

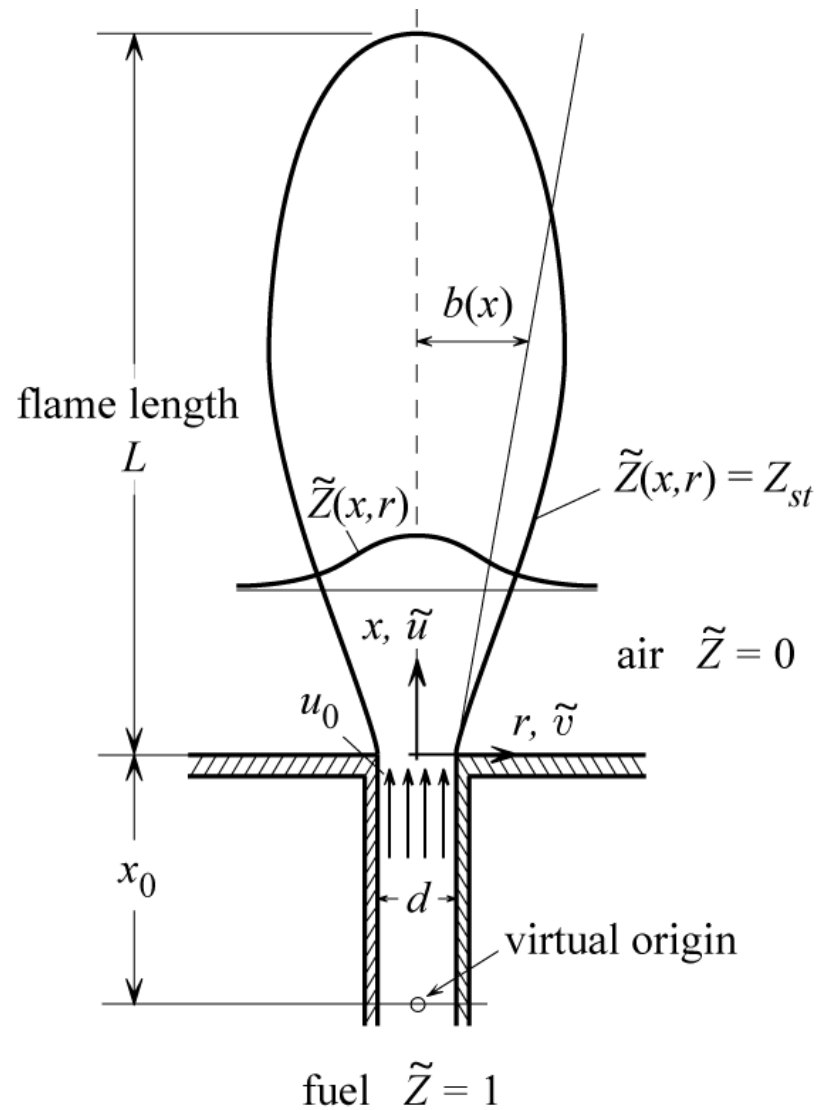
# Lecture 14

## Nonpremixed Turbulent Combustion: The Flamelet Concept

## The Round Turbulent Jet Diffusion Flame

- In many applications fuel enters into the combustion chamber as a turbulent jet, with or without swirl.
- To provide an understanding of the basic properties of jet diffusion flames, we will consider here the easiest case, the **axisymmetric jet flame without buoyancy**, for which we can obtain approximate analytical solutions
- This will enable us to determine, for instance, the flame length (Peters & Donnerhack, 1981)
- The flame length is defined as the distance from the nozzle to the point on the centerline of the flame where the mean mixture fraction is equal to  $Z_{st}$

- The flow configuration for the round turbulent jet flame



- Using Favre averaging and the **boundary layer assumption**, we obtain a system of two-dimensional axisymmetric equations, where molecular transport is neglected and a turbulent Schmidt number is introduced

- Continuity 
$$\frac{\partial}{\partial x} (\bar{\rho} \tilde{u} r) + \frac{\partial}{\partial r} (\bar{\rho} \tilde{v} r) = 0$$

- Momentum in x-direction 
$$\bar{\rho} \tilde{u} r \frac{\partial \tilde{u}}{\partial x} + \bar{\rho} \tilde{v} r \frac{\partial \tilde{u}}{\partial r} = \frac{\partial}{\partial r} \left( \bar{\rho} \nu_{tr} \frac{\partial \tilde{u}}{\partial r} \right)$$

- Mean mixture fraction 
$$\bar{\rho} \tilde{u} r \frac{\partial \tilde{Z}}{\partial x} + \bar{\rho} \tilde{v} r \frac{\partial \tilde{Z}}{\partial r} = \frac{\partial}{\partial r} \left( \frac{\bar{\rho} \nu_{tr}}{Sc_t} \frac{\partial \tilde{Z}}{\partial r} \right)$$

- System of equations very similar to that for laminar flames
- Scaling arguments predict eddy viscosity to be constant in turbulent round jet
- Model according to Effelsberg & Peters (1981)  $\nu_{tr} = \frac{u_0 d}{70}$

- Special case of round jet in quiescent air
  - Use results of laminar round jet
  - Formally same results for differently defined coordinates and parameters
- Similarity coordinate

$$\begin{array}{ccc}
 \text{Laminar} & & \text{Turbulent} \\
 \eta = \frac{\sqrt{2 \int_0^r \frac{\rho}{\rho_\infty} r dr}}{z + a} & \longrightarrow & \eta = \frac{\sqrt{2 \int_0^r \frac{\bar{\rho}}{\rho_\infty} r dr}}{z + a}
 \end{array}$$

- Chapman-Rubesin-Parameter

$$\begin{array}{ccc}
 \text{Laminar} & & \text{Turbulent} \\
 C = \frac{\rho \mu r^2}{2 \mu_\infty \int_0^r \rho r dr} & \longrightarrow & C = \frac{\bar{\rho}^2 \nu_t r^2}{2 \rho_\infty \nu_{t,ref} \int_0^r \bar{\rho} r dr}
 \end{array}$$

- For the solution then follows

$$\tilde{u}_z = \frac{2C\gamma^2\nu_{t,\text{ref}}}{\zeta \left(1 + (\gamma\eta)^2 / 4\right)^2}$$

where the jet spreading parameter is now

$$\gamma^2 = \frac{3}{64} \frac{\rho_0}{\rho_\infty} \frac{C^2}{\nu_{t,\text{ref}}} \left( \frac{u_{z,0}d}{\nu_{t,\text{ref}}} \right)^2 \quad \left( \text{laminar: } \gamma^2 = \frac{3}{64} \frac{\rho_0}{\rho_\infty} \frac{Re^2}{C^2} \right)$$

obtained from the requirement of integral momentum conservation along the axial direction

- The Favre-averaged velocity decays as for the laminar case as proportional to  $1/\zeta = 1/(z + a)$

- The mean mixture fraction is found to be

$$\tilde{Z} = \frac{\tilde{Z}_a}{\left(1 + (\gamma\eta)^2 / 4\right)^{2Sc_t}}$$

with the centerline value

$$\tilde{Z}_a = \frac{1 + 2Sc_t}{32} \frac{\rho_0}{\rho_\infty C} \left( \frac{u_{z,0} d}{\nu_{t,ref}} \right) \frac{d}{\zeta} \quad \left( \text{laminar: } Z_a = \frac{1 + 2Sc}{32} \frac{\rho_0}{\rho_\infty C} \frac{Re d}{\zeta} \right)$$

which again decays linearly with  $1/\zeta = 1/(z + a)$

- Similar centerline solution for laminar and turbulent case

- From this equation, the flame length  $L$  can be calculated by setting

$$\tilde{Z} = Z_{st} \quad \text{at} \quad x = L, r = 0$$

- We obtain

$$\frac{L + a}{d} = \frac{1 + 2Sc_t}{32Z_{st}} \left( \frac{u_{z,0}d}{\nu_{t,ref}} \right) \frac{\rho_0}{\rho_\infty C}$$

- Experimental data by Hawthorne et al. (1949) suggest that the flame length  $L$  should scale as

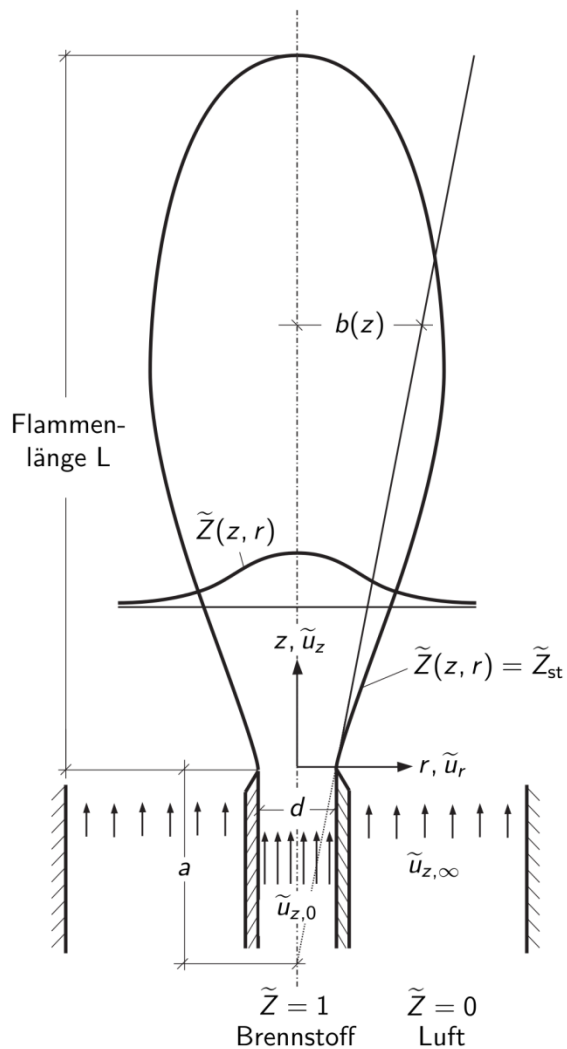
$$\frac{L + a}{d} = \frac{5,3}{Z_{st}} \sqrt{\frac{\rho_0}{\rho_\infty}}$$

- This fixes the turbulent Schmidt number as  $Sc_t=0.71$  and the Chapman-Rubesin parameter as

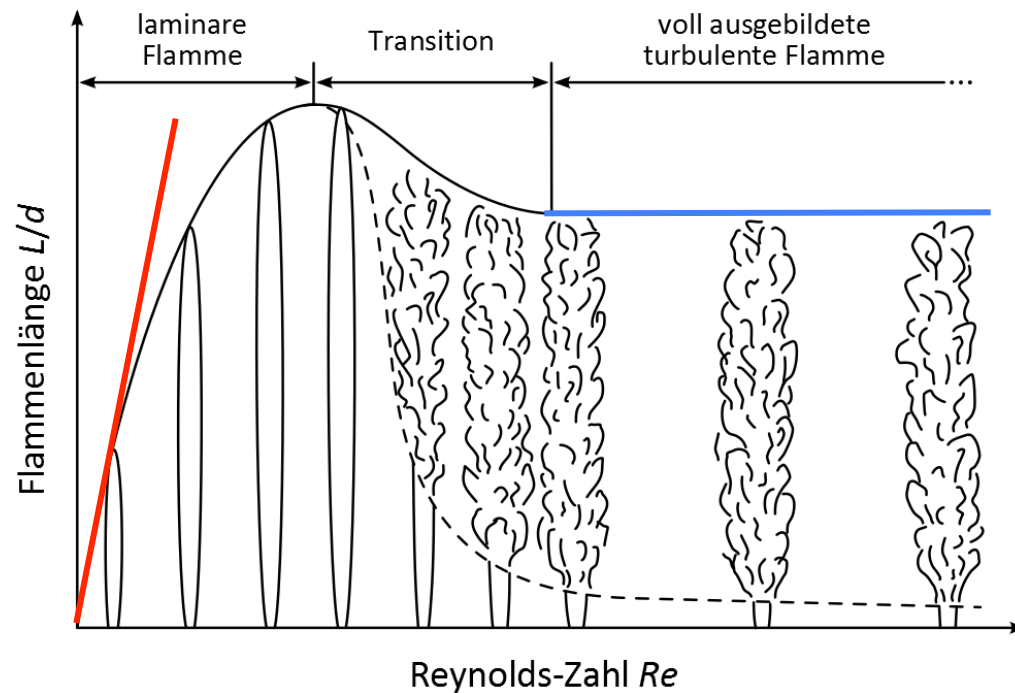
$$C = \frac{(\rho_0\rho_{st})^{1/2}}{\rho_\infty}$$



- Turbulente Freistrahldiffusionsflamme



$$\frac{L+a}{d} = \frac{1+2Sc}{32Z_{st}} \frac{\rho_0}{\rho_\infty C} \overset{\text{linear}}{\boxed{\frac{u_0 d}{\nu}}} \quad \frac{L+a}{d} = \frac{1+2Sc_t}{32Z_{st}} \frac{\rho_0}{\rho_\infty C} \overset{\text{konst.}}{\boxed{\frac{u_0 d}{\nu_{t,ref}}}} \approx 70$$



## Modeling Turbulent Non-Premixed Combustion

- Models in nonpremixed turbulent combustion are often based on the conserved scalar and the presumed shape pdf approach
- This requires the knowledge of the Favre mean mixture fraction and its variance at position  $\mathbf{x}$  and time  $t$
- Averaging of the mixture fraction equation and using the gradient transport assumption led to the equation for the Favre mean mixture fraction

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

- Molecular diffusion is much smaller than the turbulent diffusion, and has therefore been neglected

- In addition to the mean mixture fraction we have derived an equation for the Favre variance of the mixture fraction

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

where the gradient transport assumption

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

has again been used in the production term (second term of the RHS)

- For the turbulent flux of the mixture fraction variance, the gradient transport assumption

$$-\mathbf{v}'' \widetilde{Z''^2} = D_t \nabla \widetilde{Z''^2}$$

can also be used

- In

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

the mean scalar dissipation rate appears, which, as introduced in Lecture 10, will be modeled as

$$\tilde{\chi} = c_\chi \frac{\tilde{\epsilon}}{\bar{k}} \widetilde{Z''^2}$$

where the time scale ratio  $c_\chi$  is assumed to be a constant

- In the model

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

Janicka and Peters (1982) found that a value of  $c_{\chi}=2.0$  would predict the decay of scalar variance in an inert jet of methane very well

- Overholt and Pope (1996) and Juneja and Pope (1996) performing DNS studies of one and two passive scalar mixing find an increase of  $c_{\chi}$  with Reynolds number and steady state values around 2.0 and 3.0, respectively
- In the numerical simulations of Diesel engine combustion, to be presented in Lecture 15, a value of  $c_{\chi}=2.0$  has been used

- In many cases, as in turbulent jet diffusion flames in air, zero gradient boundary conditions, except at the inlet, can be imposed
- If the simplifying assumptions mentioned in Section 3.9 of Lecture 3 can be introduced, the enthalpy  $h$  can be related to the mixture fraction by the linear coupling relation

$$h = h_2 + Z(h_1 - h_2)$$

which also holds for the mean values

$$\tilde{h} = h_2 + \tilde{Z}(h_1 - h_2)$$

and where  $h_2$  is the enthalpy of air and  $h_1$  that of the fuel

- Then, no additional equation for the enthalpy is required

- A more general formulation is needed, if different boundary conditions have to be applied for the Favre mean mixture fraction and enthalpy or if heat loss due to radiation or unsteady pressure changes must be considered
- Then, an equation for the Favre mean enthalpy as an additional variable must be solved

- This equation can be obtained from the enthalpy equation

$$\rho \frac{Dh}{Dt} = \rho c_p \frac{DT}{Dt} + \sum_{i=1}^k (-\mathbf{div} \mathbf{j}_i + \dot{m}_i) h_i.$$

by averaging

$$\bar{\rho} \frac{\partial \tilde{h}}{\partial t} + \bar{\rho} \tilde{\mathbf{v}} \cdot \nabla \tilde{h} = \frac{\partial \bar{p}}{\partial t} + \nabla \cdot (\bar{\rho} D_t \nabla \tilde{h}) + \bar{q}_R$$

- Again a gradient transport model for the correlation  $-\tilde{\mathbf{v}}'' \tilde{h}''$  has been introduced



- The term describing temporal mean pressure changes  $\partial \bar{p} / \partial t$  has been retained, because it is important for modeling internal combustion engines operating under non-premixed conditions, such as Diesel engines
- The mean volumetric heat exchange term  $\overline{\dot{q}_R}$  must also be retained in many applications, where radiative heat transfer has an influence on the local enthalpy balance
- Changes of the mean enthalpy also occur due to convective heat transfer at the boundaries or due to the evaporation of a liquid fuel
- Temperature changes due to radiation within the flamelet structure also have a strong influence on the prediction of **NO<sub>x</sub> formation** (cf. Pitsch et al. ,1998)

## Presumed Shape Pdf Approach

- These model equations can be used to calculate the mean mixture fraction and the mixture fraction variance at each point of the turbulent flow field, provided that the density field is known
- In addition, of course, equations for momentum and the turbulent flow field must be solved

- In this approach, a suitable two-parameter probability density function is "presumed" in advance, thereby fixing the functional form of the pdf by relating the two parameters in terms of the known values of the mean mixture fraction and its variance at each point of the flow field
- Since in a two-feed system the mixture fraction  $Z$  varies between  $Z = 0$  and  $Z = 1$ , the [beta function pdf](#) is widely used for the Favre pdf in non-premixed turbulent combustion

- The [beta-function pdf](#) has the form

$$\tilde{P}(Z; \boldsymbol{x}, t) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1} \Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

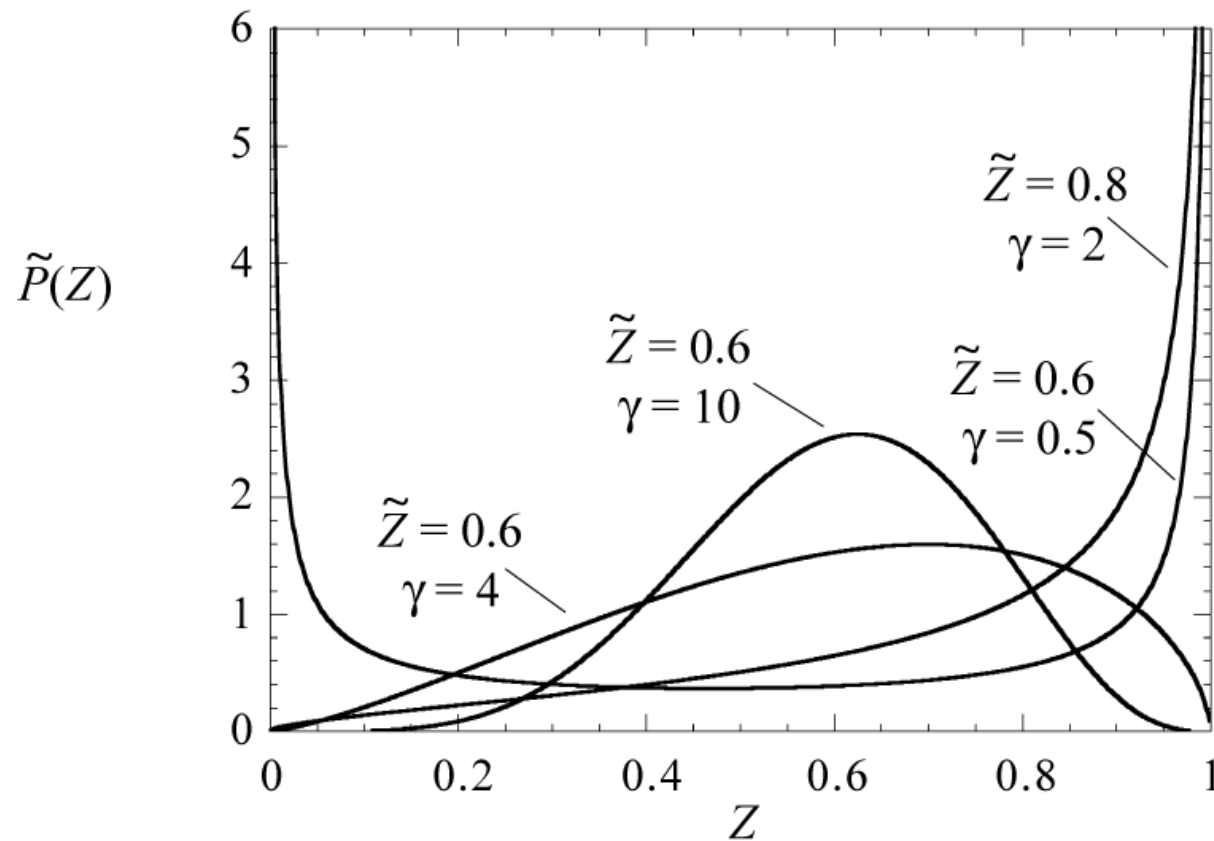
- Here  $\Gamma$  is the [gamma function](#)
- The two parameters  $\alpha$  and  $\beta$  are related to the Favre mean mixture fraction and its variance by

$$\alpha = \tilde{Z}\gamma, \quad \beta = (1 - \tilde{Z})\gamma$$

where

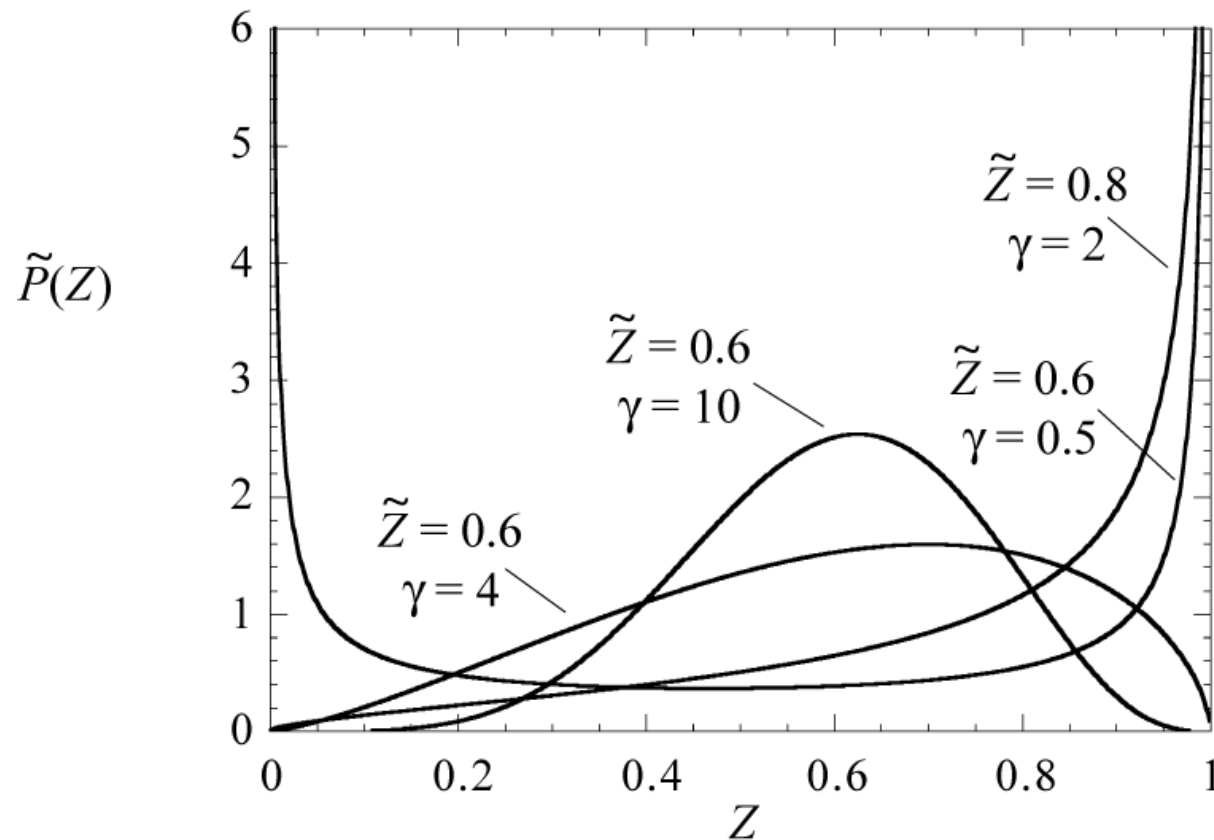
$$\gamma = \frac{\tilde{Z}(1 - \tilde{Z})}{\widetilde{Z'^2}} - 1 \geq 0$$

- The beta-function plotted for different combinations of its parameters



- It can be shown that in the limit of very small  $\tilde{Z}^{1/2}$  (large  $\gamma$ ) the beta-function approaches a [Gaussian distribution](#)

- For  $\alpha < 1$  it develops a singularity at  $Z = 0$  and for  $\beta < 1$  a singularity at  $Z = 1$



- Despite of its surprising flexibility, it is unable to describe distributions with a singularity at  $Z = 0$  or  $Z = 1$  and an additional intermediate maximum in the range  $0 < Z < 1$

- Using the presumed shape pdf approach, the moments of quantities that depend only on mixture fraction can be calculated
- For instance, the mean value of  $\psi_i$  can be obtained from

$$\tilde{\psi}_i(\mathbf{x}, t) = \int_0^1 \psi_i(Z) \tilde{P}(Z; \mathbf{x}, t) dZ$$

- A further quantity of interest is the mean density
- Since Favre averages are considered, one must take the Favre average of  $\rho^{-1}$ , which leads to

$$\widetilde{\rho^{-1}} = \frac{1}{\bar{\rho}} = \int_0^1 \rho^{-1}(Z) \tilde{P}(Z) dZ.$$

- With

$$\tilde{P}(Z; \mathbf{x}, t) = \frac{Z^{\alpha-1}(1-Z)^{\beta-1} \Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)}, \quad \alpha = \tilde{Z}\gamma, \quad \beta = (1-\tilde{Z})\gamma$$

$$\gamma = \frac{\tilde{Z}(1-\tilde{Z})}{\tilde{Z}''^2} - 1 \geq 0$$

and the [Burke-Schumann solution](#) the [Conserved Scalar Fast-Chemistry Model](#) for non-premixed combustion is formulated

- It is based on a closed set of equations, which do not require any further chemical input other than the assumption of [infinitely fast irreversible chemistry](#)



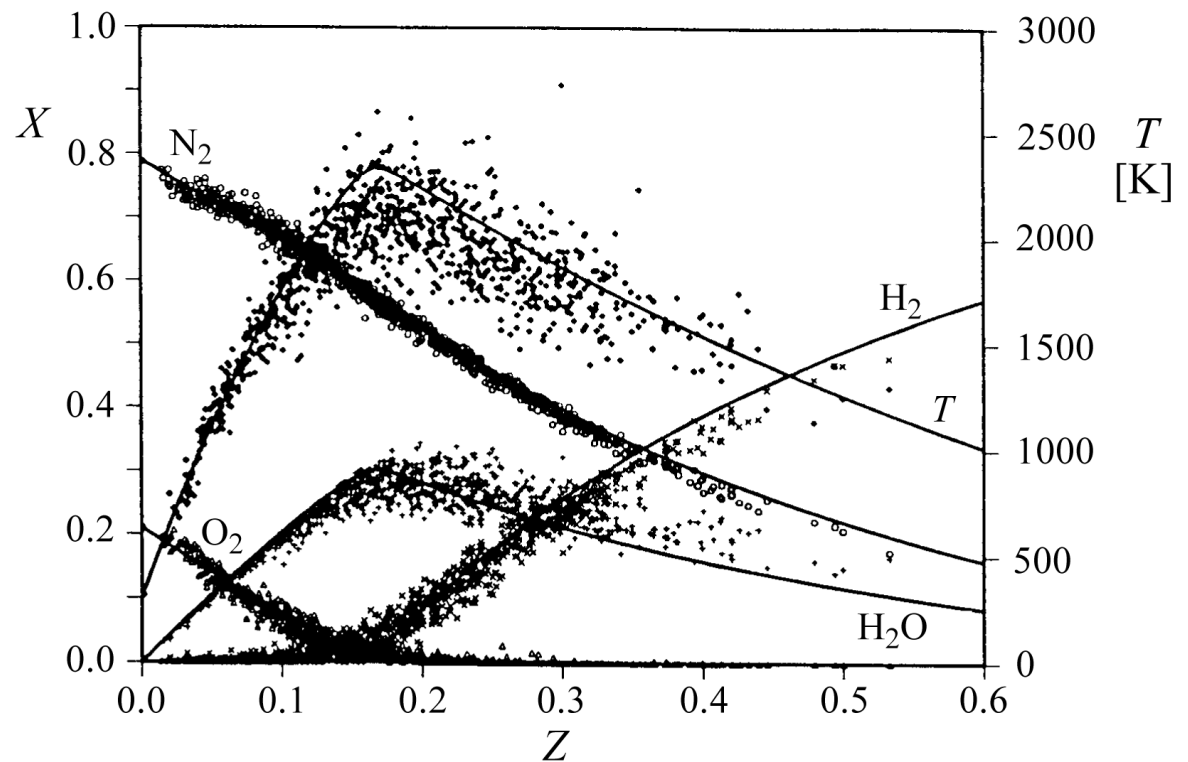
## Experimental Data from Turbulent Jet Diffusion Flames

- There is a large body of experimental data on single point measurements using Laser Rayleigh and Raman scattering techniques combined with Laser-Induced Fluorescence (LIF)
- Since a comprehensive review on the subject by Masri et al. (1996) is available, here only the example of the results by Barlow et al. (1990) obtained by the combined Raman-Rayleigh-LIF technique will be shown
- The fuel stream of the two flames that were investigated consisted of a mixture of 78 mole % H<sub>2</sub> and 22 mole % argon, the nozzle inner diameter  $d$  was 5.2 mm and the co-flow air velocity was 9.2 m/s
- The resulting flame length was approximately  $L = 60 d$

- Two cases of exit velocities were analyzed, but only the case B with  $u_0 = 150$  m/s will be considered here
- The stable species  $H_2$ ,  $O_2$ ,  $N_2$ , and  $H_2O$  were measured using Raman-scattering at a single point with light from a flash-lamp pumped dye laser
- In addition, quantitative OH radical concentrations from LIF measurements were obtained by using the instantaneous one-point Raman data to calculate quenching corrections for each laser shot
- The temperature was calculated for each laser shot by adding number densities of the major species and using the perfect gas law

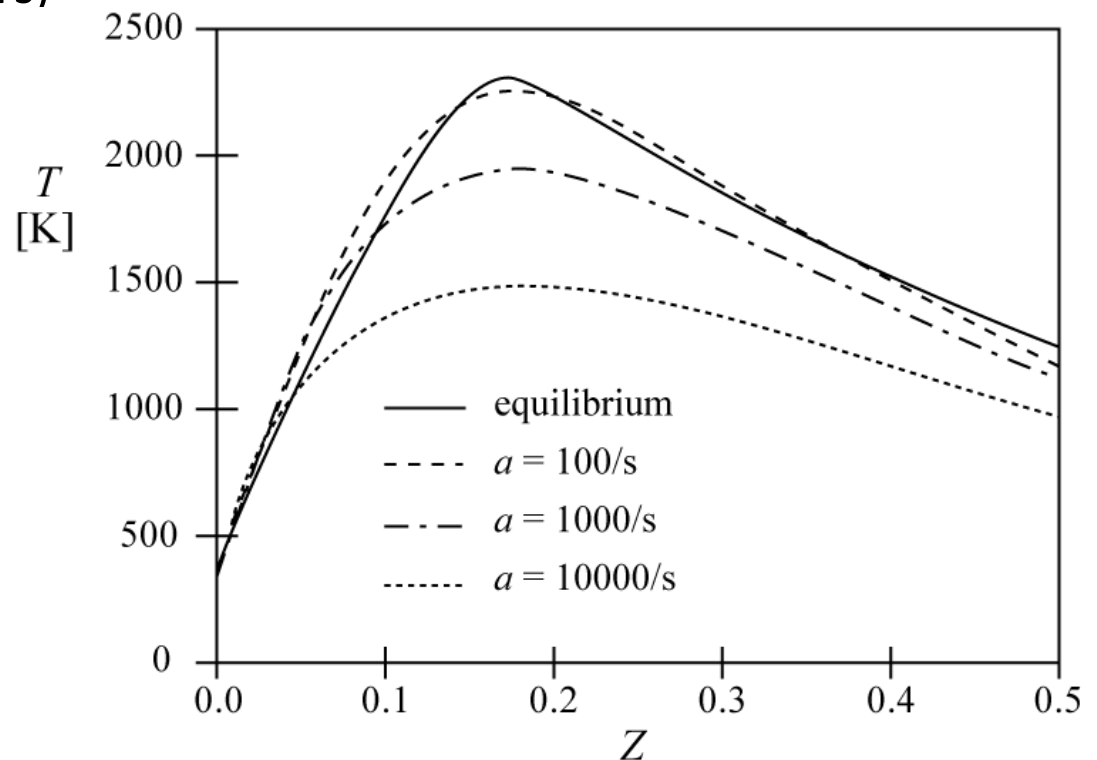
- An ensemble of one-point, one-time Raman-scattering measurements of major species and temperature plotted over mixture fraction are shown in the figure

- They were taken at  $x/d = 30$ ,  $r/d = 2$  in the case B flame
- Also shown are calculations based on the assumption of chemical equilibrium

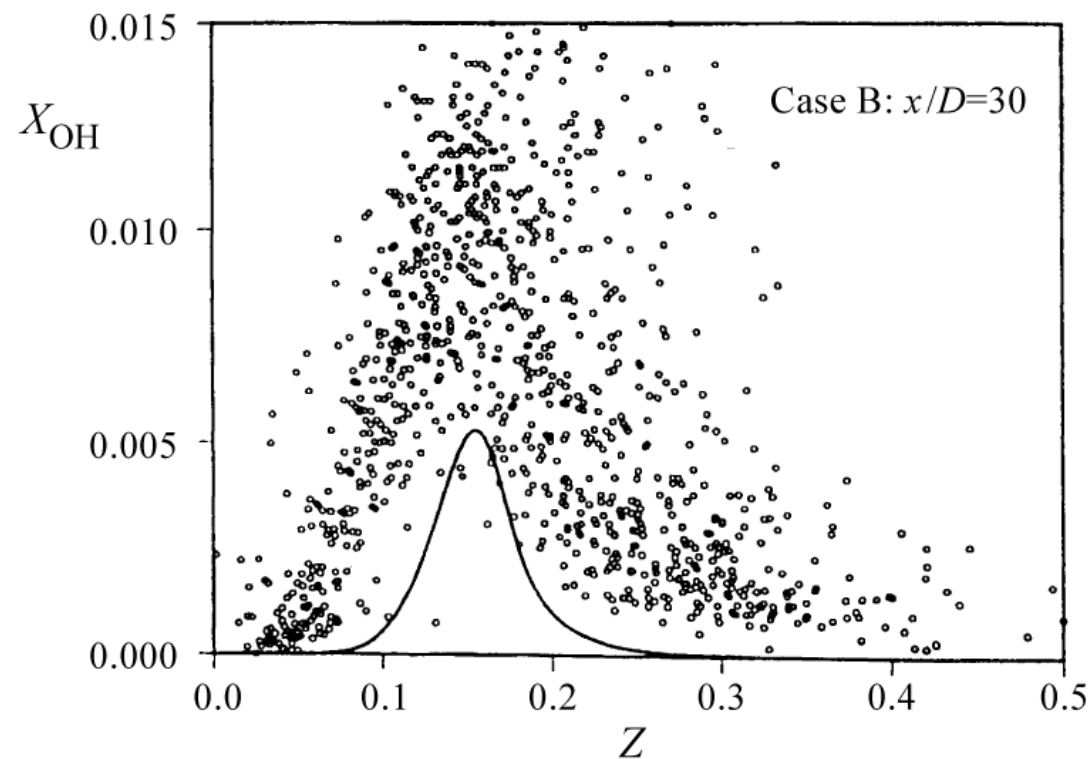


## Temperature profiles versus mixture fraction calculated for counterflow diffusion flames at different strain rates

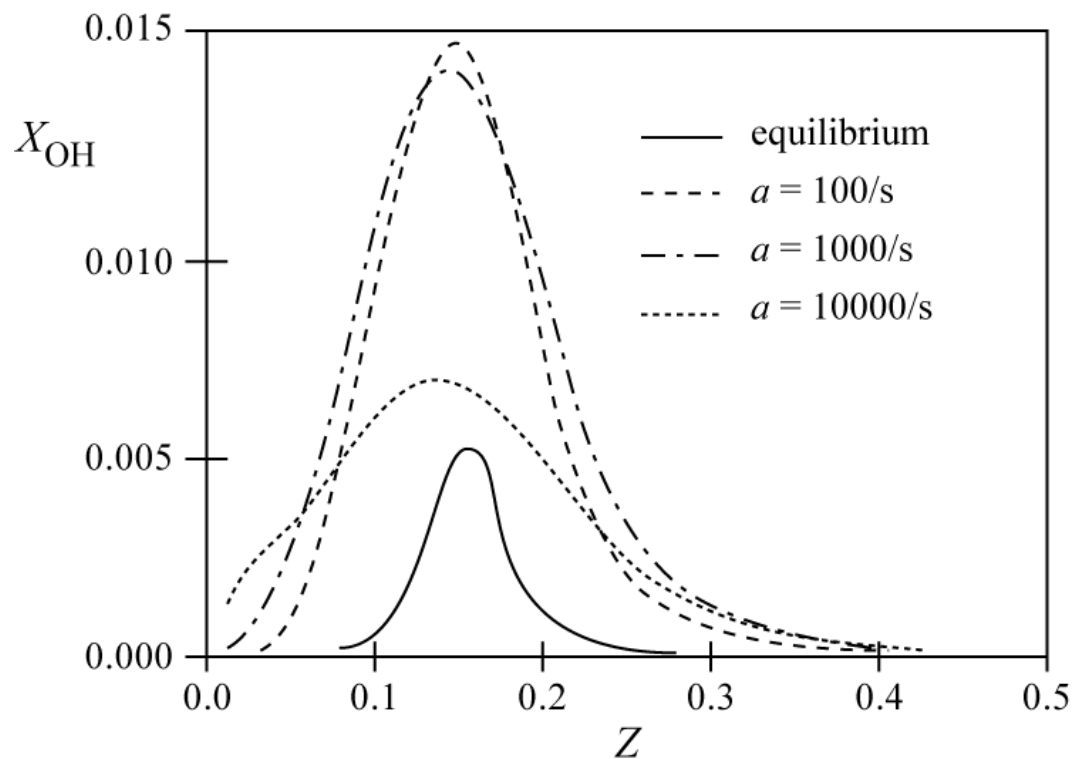
- These steady state flamelet profiles display the characteristic decrease of the maximum temperature with increasing strain rates (which corresponds to decreasing Damköhler numbers) as shown schematically by the upper branch of the S-shaped curve
- The strain rates vary here between  $a = 100/s$  which is close to chemical equilibrium and  $a = 10000/s$



- Data of OH-concentrations compared to equilibrium
- It is evident that the local OH-concentrations exceed those of the equilibrium profile by a factor up to 3



- The flamelet calculations show an increase of the maximum values by a factor of 3 already at the low strain rates  $a = 100/s$  and  $a = 1000/s$
- The maximum value of  $a = 10000/s$  is close to extinction and does not represent conditions in the turbulent hydrogen flame considered here

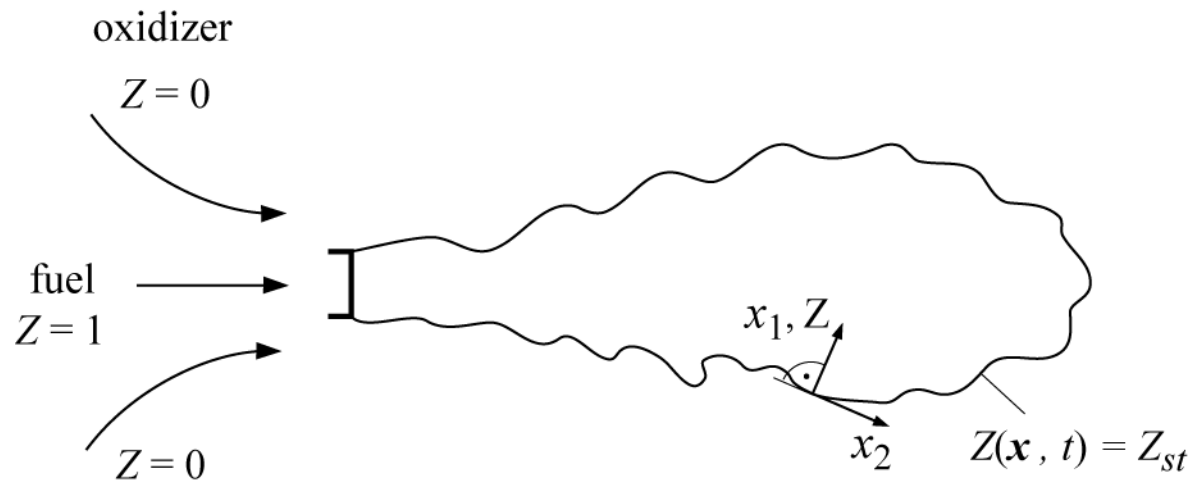


- In summary, it may be concluded that one-point, one-time experimental data in turbulent flames, when plotted as a function of mixture fraction, show qualitatively similar tendencies as laminar flamelet profiles in counterflow diffusion flames
- Non-equilibrium effects are evident in both cases and lead to an increase of radical concentrations and a decrease of temperatures
- This has an important influence on  $\text{NO}_x$  formation in turbulent diffusion flames

## Laminar Flamelet Equations for Nonpremixed Combustion

- Based on the laminar flamelet concept introduced in Lecture 8, the flame surface is defined as the surface of stoichiometric mixture which is obtained by setting  $Z(x, t) = Z_{st}$

- In the vicinity of that surface, the reactive-diffusive structure can be described by the flamelet equations



$$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho \chi}{Le_i} \frac{\partial^2 \psi_i}{\partial Z^2} + \omega_i$$

- In these equations the **instantaneous scalar dissipation rate** has been introduced



- At the flame surface, the instantaneous scalar dissipation rate takes the value  $\chi_{st}$
- If  $\chi$  is assumed to be a function of  $Z$ , this functional dependence can be parameterized by  $\chi_{st}$
- The scalar dissipation rate acts as an external parameter that is imposed on the flamelet structure by the mixture fraction field
- It has the dimension of an **inverse time** and therefore represents the **inverse of a diffusion time scale**
- It also can be thought of as a **diffusivity in mixture fraction space**

- In principle, both the mixture fraction  $Z$  and the scalar dissipation rate  $\chi$  are **fluctuating quantities** and their statistical distribution needs to be considered, if one wants to calculate statistical moments of the reactive scalars (cf. Peters, (1984))
- If the joint pdf  $\tilde{P}(Z, \chi_{st})$  is known and the steady state flamelet equations are solved to obtain  $\psi_i$  as a function of  $Z$  and  $\chi_{st}$ , for point  $\mathbf{x}$  and time  $t$ , the Favre mean of  $\psi_i$  can be obtained from

$$\tilde{\psi}_i(\mathbf{x}, t) = \int_0^1 \int_0^\infty \psi_i(Z, \chi_{st}) P(Z, \chi_{st}; \mathbf{x}, t) d\chi_{st} dZ$$

- If the unsteady term in the flamelet equation must be retained, joint statistics of  $Z$  and  $\chi_{st}$  become impractical
- Then, in order to reduce the dimension of the statistics, it is useful to introduce **multiple flamelets**, each representing a different range of the  $\chi$ -distribution
- Such multiple flamelets are used in the Eulerian Particle Flamelet Model (EPFM) by Barths et al. (1998)

- Since the dissipation rate is a fluctuating quantity, the conditional mean can be used
- The conditional Favre mean scalar dissipation rate can be determined as

$$\tilde{\chi}_Z = \frac{\langle \rho \chi | Z \rangle}{\langle \rho | Z \rangle}$$

- Then, the flamelet equations in a turbulent flow field take the form

$$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho}{\text{Le}_i} \frac{\tilde{\chi}_Z}{2} \frac{\partial \psi_i}{\partial Z} + \omega_i$$

- A mean scalar dissipation rate, however, is unable to account for those ignition and extinction events that are triggered by small and large values of  $\chi$ , respectively
- This is where [LES](#), as discussed in Lecture 10, must be used

- With  $\psi_i(Z, \tilde{\chi}_Z, t)$  obtained from solving

$$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho}{Le_i} \frac{\tilde{\chi}_Z}{2} \frac{\partial \psi_i}{\partial Z} + \omega_i$$

Favre mean values of  $\psi_i$  can be obtained at any point  $\mathbf{x}$  and time  $t$  in the flow using

$$\tilde{\psi}_i(\mathbf{x}, t) = \int_0^1 \psi_i(Z, \tilde{\chi}_Z, t) \tilde{P}(Z; \mathbf{x}, t) dZ$$

- Here the presumed shape of the pdf  $\tilde{P}(Z; \mathbf{x}, t)$  can be calculated from the mean and the variance of the turbulent mixture fraction field, as discussed in Section 14

- Then, there remains the problem on how to model the conditional scalar dissipation rate  $\tilde{\chi}_Z$
- One first relates the conditional scalar dissipation rate  $\tilde{\chi}_Z$  to that at a fixed value  $Z_{st}$  by

$$\tilde{\chi}_Z = \tilde{\chi}_{st} \frac{f(Z)}{f(Z_{st})}$$

where  $f(Z)$  is a function as in

$$\chi \propto \exp(-2[\text{erfc}^{-1}(2Z)]^2)$$

- Then, with the presumed pdf  $\tilde{P}(Z)$  being known, the unconditional average can be written as

$$\tilde{\chi} = \int_0^1 \tilde{\chi}_Z \tilde{P}(Z) dZ = \tilde{\chi}_{st} \int_0^1 \frac{f(Z)}{f(Z_{st})} \tilde{P}(Z) dZ$$

- Therefore, using the model

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

the conditional mean scalar dissipation rate  $\tilde{\chi}_{st}$  can be expressed as

$$\tilde{\chi}_{st} = \frac{\tilde{\chi} f(Z_{st})}{\int_0^1 f(Z) \tilde{P}(Z) dZ}$$

which is to be used in

$$\tilde{\chi}_Z = \tilde{\chi}_{st} \frac{f(Z)}{f(Z_{st})}$$

- Flamelet equations can also be used to describe ignition in a nonpremixed system
- As the scalar dissipation rate decreases, as for instance in a Diesel engine after injection, heat release by chemical reactions will exceed heat loss out of the reaction zone, leading to auto-ignition
- The scalar dissipation rate at auto-ignition is denoted by

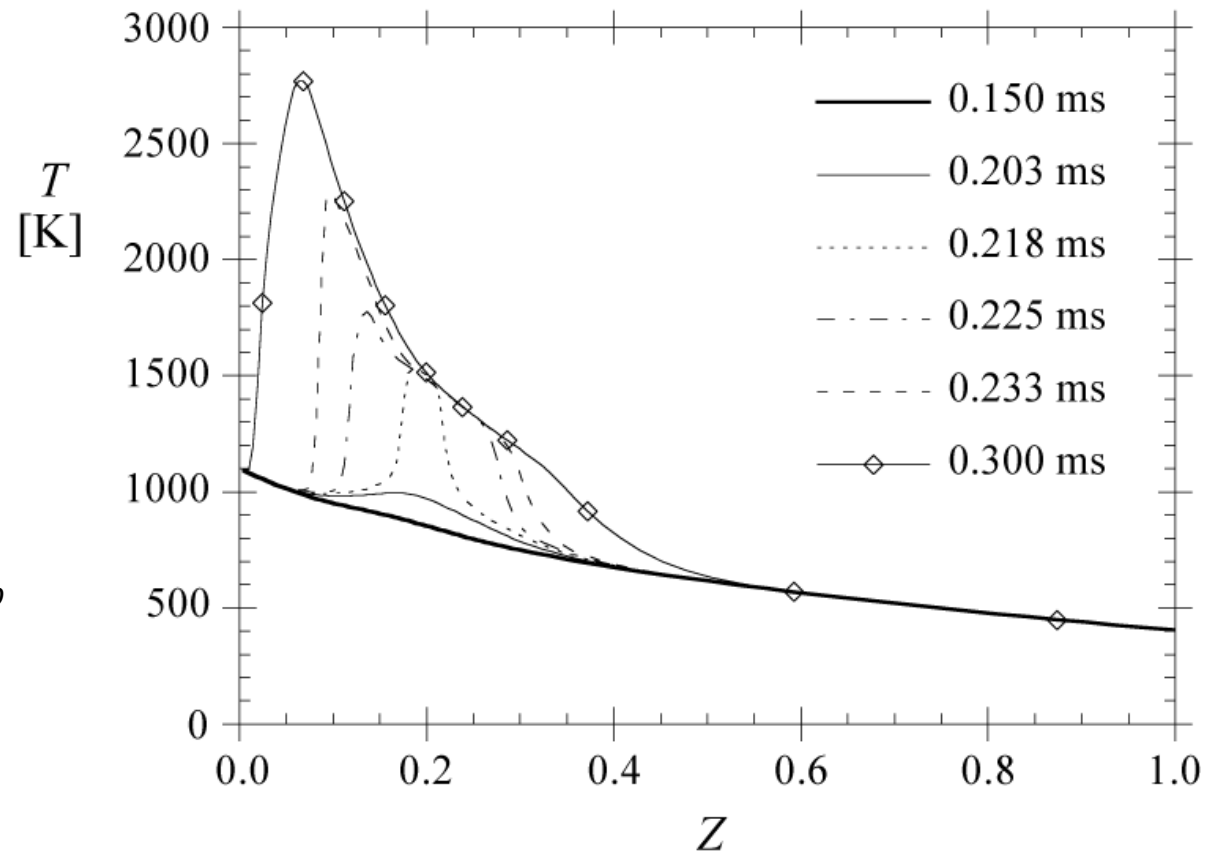
$$\chi_i = \chi_{st,ign}$$

- For ignition under Diesel engine conditions this has been investigated by Pitsch and Peters (1998)
- An example of auto-ignition of a *n*-heptane-air mixture calculated with the RIF code (cf. Paczko et al., 1999) will be shown here



- The initial air temperature is 1100 K and the initial fuel temperature is 400 K

- Mixing of fuel and air leads to a straight line for the enthalpy in mixture fraction space, but not for the temperature  $T_u(Z)$ , since the heat capacity  $c_p$  depends on temperature



- It is seen that auto-ignition starts after 0.203 ms, when the temperature profile shows already a small increase over a broad region around  $Z = 0.2$

- At  $t = 0.218$  ms, there has been a fast thermal runaway in that region, with a peak at the adiabatic flame temperature

