

# 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
    - Depends on small-scale mixing
  - 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 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 inter-diffusion
- 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 **how chemical and turbulent scales interact**

## 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**
  - For example, distribution function of a single variable of the velocity component  $u$
- 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  $u$ 
  - 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

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

- 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 **probability one**

- This 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

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

- Semicolon indicates that  $P_u$  is probability density in  $U$ -space and a function of  $\mathbf{x}$  and  $t$
- In the following we will, for simplicity of notation, not distinguish between random stochastic variable  $u$  and sample space variable  $U$ , drop the index and write the *pdf* as

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

- 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

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



- Reynolds decomposition

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

divides random variable in **deterministic mean** (overline) and **random fluctuation** (prime)

- For flows with large density changes as they occur in combustion, it is 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  $\rho$  (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  $\rho$  and averaging

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

- Favre averaging considerably simplifies the equations for the averaged quantities
- For instance, the average of the product of the density  $\rho$  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

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

- When averaging, only the first two terms remain

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

- 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](#)

- Even though it certainly is the best compromise for engineering design using RANS, the predictive power of the  $k$ - $\varepsilon$  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 
$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p - \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g}$$

- Using Favre averaging, one obtains

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

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

- This equation is similar to

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

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

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

which is called the **Reynolds stress tensor**

- An important simplification is obtained by introducing the so called **eddy viscosity**  $\nu_t$  in a model for the Reynolds stress tensor

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

where  $\mathbf{I}$  is the unit tensor

- This model for the Reynolds stress tensor then has the same form as the molecular stress
- The kinematic eddy viscosity is related to the **Favre average turbulent kinetic energy**

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

and its dissipation by  $\nu_t = c_\mu \frac{\tilde{k}^2}{\tilde{\epsilon}}$ ,  $c_\mu = 0.09$

- 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 kinetic energy dissipation rate

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

- 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  $k$ - $\varepsilon$  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)

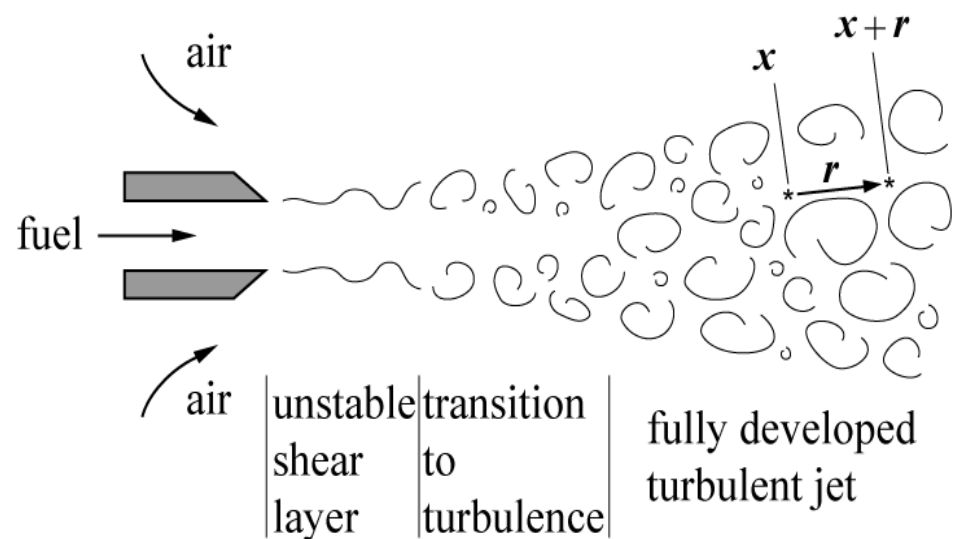
## Two-Point Velocity Correlations and Turbulent Scales

- 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

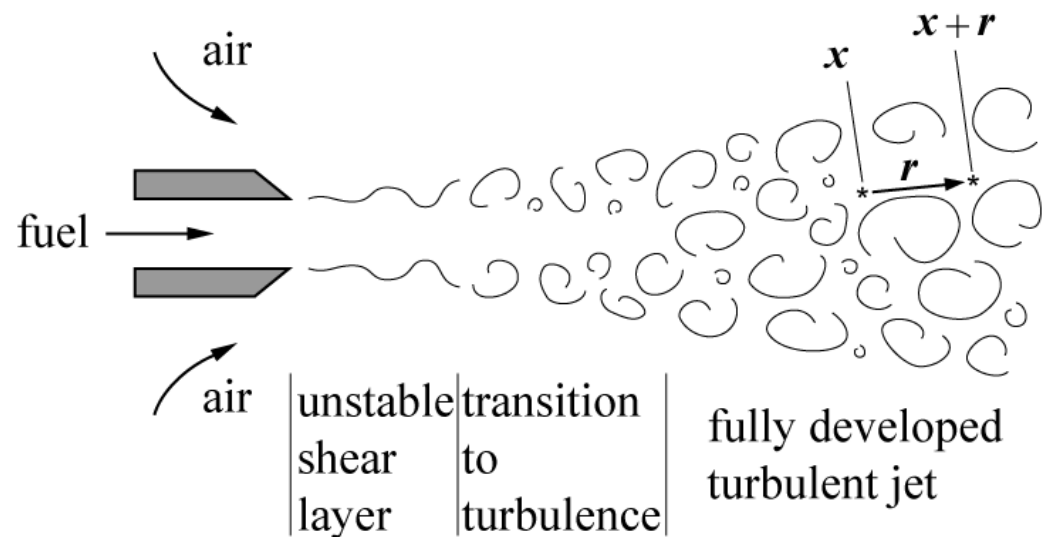
shear layer instability which after

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

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

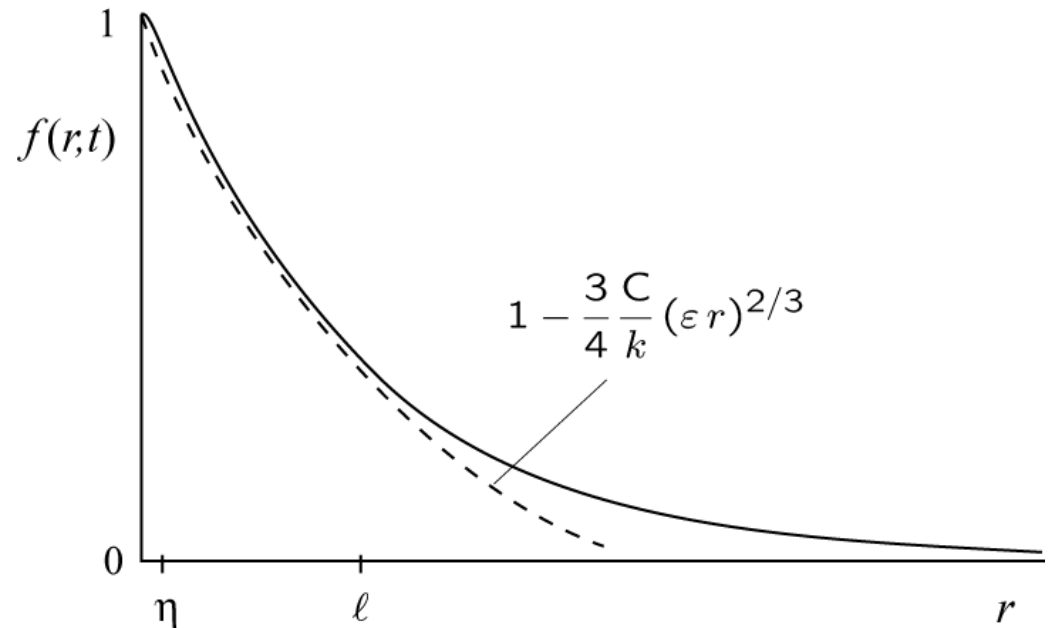


- For **homogeneous isotropic turbulence**, the location  $\mathbf{x}$  is arbitrary and  $r$  may be replaced by its absolute value  $r=|\mathbf{r}|$ .

- 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**

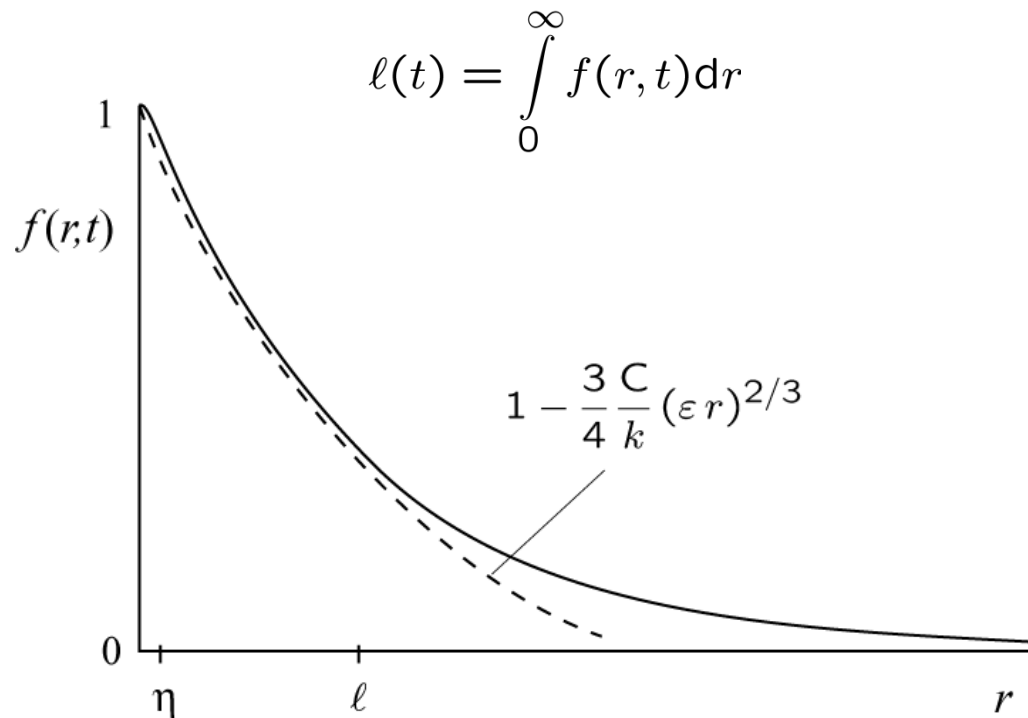
- Energy transfer rate is independent of the size of the eddies within the so called inertial range and equal to the dissipation rate
- Then, the dissipation  $\varepsilon$  is the only dimensional quantity apart from the correlation co-ordinate  $r$  that is available for the scaling of  $f(r,t)$
- Since  $\varepsilon$  has the dimension  $\text{m}^2/\text{s}^3$ , this leads to

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

where  $C$  is a universal constant called the [Kolmogorov constant](#)

## Turbulent Time, Length, and Velocity Scales

- Large scale eddies contain most of the kinetic energy
- These eddies still have 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



- 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

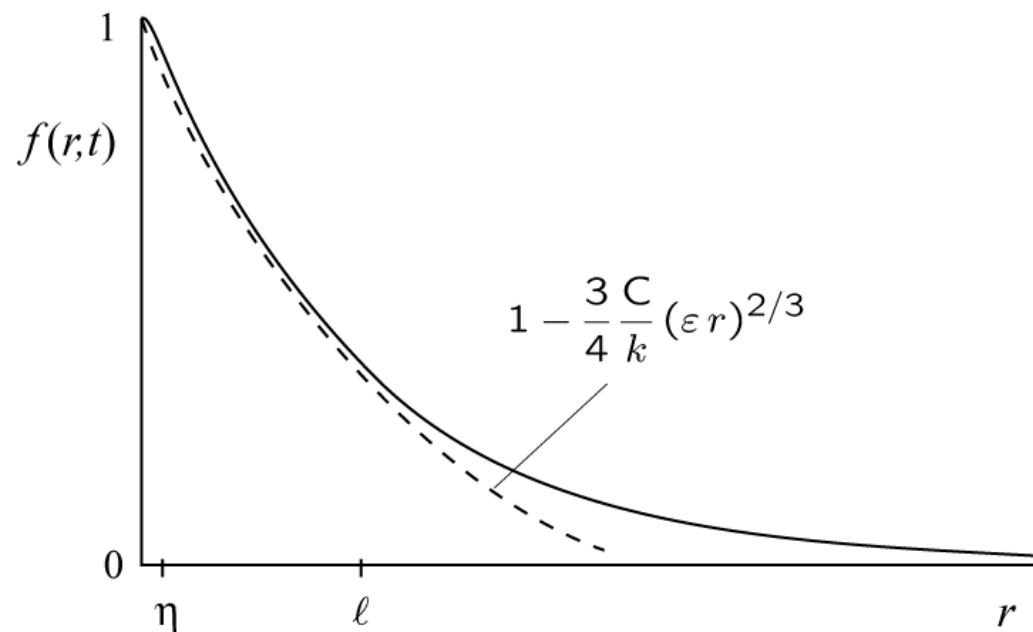
$$l/v'$$

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

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

- The motion of very small eddies is influenced by **viscosity** which provides an additional dimensional quantity for scaling

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





- In addition to  $\eta$ , 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  $\varepsilon$  directly to the turnover velocity and the length scale of the integral scale eddies

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

## Kolmogorov Scaling

- We now define a discrete sequence of eddies within the inertial sub-range by

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

- Since  $\varepsilon$  is constant within the **inertial sub-range**, dimensional analysis relates the turnover time and the velocity difference across the eddy size to  $\varepsilon$  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

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

## Energy Spectrum and $k^{-5/3}$ Law

- A Fourier transform of the **isotropic two-point correlation function** leads to 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  $v_n^2 \sim (\varepsilon \ell_n)^{2/3} = \varepsilon^{2/3} k^{-2/3}$

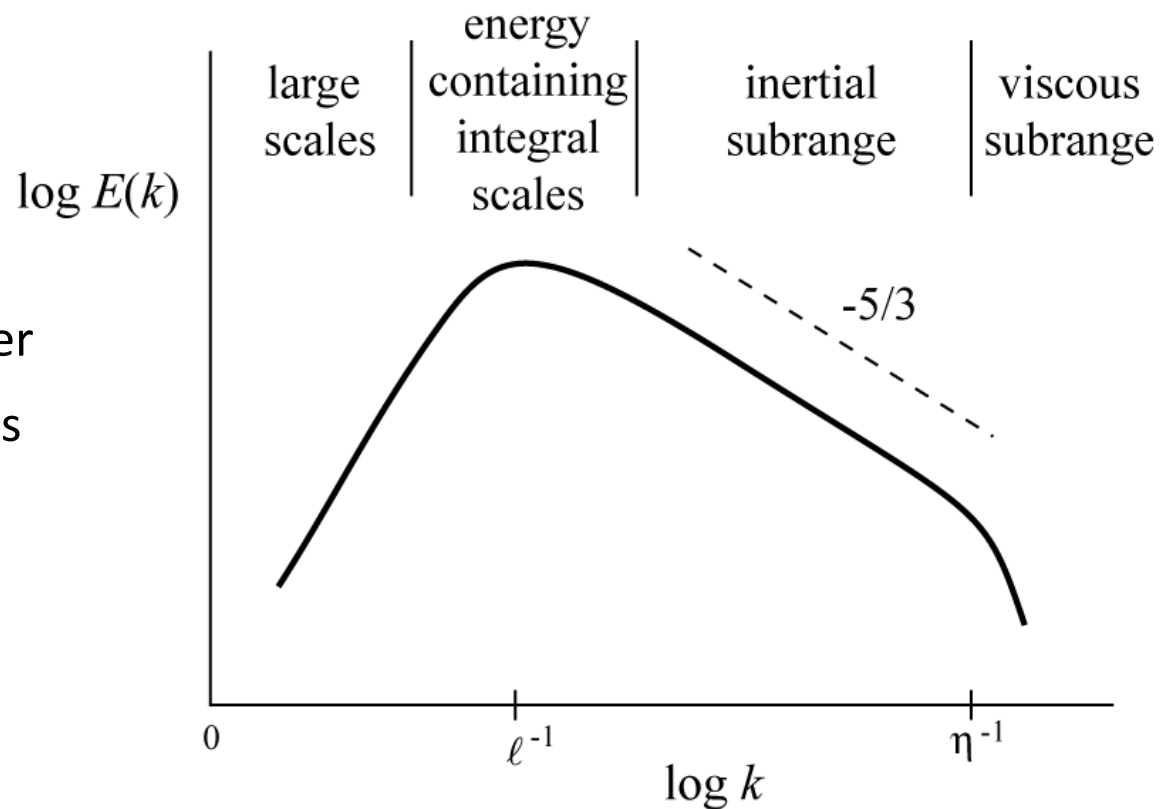
and its density in wave number space is proportional to

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

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

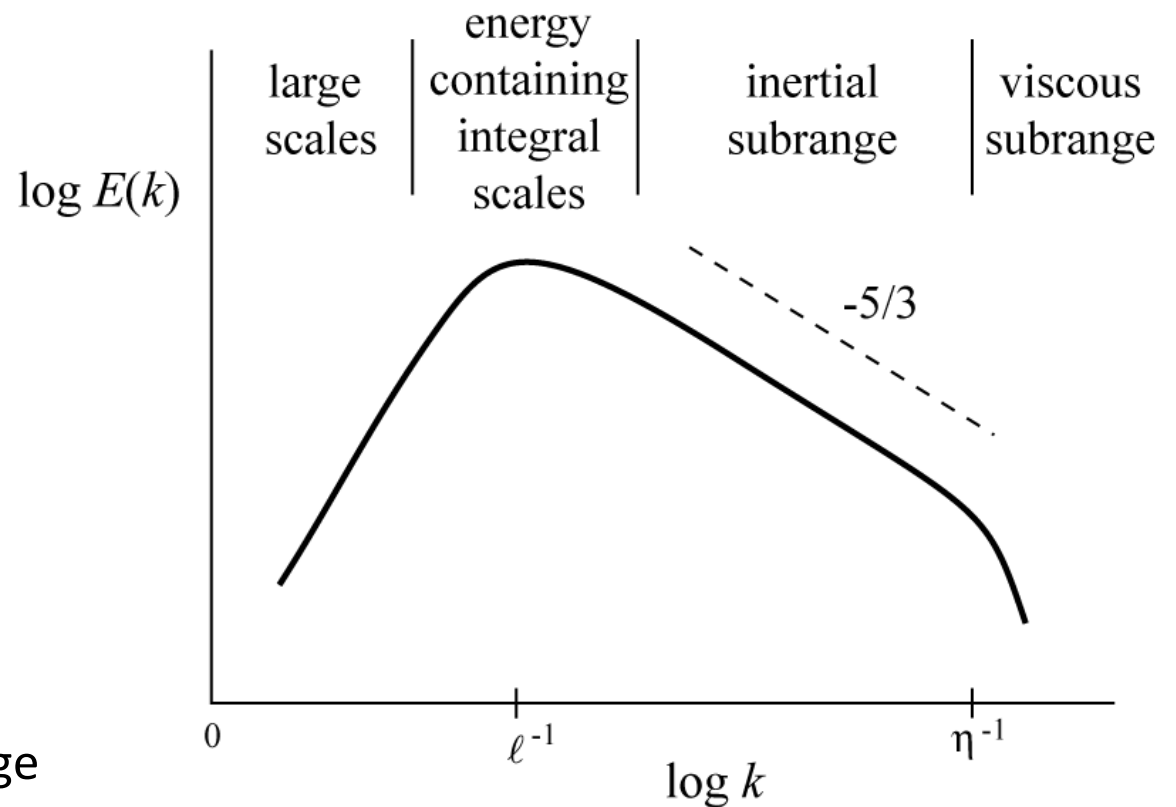
## Energy Spectrum

- 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
- $k^{-5/3}$  law in the inertial sub-range
- Cut-off due to viscous effects at the Kolmogorov scale  $\eta$ .
- Beyond this cut-off, in the range called the **viscous subrange**, the energy per unit wave number decreases exponentially due to viscous effects



## 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

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

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

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

- The balance equation for the reactive scalar  $\psi_i$  will be written

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

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,  $\sigma_i$  ( $i=1,2,\dots,k$ ) are the species source terms  $\dot{m}_i$ ,  $i = 1, 2, \dots, k$  and  $\sigma_{k+1}$  is  $\omega_T$ .
- The chemical source term will also be written as  $\sigma_i = \rho S_i$

## Moment Methods for Reactive Scalars

- Favre averaged equations for the mean of the reactive scalars can be derived as

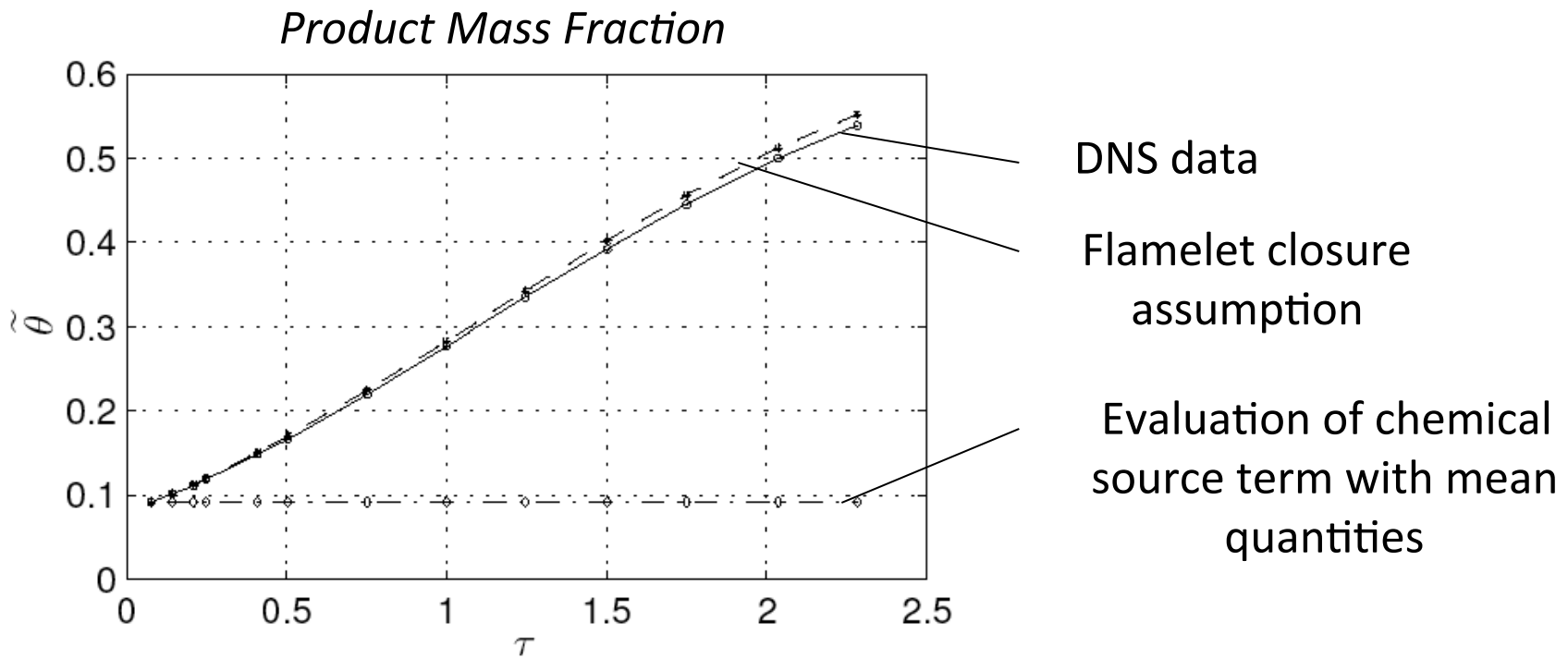
$$\bar{\rho} \frac{\partial \tilde{\psi}_i}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{\psi}_i = \nabla \cdot \overline{(\rho D_i \nabla \psi_i)} - \nabla \cdot (\bar{\rho} \tilde{\mathbf{v}}'' \tilde{\psi}_i'') + \bar{\rho} \tilde{S}_i$$

- In high Reynolds number flows the molecular transport term containing the molecular diffusivities  $D_i$  are small and can be neglected
- Two last terms on RHS need modeling



- Test of simple model for non-premixed combustion in isotropic turbulence

- Mean transport for reactive scalars in decaying isotropic turbulence  $\frac{\partial \tilde{\psi}_i}{\partial t} = \tilde{S}_i$



- Neglecting appropriate closure leads to leading order error!

## 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

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

- 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 the **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 the instantaneous equation

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

which leads to

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

- If derivatives of  $\rho$  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  $Z''^2$ .
- Using the continuity equation and averaging one obtains

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

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

- As before, the terms on the LHS describe the local change and convection
- The first term on the RHS is the turbulent transport term
- The second term on the RHS accounts for the production of scalars fluctuations
- The mean molecular transport term has been neglected, 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 scale  $\tau = \widetilde{k}/\widetilde{\varepsilon} = c_\chi \tau_Z$
- The constant of proportionality  $c_\chi$  is of order unity but varies

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

- $c_\chi = 2.0$  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
- 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  $C_{\text{EBU}}$  is the Eddy-Break-Up constant

- Problems for lean and rich regions in non-premixed combustion
- This model has been modified by Magnussen and Hjertager (1977) who replaced  $\overline{Y_P''^2}$  by the mean mass fraction of the deficient species (fuel for lean or oxygen for rich mixtures), which is then called 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

$$\bar{\omega}_{O_2} = \bar{\rho} \frac{A \bar{Y}_{O_2} \varepsilon}{\nu k}$$

and with the product mass fraction

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

in order to calculate the mean chemical source term

- $A$  and  $B$  are modeling constants and  $\nu$  is the stoichiometric oxygen to fuel mass ratio defined by

$$\frac{Y_{O_2,u}}{Y_{F,u}} \Big|_{st} = \frac{\nu'_{O_2} W_{O_2}}{\nu'_F W_F} = \nu$$

- 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  $C_{\text{EBU}}$  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, in principle, independent of the combustion regime
- A joint pdf transport equation for the velocity and the reactive scalars can be derived, 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  $\boldsymbol{\psi}$ ,

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

is the probability of finding at point  $\boldsymbol{x}$  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

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

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

- The symbol  $\nabla_v$  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  $\psi$ .
- 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
- 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 a 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

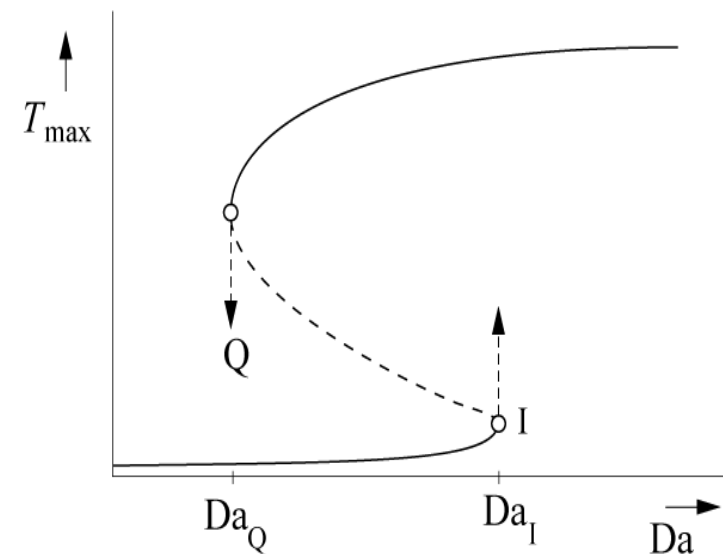
- From a numerical point of view, the most apparent property of the pdf transport equation is its high dimensionality
- Finite-volume and finite-difference techniques are not very attractive for this type of problem, as memory requirements increase roughly exponentially with dimensionality
- Therefore, 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 so called notional particles
- In the Lagrangian algorithm (Pope, 1985), the particles are not bound to grid nodes, but each particle has its own position and moves through the computational domain with its own velocity
- 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 small eddies of a certain size 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 non-premixed combustion, the mixture fraction  $Z$  is that scalar quantity, for premixed combustion the level set scalar  $G$  was introduced
- Once equations describing the statistical distributions of  $Z$  and  $G$  are solved, 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 later

## 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 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](#) (Bray & Moss, 1977) by assuming the pdf of the progress variable  $c$  to be a double delta function distribution
- This assumption only allows for states at  $c = 0$  and  $c = 1$  in a turbulent premixed flame, but is able to illustrate important features, such as 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

- A model for the chemical source term by Bray and Libby (1994) 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  $\Sigma$  is the flame surface density (flame surface per unit volume)

- A model for  $\Sigma$  has been proposed by Candel et al. (1990), which is called [Coherent Flame Model \(CFM\)](#)

- Modeling based on DNS data has led Trouve and Poinsot (1994) to the following equation for the flame surface density  $\Sigma$ :

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

- 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
- Multiplying this equation with  $s_L$  leads to an equation for  $s_L \Sigma$ , which is independent of  $s_L$
- Then also  $\bar{\omega}_c = \rho_u s_L I_0 \Sigma$  in this model is independent of  $s_L$

## Combustion Models used in Large Eddy 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)**

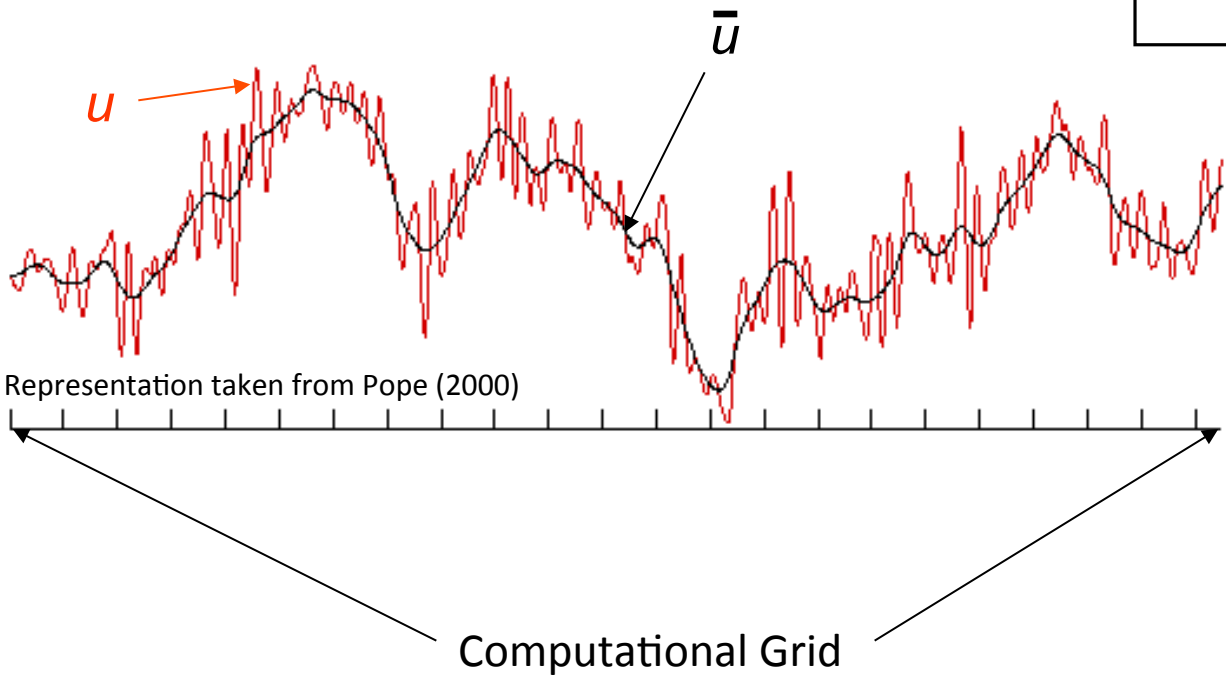
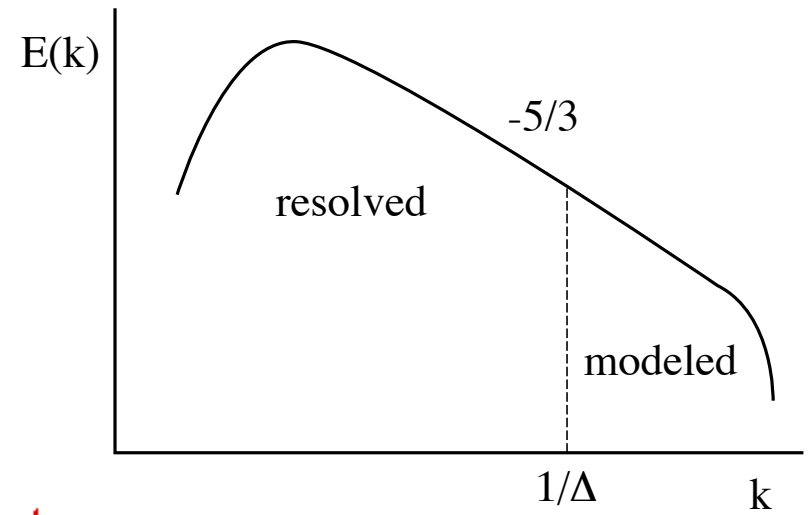


- Large Eddy Simulation does not intend to numerically resolve all turbulent length scales, but only a fraction of the larger energy containing scales within the inertial subrange
- Modeling is then applied to represent the smaller unresolved scales, which contain only a small fraction of the turbulent 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

# Concept of LES

- Spatial filtering rather than ensemble average

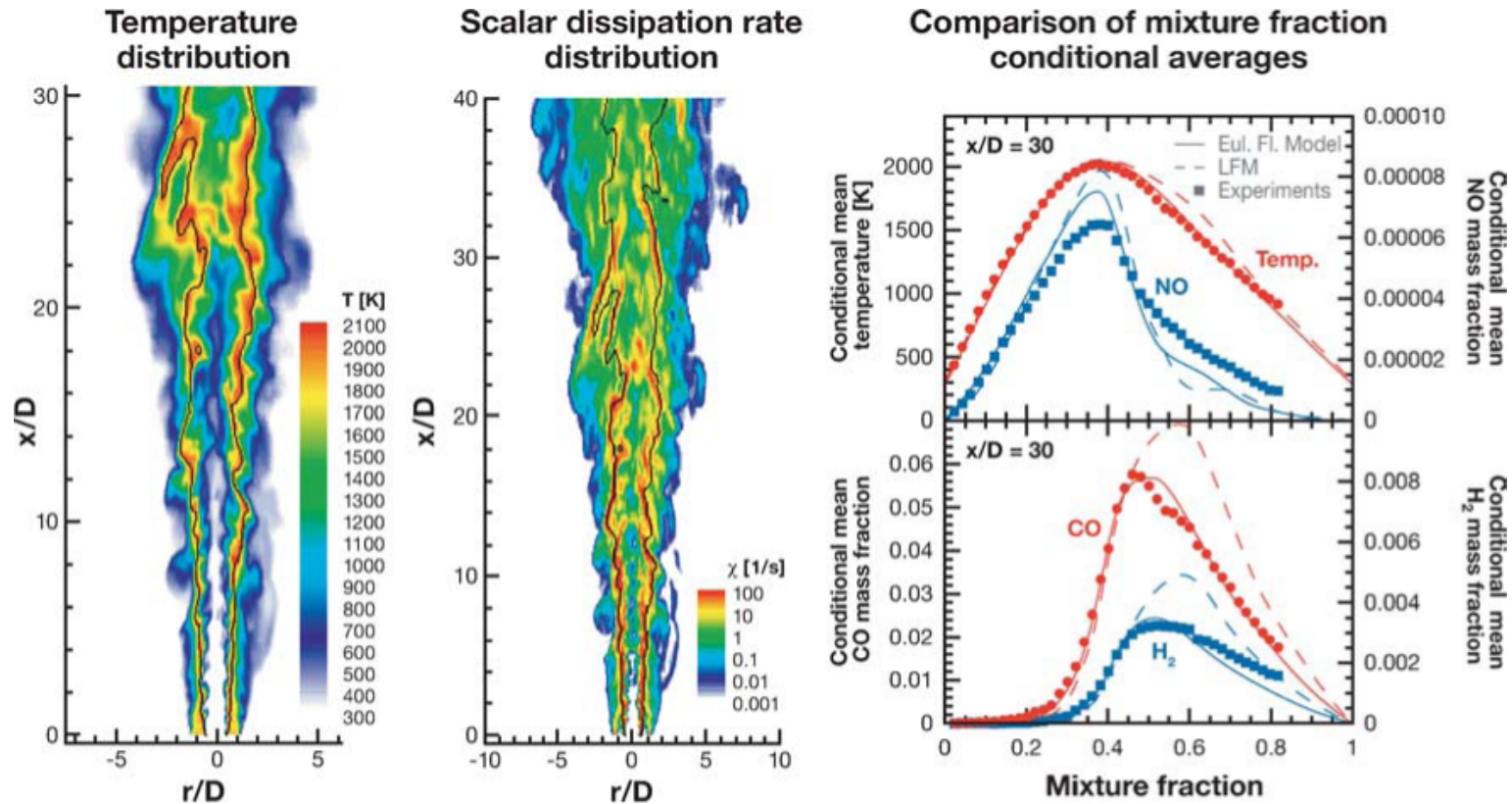
$$\bar{u} = \int G(x, x') u(x') dx'$$



- The model for the smaller scales is called the **sub-filter** or **subgrid model**
- In deriving the basic LES equations, the Navier-Stokes equations are spatially filtered with a filter of size  $\Delta$ , 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 (Pitsch, 2006)

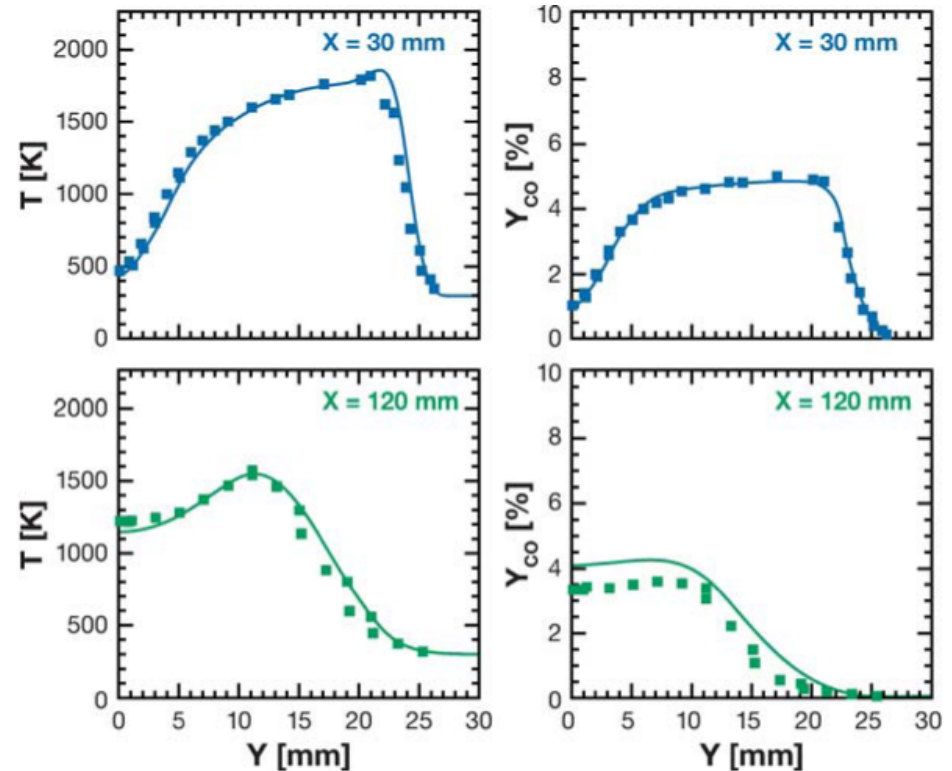
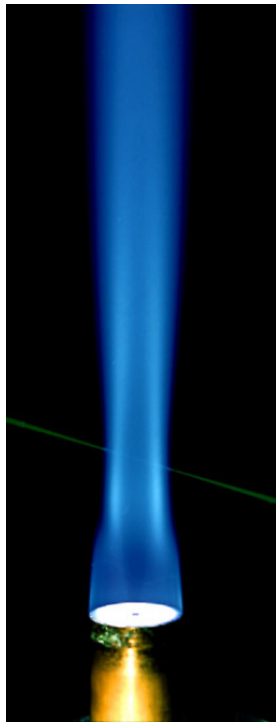
- For example, to study the importance of turbulent scalar dissipation rate fluctuations on the combustion process and to highlight the differences between RANS and LES, Pitsch (2002), compared the results of two different LES simulations using unsteady flamelet models in which the scalar dissipation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



- 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 H<sub>2</sub> at  $x/D = 30$

- 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, e.g. by Kim (2002) or Muradoglu (2003)
- Similar arguments can be made for premixed turbulent combustion LES

- 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





- 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

## 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 non-premixed 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 sub-filter scalar variance

- In RANS models, typically a transport equation is solved for the scalar variance, in which the Reynolds-averaged scalar dissipation rate  $\chi$  appears as an unclosed sink term that requires modeling
- The additional assumption of a constant ratio of the integral timescale of the velocity  $\tau_t$  and the scalar fields leads to the expression

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

where  $c_\phi$  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 sub-filter 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 sub-filter scalar flux in the production term

- The eddy diffusivity is

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

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 sub-filter scales and combining this with  $\tilde{\chi} = 2D_t(\nabla \tilde{Z})^2$  then leads to the model for the scalar variance

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

- 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  $c_\phi$  can be determined as

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

## LES of real Combustion Devices

- Several investigators have reported simulations of real combustion devices with LES
- Many 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 code
- 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 Flamelet/Progress Variable 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), Mueller (2012)

## LES of Pratt & Whitney Aircraft Engine

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

