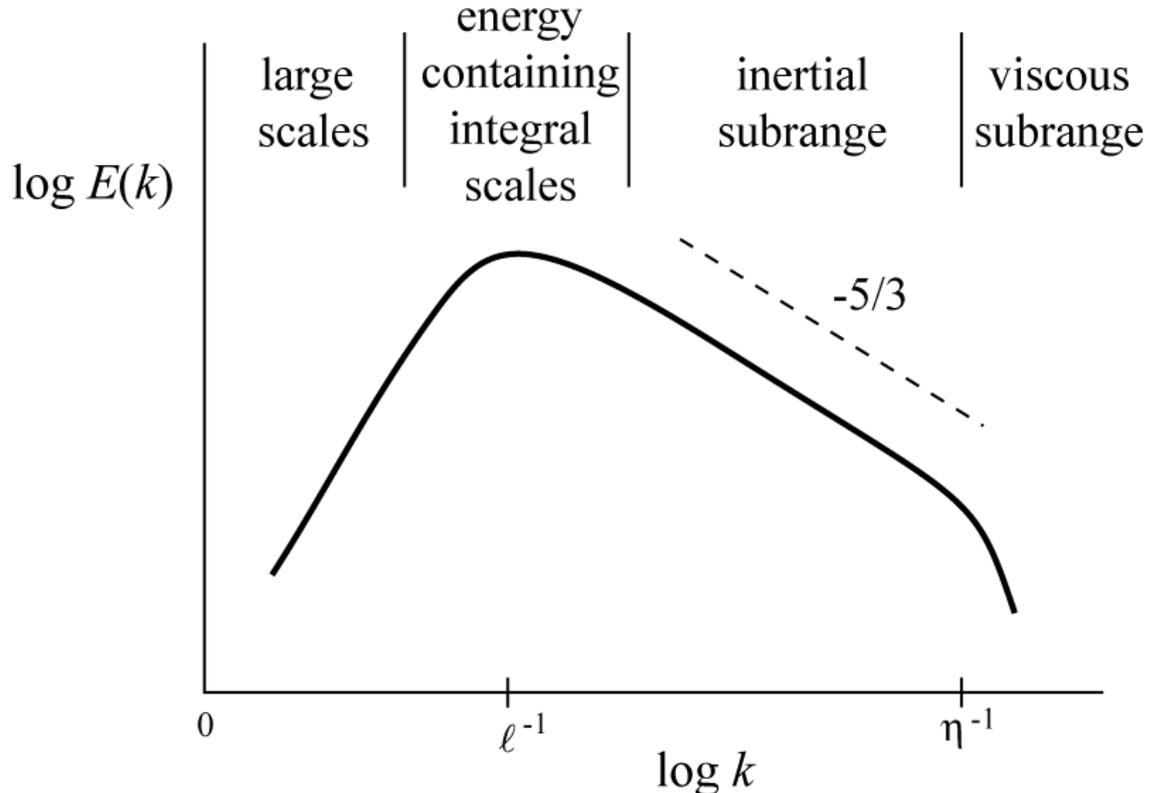
$$v_n^2 \sim (\varepsilon \ell_n)^{2/3} = \varepsilon^{2/3} k^{-2/3}$$

and its density in wave number space is proportional to $E(k) = \frac{dv_n^2}{dk} \sim \varepsilon^{2/3} k^{-5/3}$

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

If the energy spectrum is measured in the entire wave number range one obtains the behavior shown schematically in the log-log plot .

For small wave numbers
 Corresponding to large
 scale eddies the energy per
 unit wave number increases
 with a power law between
 k^2 and k^4 .



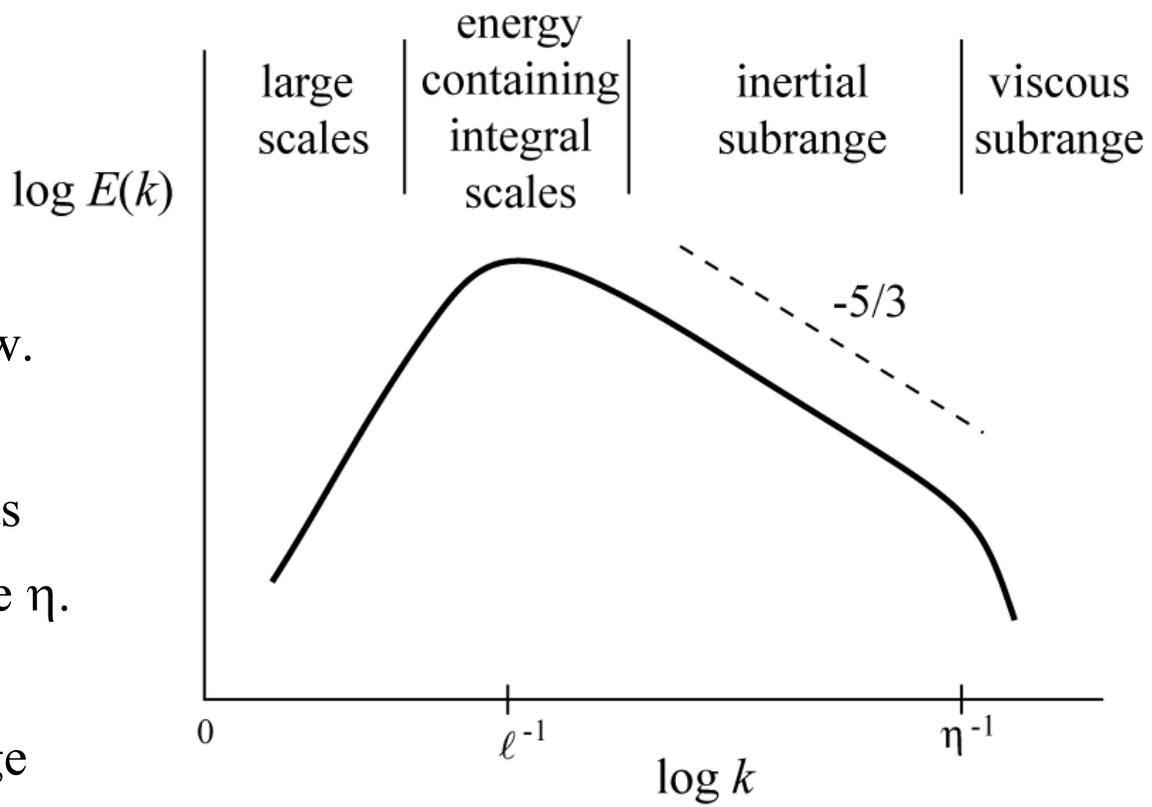
This range is not universal
 and is determined by large scale instabilities which depend on the boundary conditions
 of the flow.

The spectrum attains a maximum at a wave number that corresponds to the integral scale, since eddies of that scale contain most of the kinetic energy.

For larger wave numbers corresponding to the inertial subrange the energy spectrum decreases following the $k^{-5/3}$ law.

There is a cut-off due to viscous effects at the Kolmogorov scale η .

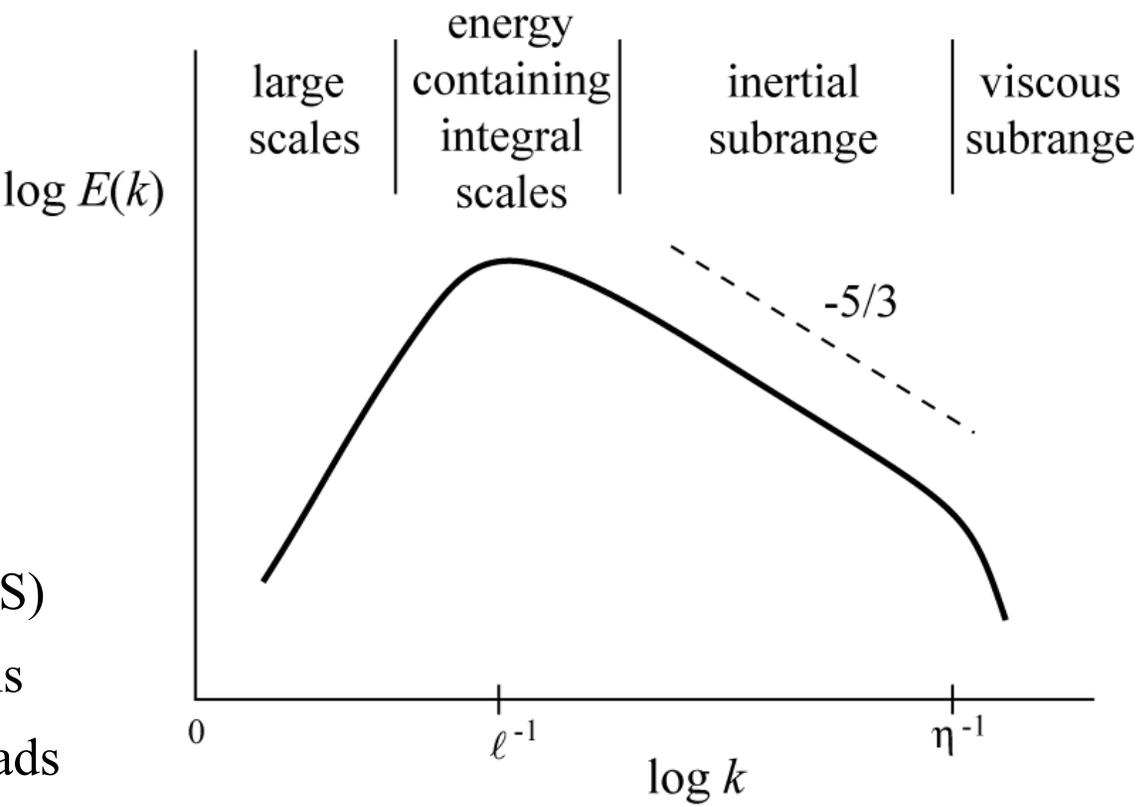
Beyond this cut-off, in the range called the **viscous subrange**, the energy per unit wave number decreases exponentially due to viscous effects.



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.

In Large Eddy Simulations (LES) the filtering over smaller regions than the integral length scale leads to different mean values and, in particular, to smaller variances.



Balance Equations for Reactive Scalars

For simplicity, we will assume that the specific heat capacities $c_{p,i}$ are all equal and constant, the pressure is constant and the heat transfer due to radiation is neglected.

Then the temperature equation for unity Lewis number becomes (cf. Lecture 3)

$$\rho \frac{\partial T}{\partial t} + \rho \mathbf{v} \cdot \nabla T = \nabla \cdot (\rho D \nabla T) + \omega_T$$

The heat release due to chemical reactions is written as

$$\omega_T = -\frac{1}{c_p} \sum_{i=1}^k h_i \dot{m}_i$$

This form of the temperature equation is similar to that for the mass fractions of species i (cf. Lecture 3), which becomes with the binary diffusion approximation

$$\rho \frac{\partial Y_i}{\partial t} + \rho \mathbf{v} \cdot \nabla Y_i = \nabla \cdot (\rho D_i \nabla Y_i) + \dot{m}_i$$

If, in addition, a one-step reaction and equal diffusivities ($D_i = D$) were assumed, coupling relations between the temperature and the species mass fractions can be derived (cf. Williams, 1985).

These assumptions are often used in mathematical analyzes of combustion problems.

In the following we will use the term "reactive scalars" for the mass fraction of all chemical species and temperature and introduce the vector

$$\psi = (Y_1, Y_2, \dots, Y_k, T)$$

Here k is the number of reactive species.

For simplicity of notation, the balance equation for the reactive scalar ψ_i will be written

$$\rho \frac{\partial \psi_i}{\partial t} + \rho \mathbf{v} \cdot \nabla \psi_i = \nabla \cdot (\rho D_i \nabla \psi_i) + \sigma_i, \quad i = 1, 2, \dots, k+1$$

where $i=1,2,\dots,k+1$. The diffusivities D_i ($i=1,2,\dots,k$) are the mass diffusivities for the species and $D_{k+1}=D$ denotes the thermal diffusivity.

Similarly, σ_i ($i=1,2,\dots,k$) are the species source terms \dot{m}_i , $i = 1, 2, \dots, k$ and σ_{k+1} is defined as ω_T .

The chemical source term will also be written as $s_i = \rho S_i$

Moment Methods for Reactive Scalars

Favre averaged equations for the mean and the variance of the reactive scalars can be derived by splitting $\psi_i(\mathbf{x}, t)$ into a Favre mean and a fluctuation

$$\psi_i(\mathbf{x}, t) = \tilde{\psi}_i(\mathbf{x}, t) + \psi_i''(\mathbf{x}, t)$$

When this is introduced into

$$\rho \frac{\partial \psi_i}{\partial t} + \rho \mathbf{v} \cdot \nabla \psi_i = \nabla \cdot (\rho D_i \nabla \psi_i) + \sigma_i, \quad i = 1, 2, \dots, k+1$$

one obtains in a similar way as for the momentum equation after averaging

$$\bar{\rho} \frac{\partial \tilde{\psi}_i}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{\psi}_i = \nabla \cdot (\overline{\rho D_i \nabla \psi_i}) - \nabla \cdot (\overline{\rho \mathbf{v}'' \psi_i''}) + \bar{\rho} \tilde{S}_i$$

In this equation the terms on the l.h.s. are closed, while those on the r.h.s. must be modeled.

In high Reynolds number flows the molecular transport term containing the molecular diffusivities D_i are small and can be neglected.

$$\bar{\rho} \frac{\partial \tilde{\psi}_i}{\partial t} + \bar{\rho} \tilde{v} \cdot \nabla \tilde{\psi}_i = \nabla \cdot (\overline{\rho D_i \nabla \psi_i}) - \nabla \cdot (\bar{\rho} \tilde{v}'' \tilde{\psi}_i'') + \bar{\rho} \tilde{S}_i$$

Closure is required for the second term on the r.h.s., the turbulent transport term, and for the last term, the mean chemical source term.

The modeling of the mean chemical source term has often been considered as the main problem of moment methods in turbulent combustion.

In order to discuss the difficulties associated with the closure of this term, we assume that coupling relations exist between the chemical species and the temperature.

As noted before, such coupling relations can easily be derived for the case of a one step reaction and equal diffusivities.

With this assumption we consider the following form of the heat release rate

$$\omega_T(T) = \rho S_T(T) = \rho B(T_b - T) \exp\left(-\frac{E}{\mathcal{R}T}\right)$$

Here B contains the frequency factor and the heat of reaction, T_b is the adiabatic flame temperature, E the activation energy.

Introducing $T = \tilde{T} + T''$ the argument of the exponential term may be expanded around $T \approx \tilde{T}$, $T'' \ll T$ as

$$\frac{E}{\mathcal{R}T} = \frac{E}{\mathcal{R}\tilde{T}} - \frac{ET''}{\mathcal{R}\tilde{T}^2}$$

If the expansion is also introduced into the preexponential term, the quantity S_T becomes

$$S_T(T) = S_T(\tilde{T}) \left(1 - \frac{T''}{T_b - \tilde{T}} \right) \exp \left(\frac{ET''}{\mathcal{R}\tilde{T}^2} \right)$$

Typically, in the reaction zone of a flame

$$E/\mathcal{R}\tilde{T} = \mathcal{O}(10), \quad 0.1 \leq T''/\tilde{T} \leq 0.3$$

Therefore the exponential term causes enhanced fluctuations of the chemical source term around its mean value evaluated with the mean temperature.

It may be concluded that moment methods for reactive scalars will fail due to the strong nonlinearity of the chemical source term.

Dissipation and Scalar Transport of Non-Reacting Scalars

As an example for a nonreactive scalar we will use the mixture fraction Z .

It is general practice in turbulent combustion to employ the gradient transport assumption for non-reacting scalars.

The scalar flux then takes the form

$$-\widetilde{v''Z''} = D_t \nabla \widetilde{Z}_i$$

Here D_t is a turbulent diffusivity which is modeled by analogy to the eddy viscosity as

$$D_t = \frac{\nu_t}{Sc_t}$$

where Sc_t is a turbulent Schmidt number.

The equation for the mean mixture fraction then reads

$$\rho \frac{\partial \tilde{Z}}{\partial t} + \rho \tilde{v} \cdot \nabla \tilde{Z} = \nabla \cdot (\bar{\rho} D_t \nabla \tilde{Z})$$

where the molecular term has been neglected.

In order to derive an equation for **mean mixture fraction variance** we first must derive an equation for the fluctuation Z'' by subtracting

$$\bar{\rho} \frac{\partial \tilde{Z}}{\partial t} + \bar{\rho} \tilde{v} \cdot \nabla \tilde{Z} = \nabla \cdot (\overline{\rho D_i \nabla Z}) - \nabla \cdot (\bar{\rho} \widetilde{v'' Z''})$$

from

$$\rho \frac{\partial Z}{\partial t} + \rho v \cdot \nabla Z = \nabla \cdot (\rho D_i \nabla Z)$$

we obtain:

$$\frac{\partial Z''}{\partial t} + (\tilde{v} + v'') \cdot \nabla Z'' + v'' \cdot \nabla \tilde{Z} = \frac{1}{\rho} \nabla \cdot (\rho D \nabla Z) - \frac{1}{\bar{\rho}} \nabla \cdot (\overline{\rho D \nabla Z}) + \nabla \cdot (\bar{\rho} \widetilde{v'' Z''})$$

If derivatives of ρ and D and their mean values are neglected for simplicity, the first two terms on the r.h.s. of

$$\frac{\partial Z''}{\partial t} + (\tilde{v} + v'') \cdot \nabla Z'' + v'' \cdot \nabla \tilde{Z} = \frac{1}{\rho} \nabla \cdot (\rho D \nabla Z) - \frac{1}{\bar{\rho}} \nabla \cdot (\overline{\rho D \nabla Z}) + \nabla \cdot (\bar{\rho} \widetilde{v'' Z''})$$

can be combined to obtain a term proportional to $D_i \Delta Z''$.

Introducing this and multiplying the equation by $2\rho Z''$ one obtains an equation for Z''^2 .

With the use of the continuity equation and averaging one obtains

$$\bar{\rho} \frac{\partial \widetilde{Z''^2}}{\partial t} + \bar{\rho} \tilde{v} \cdot \nabla \widetilde{Z''^2} = -\nabla \cdot (\bar{\rho} v'' \widetilde{Z''^2}) + 2\bar{\rho} (-v'' \widetilde{Z''}) \cdot \nabla \tilde{Z} - \bar{\rho} \tilde{\chi}$$

$$\frac{\partial Z''}{\partial t} + (\tilde{v} + v'') \cdot \nabla Z'' + v'' \cdot \nabla \tilde{Z} = \frac{1}{\rho} \nabla \cdot (\rho D \nabla Z) - \frac{1}{\bar{\rho}} \nabla \cdot (\overline{\rho D \nabla Z}) + \nabla \cdot (\bar{\rho} v'' \tilde{Z}'')$$

As before, the terms on the r.h.s. describe the local change and convection.

The first term on the r.h.s. is the turbulent transport term.

The second term on the r.h.s. accounts for the production of scalars fluctuations.

The mean molecular transport term has been neglected for simplicity but the molecular diffusivity still appears in the dissipation term.

The Favre scalar dissipation rate is defined as

$$\tilde{\chi} = 2 D (\nabla \tilde{Z}'')^2$$

An integral scalar time scale can be defined by

$$\tau_Z = \frac{\widetilde{Z}''^2}{\widetilde{\chi}}$$

It is often set proportional to the flow time $\tau = \widetilde{k}/\widetilde{\varepsilon} = c_\chi \tau_Z$

The constant of proportionality c_χ is of order unity but varies:

$$1.5 \leq c_\chi \leq 3$$

A value $c_\chi=2.0$ is often used.

Combining $\tau_Z = \frac{\widetilde{Z}''^2}{\widetilde{\chi}}$ and $\tau = \widetilde{k}/\widetilde{\varepsilon} = c_\chi \tau_Z$

leads to the model

$$\widetilde{\chi} = c_\chi \frac{\widetilde{\varepsilon}}{\widetilde{k}} \widetilde{Z}''^2$$

The Eddy Break Up and the Eddy Dissipation Model

An early attempt to provide a closure for the chemical source term is due to Spalding (1971).

Turbulent mixing may be viewed as a cascade process from the integral down to the molecular scales,
the cascade process also controls the chemical reactions as long as mixing rather than reaction is the rate determining process.

This model was called the [Eddy-Break-Up model \(EBU\)](#).

The turbulent mean reaction rate of products was expressed as

$$\bar{\omega}_P = \rho C_{\text{EBU}} \frac{\varepsilon}{k} \left(\overline{Y_P''^2} \right)^{1/2}$$

$\overline{Y_P''^2}$ is the variance of the product mass fraction and C_{EBU} is the Eddy-Break-Up constant.

This model has been modified by Magnussen and Hjertager (1977) who replaced $\overline{Y_P''^2}$ simply by the mean mass fraction of the deficient species (fuel for lean or oxygen for rich mixtures) calling it the **Eddy Dissipation Model (EDM)**.

The **Eddy Dissipation Model** takes the minimum of three rates, those defined with the mean fuel mass fraction with the mean oxidizer mass fraction

$$\bar{\omega}_{\text{O}_2} = \bar{\rho} \frac{A \bar{Y}_{\text{O}_2} \varepsilon}{\nu k}$$

and with the product mass fraction

$$\bar{\omega}_{\text{P}} = \bar{\rho} \frac{A \cdot B}{(1 + \nu)} \bar{Y}_{\text{P}} \frac{\varepsilon}{k}$$

in order to calculate the mean chemical source term.

A and B are modeling constants and ν is the stoichiometric oxygen to fuel mass ratio defined by

$$\frac{Y_{\text{O}_2,u}}{Y_{\text{F},u}} \Big|_{st} = \frac{\nu'_{\text{O}_2} W_{\text{O}_2}}{\nu'_{\text{F}} W_{\text{F}}} = \nu$$

The Eddy Break-Up model and its modifications are based on intuitive arguments.

The main idea is to replace the chemical time scale of an assumed one-step reaction by the turbulent time scale $\tau = k/\varepsilon$.

Thereby the model eliminates the influence of chemical kinetics, representing the fast chemistry limit only.

When these models are used in CFD calculations, it turns out that the constants C_{EBU} or A and B must be "tuned" within a wide range in order to obtain reasonable results for a particular problem.

The Pdf Transport Equation Model

Similar to moment methods, models based on a pdf transport equation for the velocity and the reactive scalars are usually formulated for one-point statistics.

Within that framework, however, they represent a general statistical description of turbulent reacting flows, applicable to premixed, nonpremixed and partially premixed combustion.

A joint pdf transport equation for the velocity and the reactive scalars can be derived, which is equivalent to an infinite hierarchy of one-point moment equations for these quantities, Pope (1990).

For simplicity, we will consider here the transport equation for the joint pdf of velocity and reactive scalars only.

Denoting the set of reactive scalars, such as the temperature and the mass fraction of reacting species by the vector ψ ,

$$P(\mathbf{v}, \psi; \mathbf{x}, t) d\mathbf{v} d\psi$$

is the probability of finding at point \mathbf{x} and time t the velocity components and the reactive scalars within the intervals

$$v - dv/2 < v < v + dv/2; \quad \psi - d\psi/2 < \psi < \psi + d\psi/2$$

There are several ways to derive a transport equation for the probability density $P(\mathbf{v}, \boldsymbol{\psi} ; \mathbf{x}, t)$ (cf. O'Brien, 1980) .

We refer here to the presentation in Pope (1985, 2000), but write the convective terms in conservative form

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho \mathbf{v} P) + (\rho \mathbf{g} - \nabla \bar{p}) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_{\mathbf{v}} \cdot [\langle -\nabla \cdot \boldsymbol{\tau} + \nabla \langle p' | \mathbf{v}, \boldsymbol{\psi} \rangle P] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\langle \nabla \cdot (\rho D \nabla \psi_i) | \mathbf{v}, \boldsymbol{\psi} \rangle P]$$

In deriving this equation, the equations for all reactive scalars, including that for temperature this equation have been cast into the form

$$\rho \frac{\partial \psi_i}{\partial t} + \rho \mathbf{v} \cdot \nabla \psi_i = \nabla \cdot (\rho D_i \nabla \psi_i) + \sigma_i,$$

for simplicity.

The symbol ∇_v denotes the divergence operator with respect to the three components of velocity.

The angular brackets denote conditional averages, conditioned with respect to fixed values of v and ψ .

For simplicity of presentation we do not use different symbols for the random variables describing the stochastic fields and the corresponding sample space variables which are the independent variables in the pdf equation.

The first two terms on the l.h.s. of

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho \mathbf{v} P) + (\rho \mathbf{g} - \nabla \bar{p}) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_{\mathbf{v}} \cdot [\langle -\nabla \cdot \boldsymbol{\tau} + \nabla \langle p' | \mathbf{v}, \boldsymbol{\psi} \rangle P] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\langle \nabla \cdot (\rho D \nabla \psi_i) | \mathbf{v}, \boldsymbol{\psi} \rangle P]$$

are the local change and convection of the probability density function in physical space.

The third term represents transport in velocity space by gravity and the mean pressure gradient.

The last term on the l.h.s. contains the chemical source terms.

All these terms are in closed form, since they are local in physical space.

Note that the mean pressure gradient does not present a closure problem, since the pressure is calculated independently of the pdf equation using the mean velocity field.

For chemical reacting flows it is of particular interest that the chemical source terms can be treated exactly for arbitrarily complex chemical kinetics.

It has often been argued that in this respect the transported pdf formulation has a considerable advantage compared to other formulations.

However, on the r.h.s. of the transport equation

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho \mathbf{v} P) + (\rho \mathbf{g} - \nabla \bar{p}) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_{\mathbf{v}} \cdot [\langle -\nabla \cdot \boldsymbol{\tau} + \nabla \langle p' | \mathbf{v}, \boldsymbol{\psi} \rangle P] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\langle \nabla \cdot (\rho D \nabla \psi_i) | \mathbf{v}, \boldsymbol{\psi} \rangle P]$$

there are two terms that contain gradients of quantities conditioned on the values of velocity and composition.

Therefore, if gradients are not included as sample space variables in the pdf equation, these terms occur in unclosed form and have to be modeled.

$$\frac{\partial(\rho P)}{\partial t} + \nabla \cdot (\rho \mathbf{v} P) + (\rho \mathbf{g} - \nabla \bar{p}) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\omega_i P] =$$

$$\nabla_{\mathbf{v}} \cdot [\langle -\nabla \cdot \boldsymbol{\tau} + \nabla \langle p' | \mathbf{v}, \boldsymbol{\psi} \rangle P] - \sum_{i=1}^n \frac{\partial}{\partial \psi_i} [\langle \nabla \cdot (\rho D \nabla \psi_i) | \mathbf{v}, \boldsymbol{\psi} \rangle P]$$

The first unclosed term on the r.h.s. describes transport of the probability density function in velocity space induced by the viscous stresses and the fluctuating pressure gradient.

The second term represents transport in reactive scalar space by molecular fluxes.

This term represents molecular mixing.

When chemistry is fast, mixing and reaction take place in thin layers where molecular transport and the chemical source term balance each other.

Therefore, the closed chemical source term and the unclosed molecular mixing term, being leading order terms in an asymptotic description of the flame structure, are closely linked to each other.

Pope and Anand (1984) have illustrated this for the case of premixed turbulent combustion by comparing a standard pdf closure for the molecular mixing term with a formulation, where the molecular diffusion term was combined with the chemical source term to define a modified reaction rate.

They call the former distributed combustion and the latter flamelet combustion and find considerable differences in the Damköhler number dependence of the turbulent burning velocity normalized with the turbulent intensity.

From a numerical point of view, the most apparent property of the pdf transport equation is its high dimensionality.

Finite-volume and finite-difference techniques are not very attractive for this type of problem, as memory requirements increase roughly exponentially with dimensionality.

Therefore, virtually all numerical implementations of pdf methods for turbulent reactive flows employ [Monte-Carlo simulation techniques](#) (cf. Pope, 1981, 1985),

The advantage of Monte-Carlo methods is that their memory requirements depend only linearly on the dimensionality of the problem.

Monte-Carlo methods employ a large number, N , of particles.

In the Lagrangian algorithm (Pope, 1985)) the particles are not bound to grid nodes.

Instead, each particle has its own position and moves through the computational domain with its own instantaneous velocity.

The particles should be considered as different realizations of the turbulent reactive flow problem under investigation.

The state of the particle is described by its position and velocity, and by the values of the reactive scalar that it represents as a function of time.

These particles should not be confused with real fluid elements, which behave similarly in a number of respects.

The Laminar Flamelet Concept

The view of a turbulent diffusion flame as an ensemble of stretched laminar flamelets is due to Williams (1975).

Flamelet equations based on the mixture fraction as independent variable, using the scalar dissipation rate for the mixing process, were independently derived by Peters (1980) and Kuznetsov (1982).

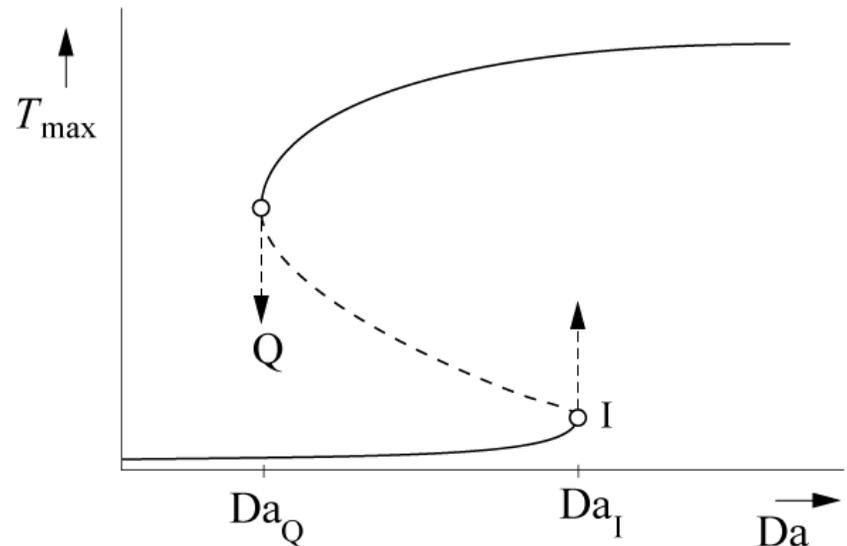
A first review of diffusion flamelet models was given by Peters (1984).

For premixed and diffusion flames the flamelet concept was reviewed by Peters (1986) and Bray and Peters (1994).

Flamelets are thin reactive-diffusive layers embedded within an otherwise non-reacting turbulent flow field.

Once ignition has taken place, chemistry accelerates as the temperature increases due to heat release.

When the temperature reaches values that are of the order of magnitude of those of the close-to-equilibrium branch the reactions that determine fuel consumption become very fast.



For methane combustion, for example, the time scale of the rate determining reaction in the fuel consumption layer was estimated in Lecture 1.

Since the chemical time scale of this reaction is short, chemistry is active only within a thin layer, namely the fuel consumption or inner layer.

If this layer is thin compared to the size of a Kolmogorov eddy, it is embedded within the quasi-laminar flow field of such an eddy and the assumption of a laminar flamelet structure is justified.

If, on the contrary, turbulence is so intense, that Kolmogorov eddies become smaller than the inner layer and can penetrate into it, they are able to destroy its structure.

Under these conditions the entire flame is likely to extinguish.

The location of the inner layer defines the flame surface.

Differently from moment methods or methods based on a pdf transport equation, statistical considerations in the flamelet concept focus on the location of the flame surface and not on the reactive scalars themselves.

That location is defined as an iso-surface of a non-reacting scalar quantity, for which a suitable field equation is derived.

For nonpremixed combustion the mixture fraction Z is that scalar quantity, for premixed combustion the scalar G will be introduced.

Once equations that describe the statistical distributions of Z and G are resolved, the profiles of the reactive scalars normal to the surface are calculated using flamelet equations.

These profiles are assumed to be attached to the flame surface and are convected with it in the turbulent flow field.

Therefore the statistical moments of the reactive scalars can be obtained from the statistical distribution of the scalar quantities Z and G .

Details of this procedure will be discussed in Lecture 12.

The BML-Model and the Coherent Flamelet Model

For premixed combustion, flamelet models are typically based on the progress variable c .

The progress variable c is defined as a normalized temperature or normalized product mass fraction

$$c = \frac{T - T_u}{T_b - T_u} \quad \text{or} \quad c = \frac{Y_P}{Y_{P,b}}$$

which implies a one-step reaction A to P and a corresponding heat release raising the temperature from T_u to T_b .

In flamelet models based on the progress variable the flame structure is assumed to be infinitely thin and no intermediate values of temperature are resolved.

This corresponds to the fast chemistry limit.

The progress variable therefore is a step function that separates unburnt mixture and burnt gas in a given flow field.

The classical model for premixed turbulent combustion, the **Bray-Moss-Libby (BML) model**, was initiated by Bray and Moss (1977) by assuming the pdf of the progress variable c to be a two delta function distribution.

This assumption only allows for entries at $c = 0$ and $c = 1$ in a turbulent premixed flame, but it illustrates important features, like counter-gradient diffusion of the progress variable.

This appears in the equation for the Favre mean progress variable

$$\bar{\rho} \frac{\partial \tilde{c}}{\partial t} + \bar{\rho} \mathbf{v} \cdot \nabla \tilde{c} + \nabla \cdot (\bar{\rho} \widetilde{v'' c''}) = \bar{w}_c$$

where the molecular diffusion term has been neglected.

This equation

$$\bar{\rho} \frac{\partial \tilde{c}}{\partial t} + \bar{\rho} \mathbf{v} \cdot \nabla \tilde{c} + \nabla \cdot (\bar{\rho} \widetilde{\mathbf{v}'' c''}) = \bar{\omega}_c$$

requires the modeling of the turbulent transport term and the mean reaction term

$$\nabla \cdot (\bar{\rho} \widetilde{\mathbf{v}'' c''}), \quad \bar{\omega}_c$$

Libby and Bray (1981) and Bray et al. (1981) have shown that a gradient transport assumption like

$$\widetilde{\mathbf{v}'' Z''} = -D_t \nabla \tilde{Z}_i$$

is not applicable to $\widetilde{\mathbf{v}'' c''}$.

This is due to gas expansion effects at the flame surface and is called counter-gradient diffusion.

Counter-gradient diffusion has been found in many experiments and in many one-dimensional numerical analyzes.

However, there is no model available that could be used in three-dimensional calculations solving

$$\bar{\rho} \frac{\partial \tilde{c}}{\partial t} + \bar{\rho} \mathbf{v} \cdot \nabla \tilde{c} + \nabla \cdot (\bar{\rho} \widetilde{\mathbf{v}'' c''}) = \bar{w}_c$$

With counter-gradient diffusion included.

Models for the mean reaction rate by Bray et al.(1984) and Bray and Libby (1986) focus on a time series of step function events of the progress variable.

This makes the mean source term proportional to the flamelet crossing frequency.

Further modeling, discussed in more detail in Bray and Libby (1994), then leads to the expression

$$\bar{\omega}_c = \rho_u s_L I_0 \Sigma$$

where s_L is the laminar burning velocity, I_0 is a stretch factor and Σ is the flame surface density (flame surface per unit volume).

A model for Σ has been proposed by Candel et al. (1990).

This is called the [Coherent Flame Model \(CFM\)](#).

A comparison of the performance of different formulations of the model for one-dimensional turbulent flames was made by Duclos et al. (1993).

Modeling based on DNS data has led Trounev and Poinso (1994) to the following equation for the flame surface density Σ :

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\tilde{v} \Sigma) = \nabla \cdot (D_t \nabla \Sigma) + C_1 \frac{\varepsilon}{k} \Sigma - C_2 s_L \frac{\Sigma^2}{1 - \bar{c}}$$

The terms on the l.h.s. represent the local change and convection, the first term on the r.h.s. represents turbulent diffusion, the second term production by flame stretch and the last term flame surface annihilation.

The stretch term is proportional to the inverse of the integral time scale $\tau = k/\varepsilon$ which is to be evaluated in the unburnt gas.

Combustion Models used in LargeEddy Simulation

Turbulence models based on Reynolds Averaged Navier-Stokes Equations (RANS) employ turbulent transport approximations with an effective turbulent viscosity that is by orders of magnitude larger than the molecular viscosity.

In particular if steady state versions of these equations are used, this tends to suppress large scale instabilities which occur in flows with combustion even more frequently than in non-reacting flows.

If those instabilities are to be resolved in numerical simulations, it is necessary to recur to more advanced, but computationally more expensive methods such as [Large Eddy Simulation \(LES\)](#).

Large Eddy Simulation does not intend to numerically resolve all turbulent length scales, but only a fraction of the larger energy containing scales within the inertial subrange.

Modeling is then applied to represent the smaller unresolved scales which contain only a small fraction of the turbulent kinetic energy.

Therefore the computed flows are usually less sensitive to modeling assumptions.

The distinction between the resolved large scales and the modeled small scales is made by the grid resolution that can be afforded.

The model for the smaller scales is called the [subgrid model](#).

In deriving the basic LES equations, the Navier-Stokes equations are spatially filtered with a filter of size Δ , which is of the size of the grid cell (or a multiple thereof) in order to remove the direct effect of the small scale fluctuations (cf. Ghosal and Moin, 1995).

These show up indirectly through nonlinear terms in the [subgrid-scale stress](#) tensor as subgrid-scale Reynolds stresses, [Leonard stresses](#), and subgrid-scale cross stresses.

The latter two contributions result from the fact that, unlike with the traditional Reynolds averages, a second filtering changes an already filtered field.

In a similar way, after filtering the equations for non-reacting scalars like the mixture fraction, one has to model the filtered scalar flux vectors which contain subgrid scalar fluxes, Leonard fluxes, and subgrid-scale cross fluxes.

The reason why LES still provides substantial advantages for modeling turbulent combustion is that the scalar mixing process is of paramount importance in chemical conversion.

Nonreactive and reactive system studies show that LES predicts the scalar mixing process and dissipation rates with considerably improved accuracy compared to RANS, especially in complex flows.

For example, to study the importance of turbulent scalar dissipation rate fluctuations on the combustion process and to highlight the differences between RANS and LES, Pitsch (2002), compared the results of two different LES simulations using unsteady flamelet models in which the scalar dissipation rate appears as a parameter.

The only difference between the simulations was that only the Reynolds-averaged dissipation rate was used in one simulation, Pitsch (2000), whereas the other considered the resolved fluctuations of the filtered scalar dissipation rate predicted by LES.

The results show substantially improved predictions, especially for minor species, when fluctuations are considered.

Another such example is the simulation of a bluff-body stabilized flame, Raman (2005), where a simple steady-state diffusion flamelet model in the context of an LES with a recursive filter refinement method led to excellent results.

Such accuracy has not been achieved with RANS simulations of the same configuration , Kim (20020}, Muradoglu (2003).

Both studies are discussed in more detail below. Similar arguments can be made for premixed turbulent combustion LES.

In RANS modeling it has long been realized that the direct closure of the mean chemical source term in the averaged species transport equations can hardly be accomplished, and conserved scalar methods have been used in many applications.

Using so-called coupling functions, the rate of mixing of fuel and oxidizer can be described by a nonreactive scalar, the mixture fraction. Different definitions have been used for the mixture fraction, Bilger (1976), Pitsch (1998), but essentially the mixture fraction is a measure of the local equivalence ratio.

Hence, the mixture fraction is a conserved scalar, independent of the chemistry.

This leads to the so-called conserved scalar method, which forms the basis for most of the combustion models for nonpremixed turbulent combustion.

Considering the simplest case of infinitely fast chemistry, all species mass fractions and the temperature are a function of mixture fraction only.

If the subfilter probability distribution of the mixture fraction is known, the Favre-filtered mass fractions, for instance, can then be obtained as

$$\tilde{Y}_i = \int_0^1 Y_i(Z) f(Z) dZ$$

where Z is the mixture fraction and $f(Z)$ is the marginal density-weighted filter probability density function (FPDF) of the mixture fraction.

Applications of simple conserved scalar models in LES have been based on infinitely fast irreversible chemistry Pierce (1998) and equilibrium chemistry Cook (1994}.

The flamelet model is a conserved scalar model that can account for finite-rate chemistry effects.

Many models that have been formulated for LES are variants of these and some are discussed below.

These models essentially provide state relationships for the reactive scalars as functions of mixture fraction and other possible parameters, such as the scalar dissipation rate.

Filtered quantities are then obtained by a relation similar to

$$\tilde{Y}_i = \int_0^1 Y_i(Z) f(Z) dZ$$

but using a presumed joint FPDF of the mixture fraction and, for example, the scalar dissipation rate.

Because the probability density function (PDF) plays a central role in most models for nonpremixed combustion, it is necessary to emphasize the special meaning of the FPDF in LES.

Here, the example of the marginal FPDF of the mixture fraction is discussed, but similar arguments can be made for the joint composition FPDF.

In Reynolds-averaged methods, a one-point PDF can be determined by repeating an experiment many times and recording the mixture fraction at a given time and position in space.

For a sufficiently large number of samples, the PDF of the ensemble can be determined with good accuracy.

In LES, assuming a simple box filter, the data of interest is a one-time, one-point probability distribution in a volume corresponding to the filter size surrounding the point of interest.

If an experimentally observed spatial mixture fraction distribution is considered at a given time, the FPDF cannot simply be evaluated from these data, because the observed distribution is characteristic of this particular realization and it is not a statistical property.

As a statistical property, the FPDF must be defined by an ensemble that can potentially have an arbitrary large number of samples. In the context of transported PDF model formulations for LES, which are discussed below, Pope (1990) introduced the notion of the filtered density function (FDF), which describes the local subfilter state of the considered experiment.

The FDF is not an FPDF, because it describes a single realization.

The FPDF is defined only as the average of the FDF of many realizations given the same resolved field, Fox (2003).

It is important to distinguish between the FDF and the FPDF, especially in using direct numerical simulation (DNS) data to evaluate models, and in the transported FDF models discussed below.

Only the FDF can be evaluated from typical DNS data, whereas the FPDF is required for subfilter modeling.

For conserved scalar models, a presumed shape of the FPDF has to be provided.

Similar to RANS models, a beta-function distribution is usually assumed for the marginal FPDF of the mixture fraction, and parameterized by the first two moments of the mixture fraction.

The filtered mixture fraction is determined by the solution of a transport equation, whereas algebraic models are mostly used for the subfilter scalar variance.

The beta-function is expected to be a better model for the FPDF in LES than for the PDF in RANS, because the FPDF is generally more narrow, and hence the exact shape is less important. It can also be expected that intermittency, which is a main source of error when using the beta-function in RANS, will mostly occur on the resolved scales.

The validity of the beta-function representation of the FPDF of the mixture fraction has been investigated by several authors using DNS data of nonpremixed reacting flows of both constant and variable density Cook (1994), Jimenez (1997), Wall (2000).

The main conclusion of these studies is that the beta-function distribution provides a good estimate for the FPDF of the mixture fraction and that this estimate is even better in LES than in RANS models.

Furthermore, the model is particularly good when evaluated using the mixture fraction variance taken from DNS data, suggesting that the beta-function as a model for the statistical distribution of the mixture fraction performs much better than the commonly used subgrid-scale models for the mixture fraction variance.

However, recent studies by Tong (2001, 2005) show that the FPDF often substantially deviates from the beta-function. This is discussed in more detail below.

In the following, different variants of the flamelet model are discussed.

Because all such models require the scalar dissipation rate, modeling of this quantity is discussed first.

We follow the presentation in Pitsch (2006).

Modeling the Scalar Dissipation Rate

Although different conceptual ideas and assumptions are used in the combustion models discussed here, most of them need a model for the scalar dissipation rate.

The dissipation rate of the mixture fraction is a fundamental parameter in nonpremixed combustion, which determines the filtered reaction rates, if combustion is mixing controlled.

High rates of dissipation can also lead to local or global flame extinction.

Models based on presumed FPDFs also require a model for the subfilter scalar variance.

Here, the most commonly used model formulations for LES are reviewed briefly, differences with the typical RANS models are pointed out, and potential areas of improvement are discussed.

An illustration of the importance of the scalar variance and dissipation rate in LES of nonpremixed combustion modeling is given by the following example.

Pope (2004) pointed out that LES is an incomplete model if the filter size can be arbitrarily specified.

This is an important issue, especially for combustion LES, because of the importance of the subfilter models.

To fix the arbitrariness of the filter, Raman (2005) proposed a recursive filter refinement method, where the local filter width is determined such that the ratio of subfilter scalar variance to the maximum possible variance is smaller than a specified value.

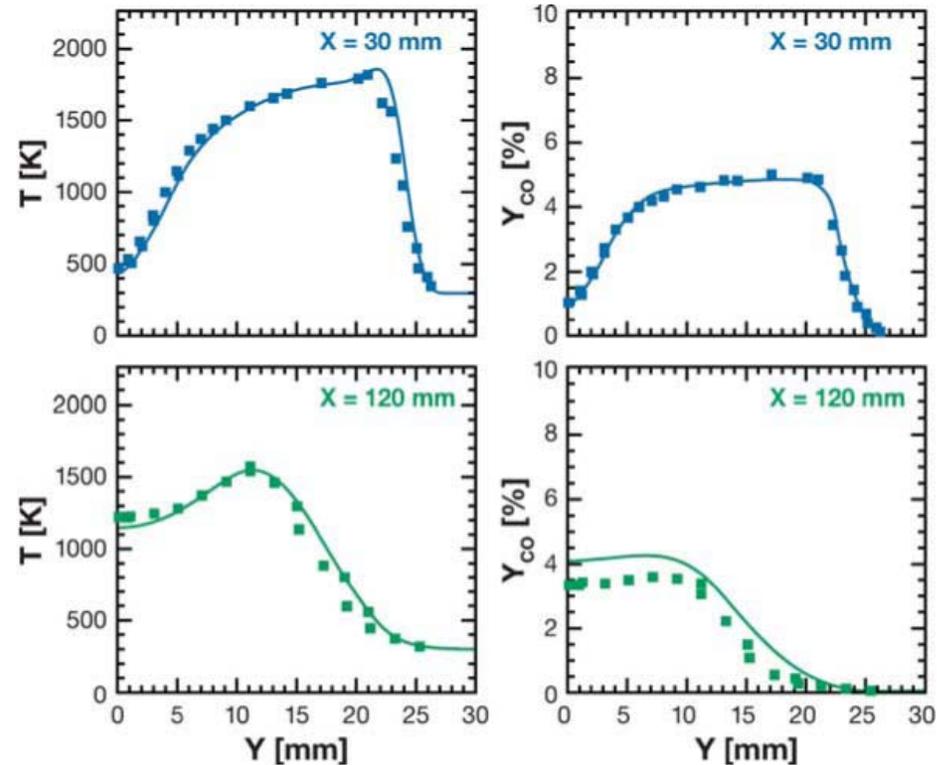
The maximum possible variance can be expressed in terms of the resolved mixture fraction as

$$\tilde{Z}(1 - \tilde{Z})$$

It was demonstrated in the simulation of a bluff-body stabilized flame that this method better resolves high scalar variance and dissipation regions, which leads to significant improvement in results.

Results from large-eddy simulation of the Sydney bluff-body flame Raman (2005)
Flame representation from simulation results (left) and time-averaged radial profiles of temperature and CO mass fraction.

The left figure shows computed chemiluminescence emissions of CH collected in an observation plane with a ray tracing technique.



In RANS models, typically a transport equation is solved for the scalar variance, in which the Reynolds-averaged scalar dissipation rate χ appears as an unclosed sink term that requires modeling.

The additional assumption of a constant ratio of the integral timescale of the velocity τ_t and the scalar fields leads to the expression

$$\langle \chi \rangle = c_\phi \frac{1}{\tau_t} \langle Z'^2 \rangle$$

where c_ϕ is the so-called timescale ratio.

In the models most commonly used in LES Girimaji (1996), Pierce (1998), the scalar variance transport equation and the timescale ratio assumption are actually used in the opposite sense.

Instead of solving the subfilter variance equation, the assumption that the scalar variance production appearing in that equation equals the dissipation term leads to an algebraic model for the dissipation rate of the form

$$\tilde{\chi} = 2D_t(\nabla \tilde{Z})^2$$

where an eddy diffusivity model was used for the subfilter scalar flux in the production term.

$$D_t = (c_Z \nabla)^2 \tilde{S}$$

is the eddy diffusivity, where c_Z can be determined using a dynamic procedure and

$$\tilde{S} = |2\tilde{S}_{ij}\tilde{S}_{ij}|^{1/2}$$

is the characteristic Favre-filtered rate of strain.

Writing $\langle \chi \rangle = c_\phi \frac{1}{\tau_t} \langle Z'^2 \rangle$ for the subfilter scales and combining it with

$\tilde{\chi} = 2D_t(\nabla \tilde{Z})^2$ then leads to the model for the scalar variance

$$\tilde{Z}'^2 = c_V \Delta^2 (\nabla \tilde{Z})^2$$

is assumed, and a new coefficient c_V is introduced, which can be determined dynamically following Pierce (1998).

From $\langle \chi \rangle = c_\phi \frac{1}{\tau_t} \langle Z'^2 \rangle$, $\tilde{\chi} = 2D_t(\nabla \tilde{Z})^2$ and the dynamically determined coefficients of the eddy diffusivity and the scalar variance, the timescale ratio c_ϕ can be determined as

$$c_\phi = 2c_Z^2/c_V$$

Pitsch (2000) used the Lagrangian flamelet model (LFM), Pitsch (1998) as a subfilter combustion model for LES in an application to a piloted methane/air diffusion flame Barlow (1998) using a 20-step reduced chemical scheme based on the GRI 2.11 mechanism Bowman (1995).

The unsteady flamelet equations are solved coupled with the LES solution to provide the filtered density and other filtered scalar quantities using a presumed FPDF of the mixture fraction.

The scalar dissipation rate χ required to solve the flamelet equation

$$\frac{\partial Y_i}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} = \dot{m}_i$$

is determined from the LES fields as a cross-sectional conditionally averaged value using a model similar to the conditional source term estimation method by Bushe (1999), which is described below.

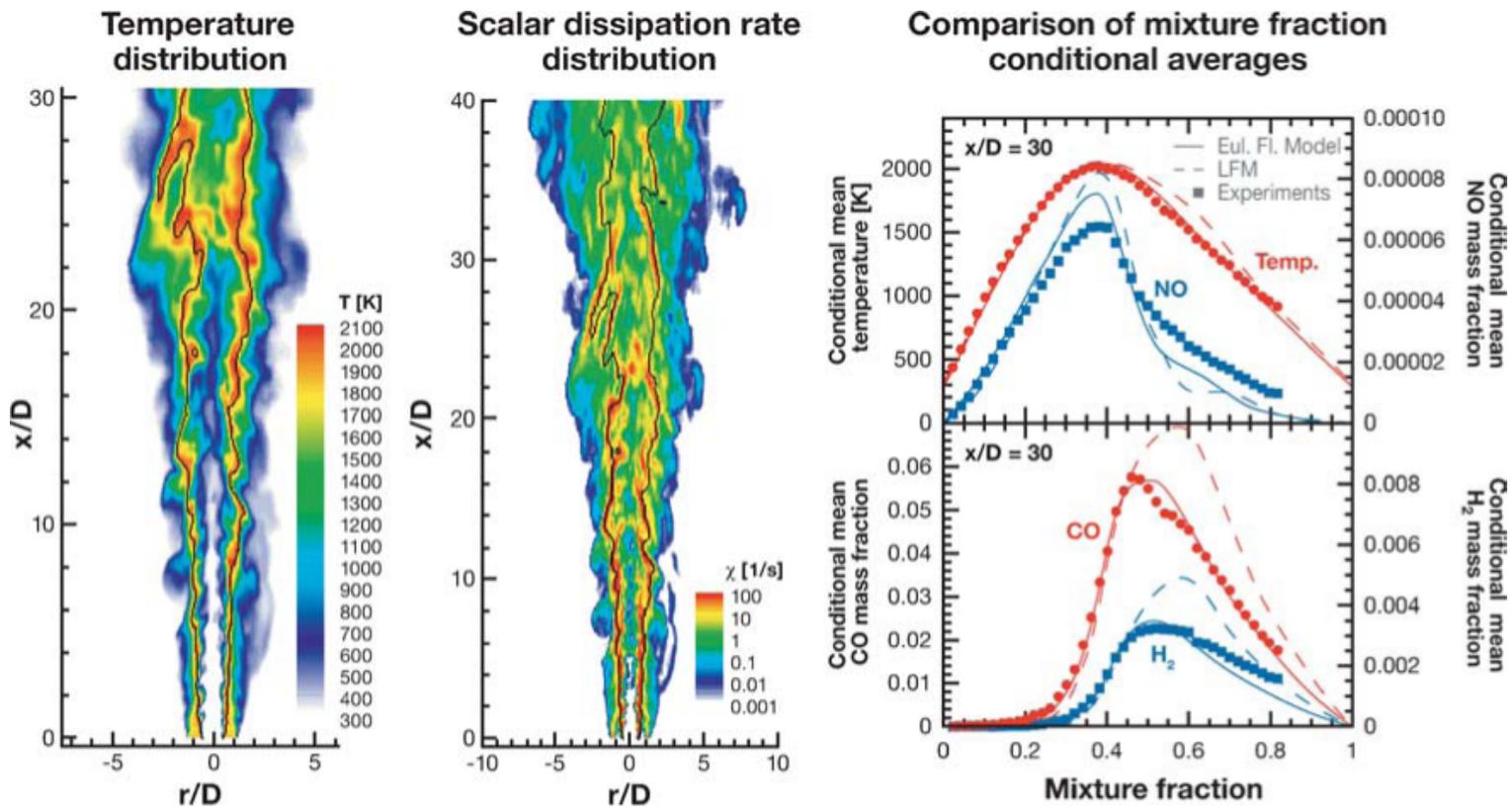
The unconditional scalar dissipation rate was determined from a dynamic model Pierce (1998).

This study is the first demonstration of combustion LES of a realistic configuration using a detailed description of the chemistry.

The results are promising, especially for NO, but because of the cross sectional averaging of the scalar dissipation rate, local fluctuations of this quantity are not considered and the potential of LES is not fully realized.

Also, this model cannot be easily applied in simulations of more complex flow fields.

In a more recent formulation, the Eulerian flamelet model Pitsch (2002), the flamelet equations are rewritten in an Eulerian form, which leads to a full coupling with the LES solver, and thereby enables the consideration of the resolved fluctuations of the scalar dissipation rate in the combustion model.



Results from large-eddy simulation of Sandia flame D (Pitsch, 2002,2000), using the Eulerian flamelet model (solid lines) and the Lagrangian flamelet model (dashed lines) compared with experimental data of Barlow (1998). Temperature distribution (left), scalar dissipation rate distribution (center), and comparison of mixture fraction–conditioned averages of temperature and mass fractions of NO, CO, and H₂ at $x/D = 30$. Courtesy of Pitsch (2006)

The resolved scalar dissipation rate field is dominated by features occurring on the large scale of the turbulence. Layers of high dissipation rate alternate with low dissipation rate regions.

In the LFM results, as well as in several earlier RANS-type modeling studies Barlow (2000), where these fluctuations are not considered, some heat release occurs on the rich partially premixed side of the flame, which leads to strong CO formation in these regions.

Accounting for the richness of the predicted spatial distribution of the scalar dissipation rate substantially improves the comparison with the experimental data by suppressing the heat release in the rich regions, and hence the formation of CO.

LES of real Combustion Devices

Several investigators have reported simulations of real combustion devices with LES.

Most of these use either structured or block-structured curvi-linear meshes, which cannot deal with very complex geometries. Simulations of gas turbines, for instance, typically require unstructured meshing strategies, for which the formulation of energy conserving and accurate numerical algorithms, of particular importance for combustion

LES, proves to be even more difficult. Among the few fully unstructured multiphysics LES codes are the AVBP code of CERFACS, which has been applied in many studies on combustion instabilities and flashback in premixed gas turbines Selle (2004), Sommerer (2004), and the Stanford CDP code¹ CDP solves both low-Ma number variable-density and fully compressible LES equations using the unstructured collocated finite volume discretization of Mahesh (2004) and its subsequent improvements by Ham (2004).

It applies Lagrangian particle tracking with adequate models for breakup, particle drag, and evaporation for liquid fuel sprays.

Closure for subfilter transport terms and other turbulence statistics is accomplished using dynamic models.

The FPV combustion model is applied to model turbulence/chemistry interactions.

The code is parallelized with advanced load balancing procedures for both gas and particle phases.

Computations have been conducted with over two billion cells using several thousand processors.

A state-of-the-art simulation of a section of a modern Pratt & Whitney gas turbine combustor that uses all these capabilities has been performed Mahesh (2005), Apte (2005).

The figure shows the spray and temperature distribution and demonstrates the complexity of the geometry and the associated flow physics.

