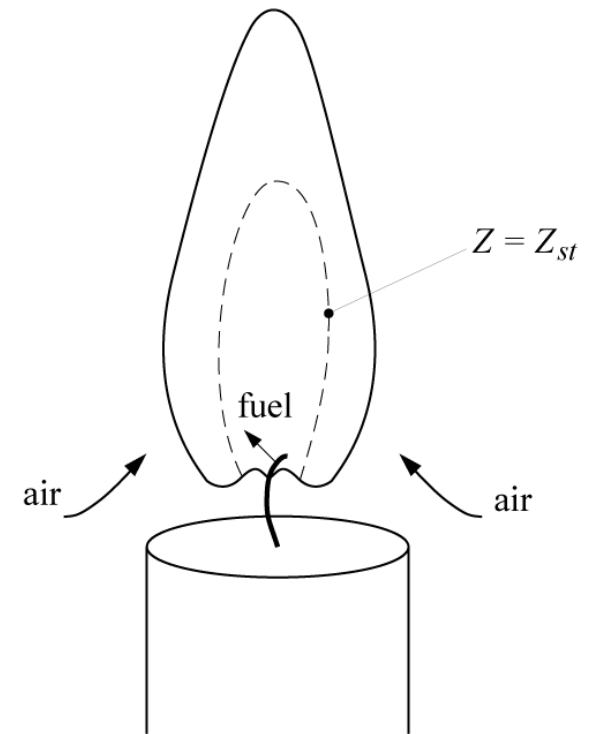


Lecture 8

Laminar Diffusion Flames: Diffusion Flamelet Theory

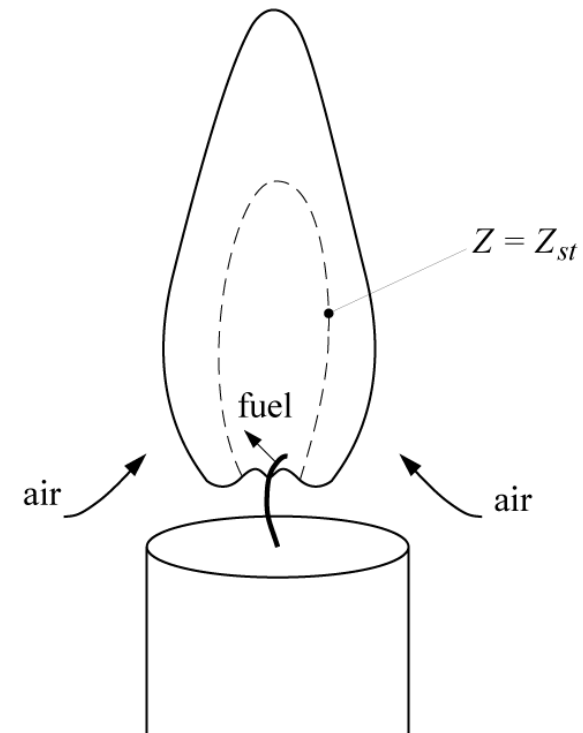
- Systems, where fuel and oxidizer enter **separately** into the combustion chamber
- Mixing takes place by convection and diffusion
- Only where fuel and oxidizer are mixed on the molecular level, chemical reactions can occur
- The time scale of reaction is much shorter than the time scale for diffusion
→ **diffusion is rate determining**
- This is why flames in non-premixed combustion are called diffusion flames



Candle flame:
A classical example of a
diffusion flame

Example: Candle Flame

- The flow entraining the air into the flame is driven by buoyancy
- The paraffin of the candle first melts due to radiative heat from the flame to the candle
- It mounts by capillary forces into the wick and evaporates to become paraffin vapor, a gaseous fuel
- The combustion zones in a diffusion flame are best described by an [asymptotic expansion for very fast chemistry](#) starting from the limit of complete combustion



- To leading order one obtains the **adiabatic flame temperature**, which is a function of mixture fraction only
- The asymptotic expansion around this limit will then describe the influence of **finite rate chemistry**
- If the expansion takes the temperature sensitivity of the chemistry into account **diffusion flame quenching** can also be described
- By introducing the **mixture fraction as an independent coordinate** for all reacting scalars, a universal coordinate transformation leads in the limit of sufficiently fast chemistry to a **one-dimensional problem for the reaction zone**
- This is the basis of the **flamelet** formulation for non-premixed combustion

Flamelet Structure of a Diffusion Flame

- Assumptions: Equal diffusivities of chemical species and temperature

$$\text{Le}_i = \lambda / (c_p \rho D_i) = 1, \quad i = 1, 2, \dots, k \quad \Rightarrow \quad D = \lambda / (\rho c_p)$$

- The balance equation for mixture fraction, temperature and species read

$$\rho \frac{\partial Z}{\partial t} + \rho v_\alpha \frac{\partial Z}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial Z}{\partial x_\alpha} \right) = 0$$

$$\rho \frac{\partial T}{\partial t} + \rho v_\alpha \frac{\partial T}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial T}{\partial x_\alpha} \right) = \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_i}{\partial t} + \rho v_\alpha \frac{\partial Y_i}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left(\rho D \frac{\partial Y_i}{\partial x_\alpha} \right) = \dot{m}_i \quad i = 1, 2, \dots, k$$

- Here the **low Mach number limit** that leads to zero spatial pressure gradients has been employed, but the temporal pressure change has been retained

Flamelet Structure of a Diffusion Flame

- The equation for the mixture fraction

$$\rho \frac{\partial Z}{\partial t} + \rho v_{\alpha} \frac{\partial Z}{\partial x_{\alpha}} - \frac{\partial}{\partial x_{\alpha}} \left(\rho D \frac{\partial Z}{\partial x_{\alpha}} \right) = 0$$

does not contain a chemical source term, since elements are conserved in chemical reactions

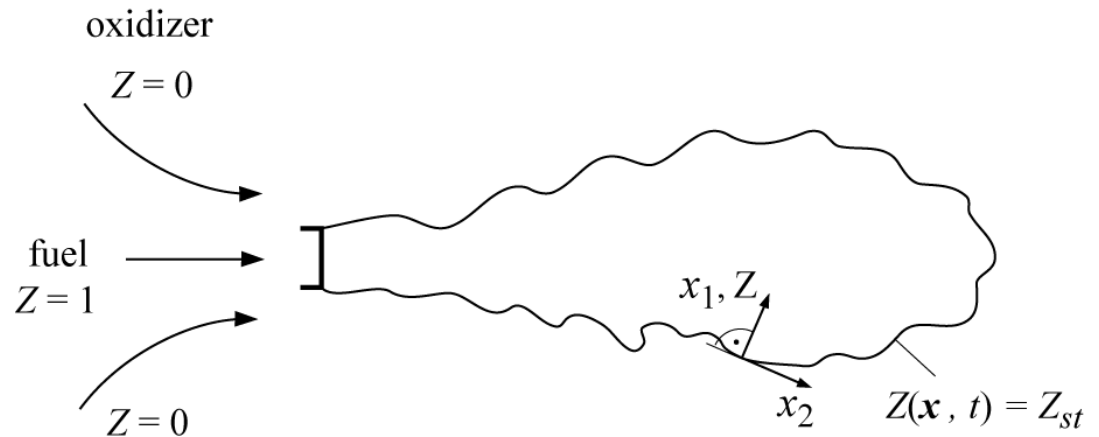
- We assume the mixture fraction Z to be given in the flow field as a function of space and time: $Z=Z(x_{\alpha},t)$

- Then the surface of the stoichiometric mixture can be determined as

$$Z(x_\alpha, t) = Z_{st}$$

- Combustion occurs in a thin layer in the vicinity of this surface if the local mixture fraction gradient is sufficiently high

- Let us locally introduce an orthogonal coordinate system x_1, x_2, x_3 attached to the surface stoichiometric mixture



- x_1 points normal to the surface Z_{st} , x_2 and x_3 lie within the surface
- We replace the coordinate x_1 by the mixture fraction Z and x_2, x_3 and t by $Z_2 = x_2, Z_3 = x_3$ and $t = \tau$
- This is a coordinate transformation of the Crocco type

- Here the temperature T , and similarly the mass fractions Y_j , will be expressed as a function of the mixture fraction Z
- By definition, the new coordinate Z is locally normal to the surface of stoichiometric mixture
- With the transformation rules

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z}, \quad \frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1} + \frac{\partial}{\partial Z}$$

$$\frac{\partial}{\partial x_\alpha} = \frac{\partial}{\partial Z_\alpha} + \frac{\partial Z}{\partial x_\alpha} \frac{\partial}{\partial Z} \quad (\alpha = 2, 3)$$

we obtain the temperature equation in the form

$$\begin{aligned} & \rho \frac{\partial T}{\partial \tau} + \rho v_2 \frac{\partial T}{\partial Z_2} + \rho v_3 \frac{\partial T}{\partial Z_3} - \frac{\partial(\rho D)}{\partial x_2} \frac{\partial T}{\partial Z_2} - \frac{\partial(\rho D)}{\partial x_3} \frac{\partial T}{\partial Z_3} + \\ & - \rho D \left(\left(\frac{\partial Z}{\partial x_\alpha} \right)^2 \frac{\partial^2 T}{\partial Z^2} + 2 \frac{\partial Z}{\partial x_2} \frac{\partial^2 T}{\partial Z \partial Z_2} + 2 \frac{\partial Z}{\partial x_3} \frac{\partial^2 T}{\partial Z \partial Z_3} + \frac{\partial^2 T}{\partial Z_2^2} + \frac{\partial^2 T}{\partial Z_3^2} \right) = \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t} \end{aligned}$$

- The transformation of the equation for the mass fraction is similar

- If the flamelet is **thin in the Z direction**, an order-of-magnitude analysis similar to that for a boundary layer shows that

$$\left(\frac{\partial Z}{\partial x_\alpha}\right)^2 \frac{\partial^2 T}{\partial Z^2}$$

is the dominating term of the spatial derivatives

- This term must balance the terms on the right-hand side

$$\rho \frac{\partial T}{\partial \tau} - \rho D \left(\frac{\partial Z}{\partial x_\alpha}\right)^2 \frac{\partial^2 T}{\partial Z^2} \approx \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

- All other terms containing spatial derivatives can be neglected to leading order
- This is equivalent to the assumption that the temperature derivatives normal to the flame surface are much larger than those in tangential direction

$$\rho \frac{\partial T}{\partial \tau} - \rho D \left(\frac{\partial Z}{\partial x_\alpha} \right)^2 \frac{\partial^2 T}{\partial Z^2} \approx \sum_{i=1}^k \dot{m}_i \frac{h_i}{c_p} + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

- The term containing the time derivative $\partial T / \partial \tau$ is important if very rapid changes, such as extinction, occur
- Formally, this can be shown by introducing the stretched coordinate ξ and the fast time scale σ

$$\xi = (Z - Z_{st}) / \varepsilon, \quad \sigma = \tau / \varepsilon^2$$

- ε is a small parameter, the inverse of a large Damköhler number or a large activation energy, for example, representing the width of the reaction zone

- If the time derivative term is retained, the flamelet structure is to leading order described by the one-dimensional time-dependent equations

$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

$$\rho \frac{\partial Y_i}{\partial t} - \rho \frac{\chi_{st}}{Z} \frac{\partial Y_i}{\partial Z^2} = \dot{m}_i \quad i = 1, 2, \dots, k.$$

- Here

$$\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_\alpha} \right)_{st}^2$$

is the **instantaneous scalar dissipation** rate at stoichiometric conditions

- It has the dimension 1/s and may be interpreted as the **inverse of a characteristic diffusion time**
- It may depend on t and Z and acts as a prescribed parameter, representing the flow and the mixture field

- As a result of the transformation, the scalar dissipation rate

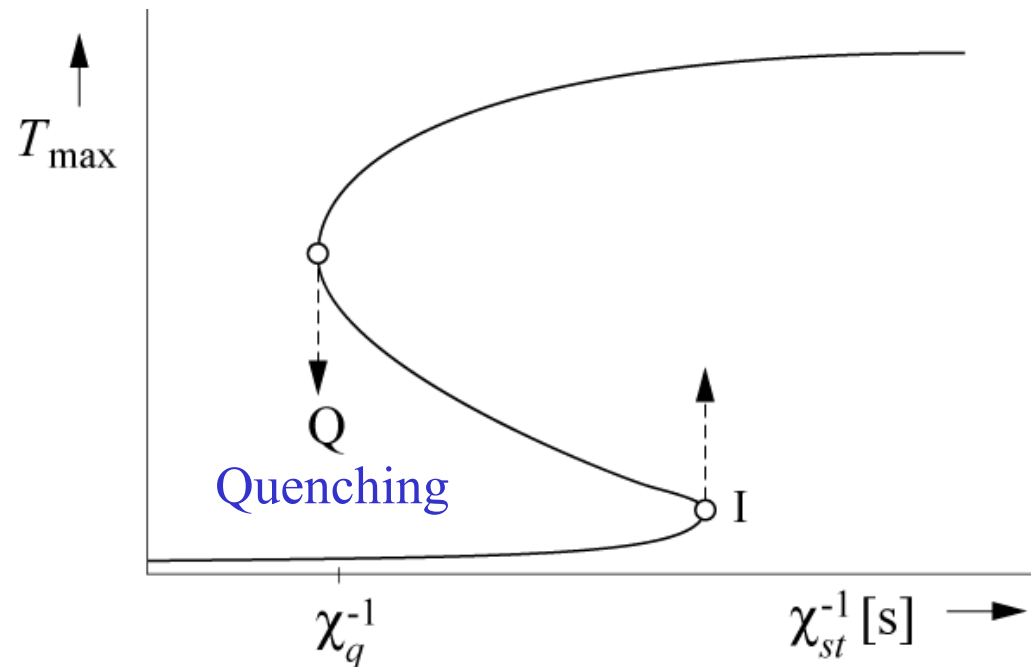
$$\chi_{st} = 2D \left(\frac{\partial Z}{\partial x_\alpha} \right)_{st}^2$$

implicitly incorporates the influence of convection and diffusion normal to the surface of the stoichiometric mixture

- In the limit $\chi_{st} \rightarrow 0$, equations for the **homogeneous reactor** are obtained

Steady Solutions of the Flamelet Equation: The S-Shaped Curve

- Burning flamelet correspond to the upper branch of the S-shaped curve
- If χ_{st} is increased, the curve is traversed to the left until χ_q is reached, beyond which value only the lower, nonreacting branch exists
- Thus at $\chi_{st} = \chi_q$ the **quenching** of the diffusion flamelet occurs
- The transition from the point Q to the lower state corresponds to the unsteady transition



- The neglect of all spatial derivatives tangential to the flame front is formally only valid in the thin reaction zone around $Z = Z_{st}$
- There are, however, a number of typical flow configurations, where

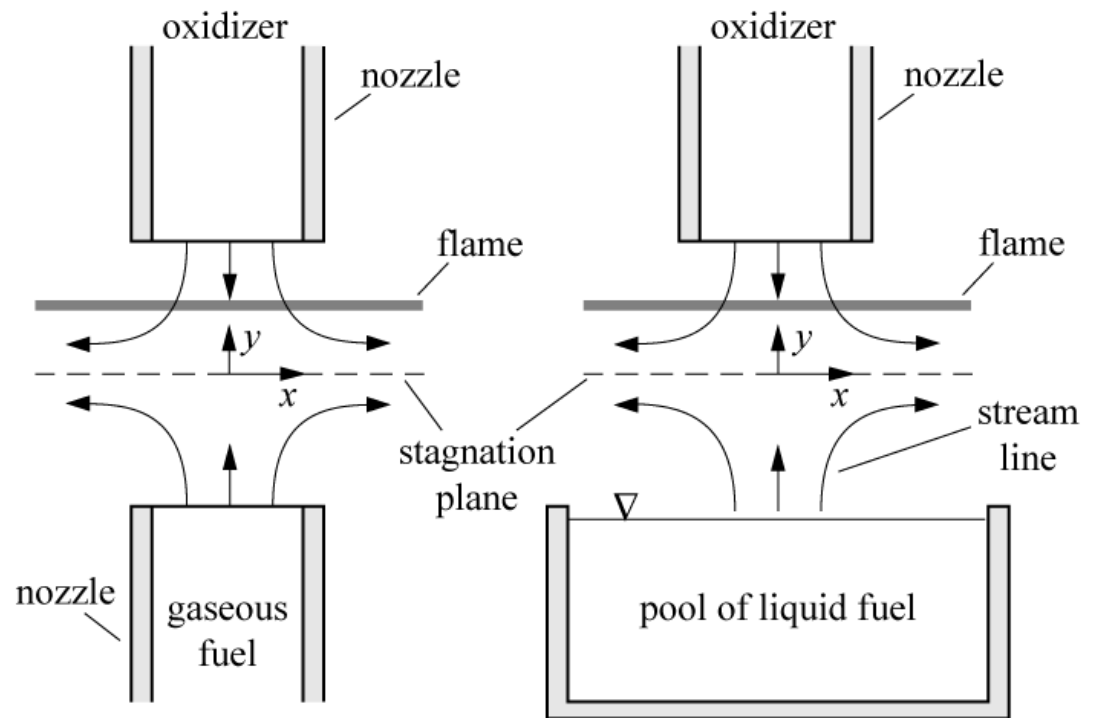
$$\rho \frac{\partial T}{\partial t} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \sum_{l=1}^r \frac{Q_l}{c_p} \omega_l + \frac{\dot{q}_R}{c_p} + \frac{1}{c_p} \frac{\partial p}{\partial t}$$

is valid in the entire Z-space

- As example, the analysis of a [planar counterflow diffusion flame](#) is included in the lecture notes

The Planar Counterflow Diffusion Flame

- Counterflow diffusion flames are very often used experimentally because they represent an essentially one-dimension diffusion flame structures
- If one assumes that the flow velocities of both streams are sufficiently large and sufficiently removed from the stagnation plane, the flame is embedded between two **potential flows**, one coming from the oxidizer and one from the fuel side



Flow equations and boundary conditions

- Prescribing the potential flow velocity gradient in the oxidizer stream

$$a = -\frac{\partial v_{\infty}}{\partial y}$$

the velocities and the mixture fraction are there

$$y \rightarrow \infty : \quad v_{\infty} = -ay, \quad u_{\infty} = ax, \quad Z = 0$$

- Equal stagnation point pressure for both streams requires that the velocities in the fuel stream are

$$y \rightarrow -\infty : \quad v_{-\infty} = -\sqrt{\frac{\rho_{\infty}}{\rho_{-\infty}}} ay, \quad u_{-\infty} = \sqrt{\frac{\rho_{\infty}}{\rho_{-\infty}}} ax, \quad Z = 1.$$

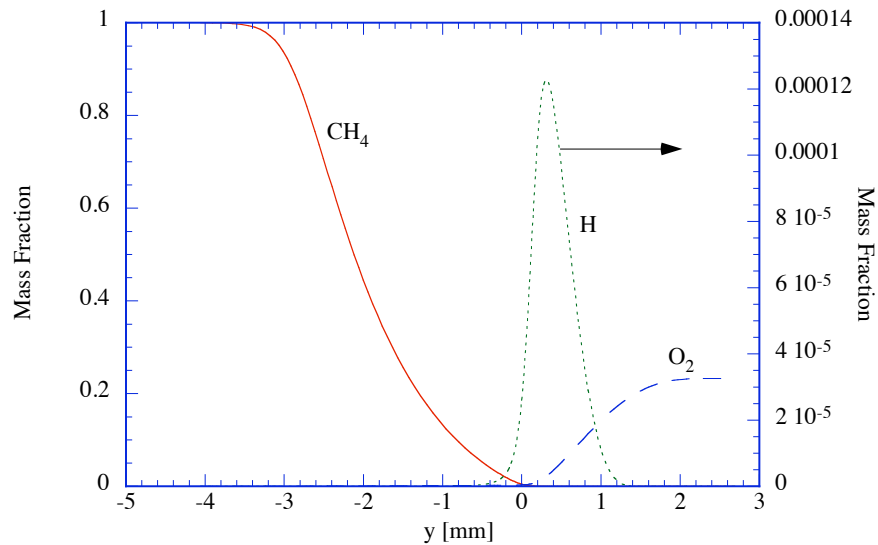
- The equations for continuity, momentum and mixture fraction are given by

$$\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0$$

$$\rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right)$$

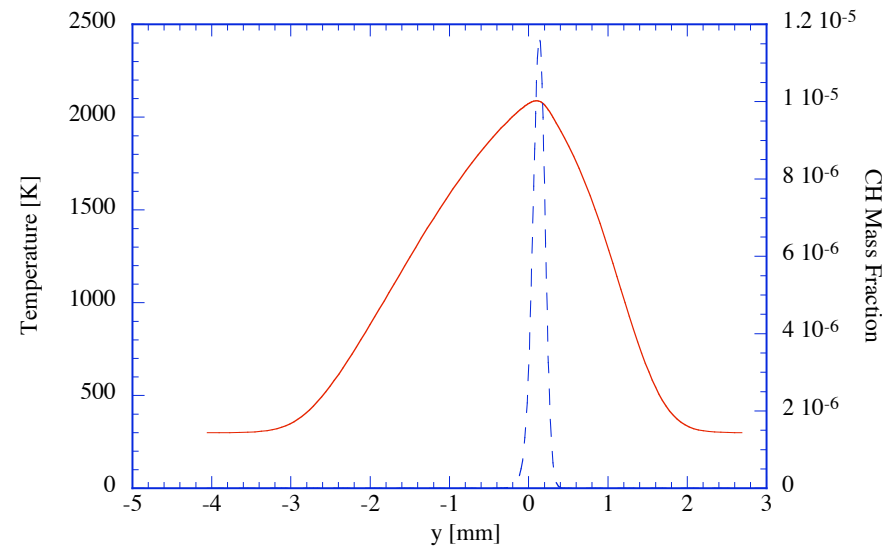
$$\rho u \frac{\partial Z}{\partial x} + \rho v \frac{\partial Z}{\partial y} = \frac{\partial}{\partial y} \left(\rho D \frac{\partial Z}{\partial y} \right)$$

Numerical Simulation of Counterflow Diffusion Flame



- **Oxygen leakage** at high strain rate

Atmospheric Methane Counterflow Diffusion Flame at $a = 100 \text{ s}^{-1}$



Example: Analysis of the Counterflow Diffusion Flame

- Introducing the similarity transformation $\eta = \left(\frac{a}{(\rho\mu)_\infty} \right)^{1/2} \int_0^y \rho dy, \quad \xi = x$

one obtains the system of ordinary differential equations

$$f = \int_0^\eta f' d\eta$$

$$\frac{\partial}{\partial \eta} \left(C \frac{\partial f'}{\partial \eta} \right) + f \frac{\partial f'}{\partial \eta} + \frac{\rho_\infty}{\rho} - f'^2 = 0$$

$$\frac{\partial}{\partial \eta} \left(\frac{C}{Sc} \frac{\partial Z}{\partial \eta} \right) + f \frac{\partial Z}{\partial \eta} = 0$$

in terms of the non-dimensional stream function

$$f = \frac{\rho v}{\sqrt{(\rho\mu)_\infty a}}$$

and the normalized tangential velocity $f' = \frac{u}{ax}$

- Furthermore the Chapman-Rubensin parameter C and the Schmidt number Sc are defined

$$C = \frac{\rho\mu}{(\rho\mu)_\infty}, \quad Sc = \frac{\mu}{\rho D}.$$

- The boundary equations are

$$\eta = +\infty : \quad f' = 1, \quad Z = 0$$

$$\eta = -\infty : \quad f' = \sqrt{\rho_\infty/\rho_{-\infty}}, \quad Z = 1$$

- An integral of the Z-equation is obtained as where the integral $I(\eta)$ is defined as

$$Z = \frac{1}{2} \frac{I(\infty) - I(\eta)}{I(\infty)}$$

$$I(\eta) = \int_0^\eta \frac{Sc}{C} \exp \left\{ - \int_0^\eta f \frac{Sc}{C} d\eta \right\} d\eta$$

- For constant properties $\rho = \rho_\infty$, $C = 1$ $f = \eta$ satisfies

$$\frac{\partial}{\partial \eta} \left(C \frac{\partial f'}{\partial \eta} \right) + f' \frac{\partial f'}{\partial \eta} + \frac{\rho_\infty}{\rho} - f'^2 = 0$$

and

$$Z = \frac{1}{2} \operatorname{erfc} \left(\eta / \sqrt{2} \right).$$

- The instantaneous scalar dissipation rate is here

$$\chi = 2D \left(\frac{\partial Z}{\partial y} \right)^2 = 2 \left(\frac{C}{Sc} \right) a \left(\frac{\partial Z}{\partial \eta} \right)^2$$

where

$$\eta = \left(\frac{a}{(\rho\mu)_\infty} \right)^{1/2} \int_0^y \rho \, dy, \quad \xi = x \quad \text{and} \quad C = \frac{\rho\mu}{(\rho\mu)_\infty}, \quad Sc = \frac{\mu}{\rho D}. \quad \text{have been used}$$

- When the scalar dissipation rate is evaluated with the assumptions that led to

$$Z = \frac{1}{2} \operatorname{erfc}\left(\eta/\sqrt{2}\right).$$

one obtains

$$\chi = \frac{a}{\pi} \exp[-\eta^2(Z)] = \frac{a}{\pi} \exp(-2[\operatorname{erfc}^{-1}(2Z)]^2)$$

- For small Z one obtains with l' Hospital's rule

$$\frac{dZ}{d\eta} = -\frac{1}{2} \frac{dI}{d\eta} \frac{1}{I(\infty)} = \frac{dI}{d\eta} \frac{Z}{I(\infty) - I(\eta)} = -\frac{Sc}{C} f Z.$$

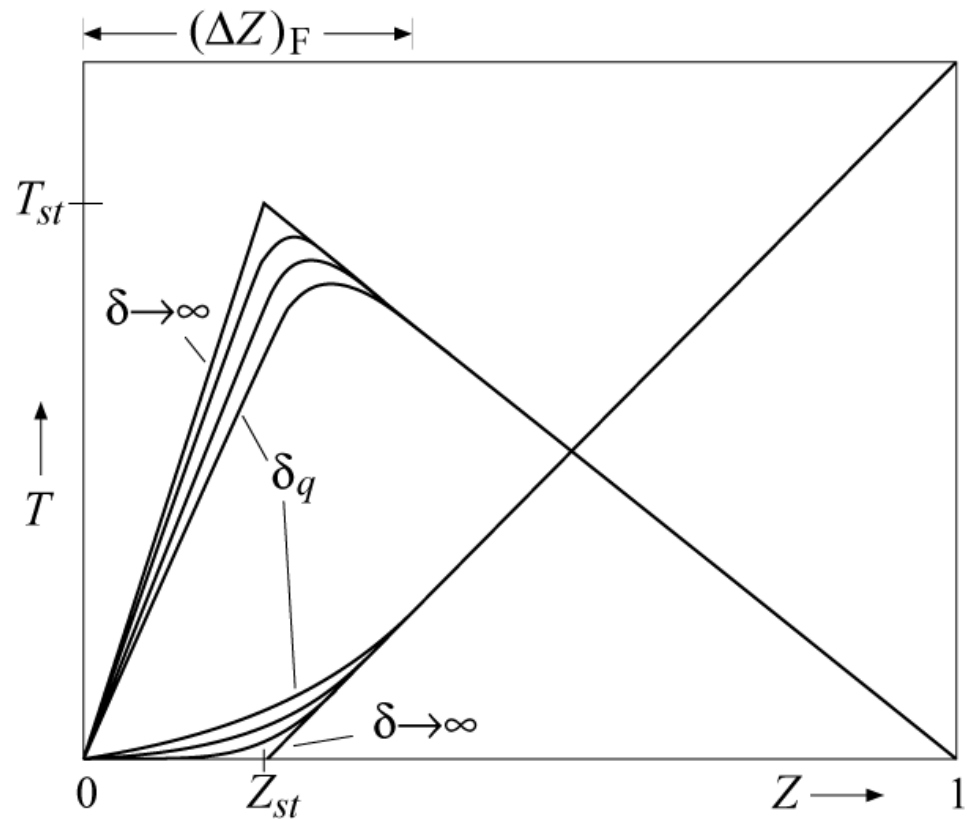
- Therefore, in terms of the velocity gradient a the scalar dissipation rate becomes

$$\chi = 2af^2 Z^2 (Sc/C)$$

showing that χ increases as Z^2 for small Z

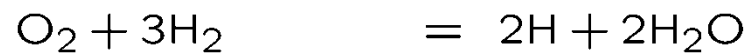
Diffusion Flame Structure of Methane-Air Flames

- Classical Linan one-step model with a large activation energy is able to predict important features such as extinction, but for small values of Z_{st} , it predicts the leakage of fuel through the reaction zone



- However, experiments of methane flames, on the contrary, show **leakage of oxygen** rather than of fuel through the reaction zone

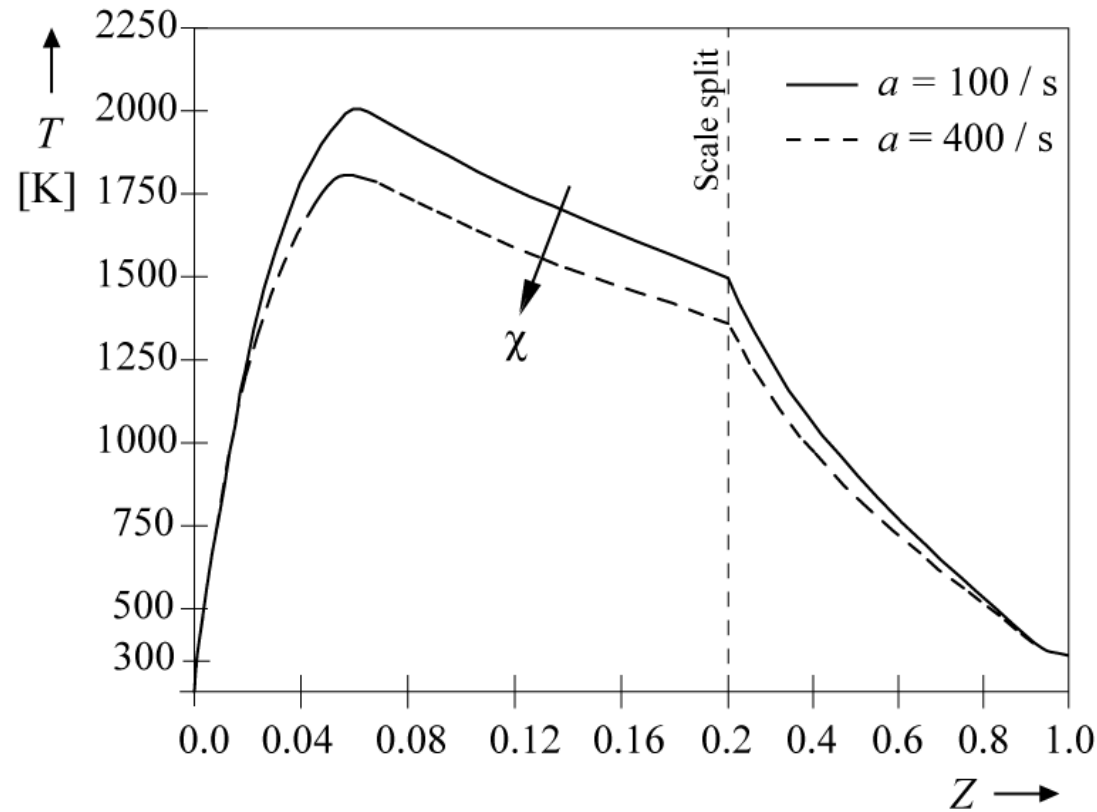
- A numerical calculation with the four-step reduced mechanism



has been performed for the counter-flow diffusion flame in the stagnation region of a porous cylinder

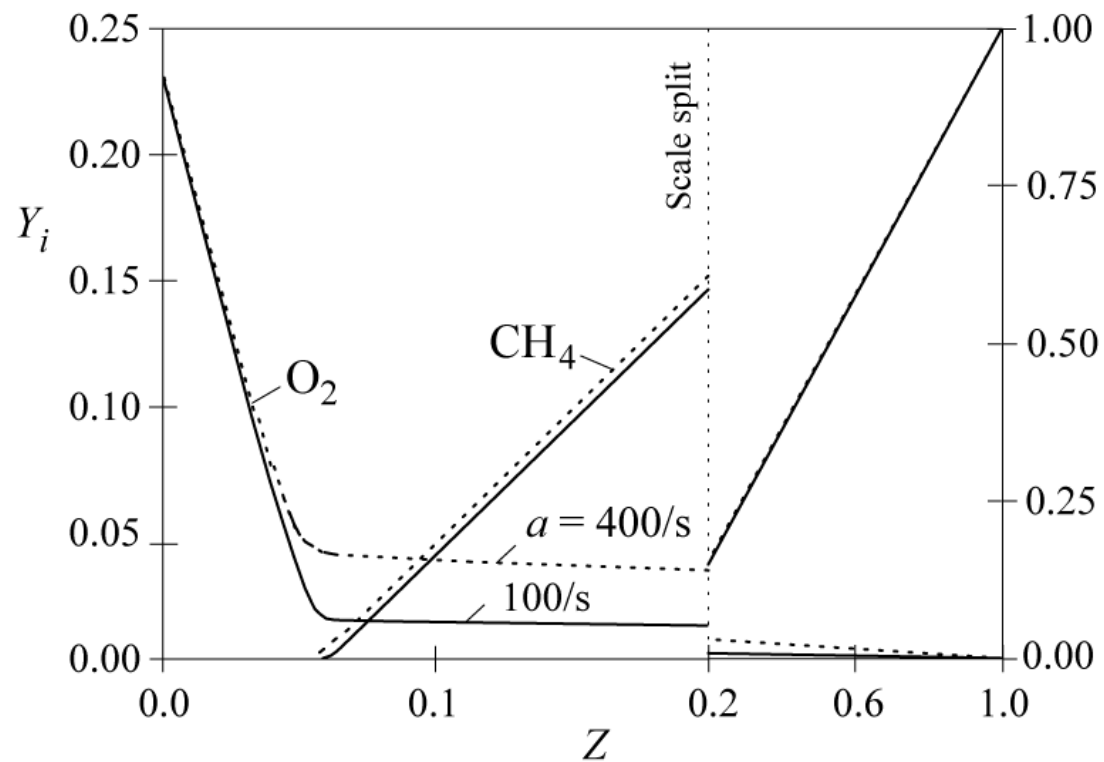
- This flow configuration, initially used by Tsuji and Yamaoka, will be presented in the next lecture

- Temperature profiles for methane-air flames



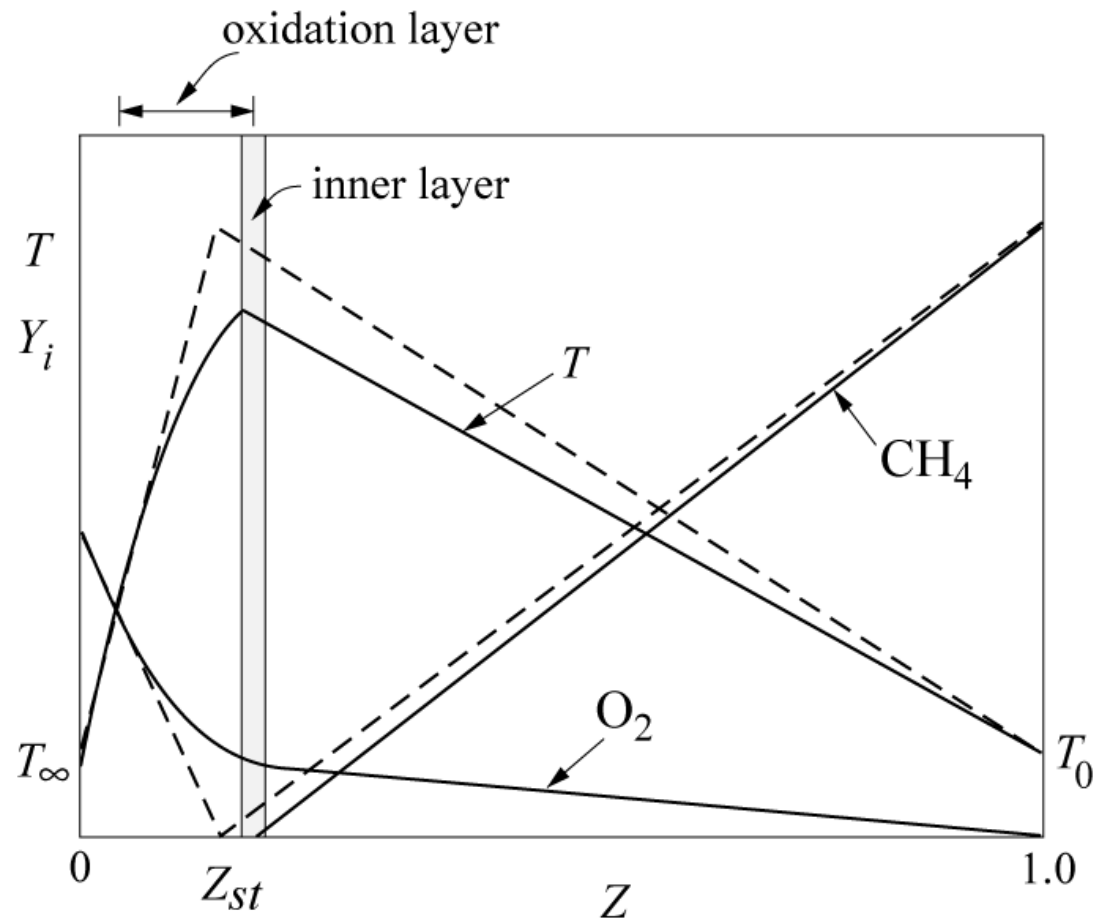
- The second value of the strain rate corresponds to a condition close to extinction
- It is seen that the temperature in the reaction zone decreases

- Fuel and oxygen mass fraction profiles for methane-air flames

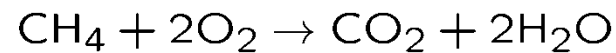


- The oxygen leakage increases as extinction is approached

- An asymptotic analysis by Seshadri (1988) based on the four-step model shows a close correspondence between the different layers identified in the premixed methane flame and those in the diffusion flame



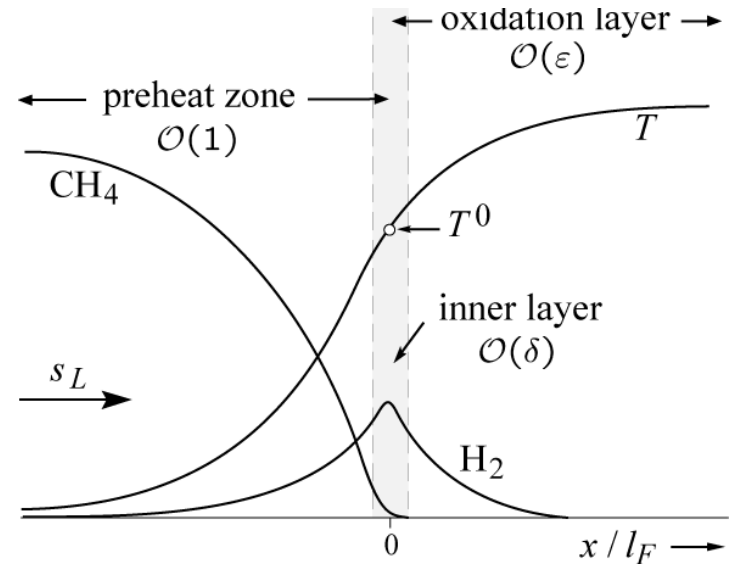
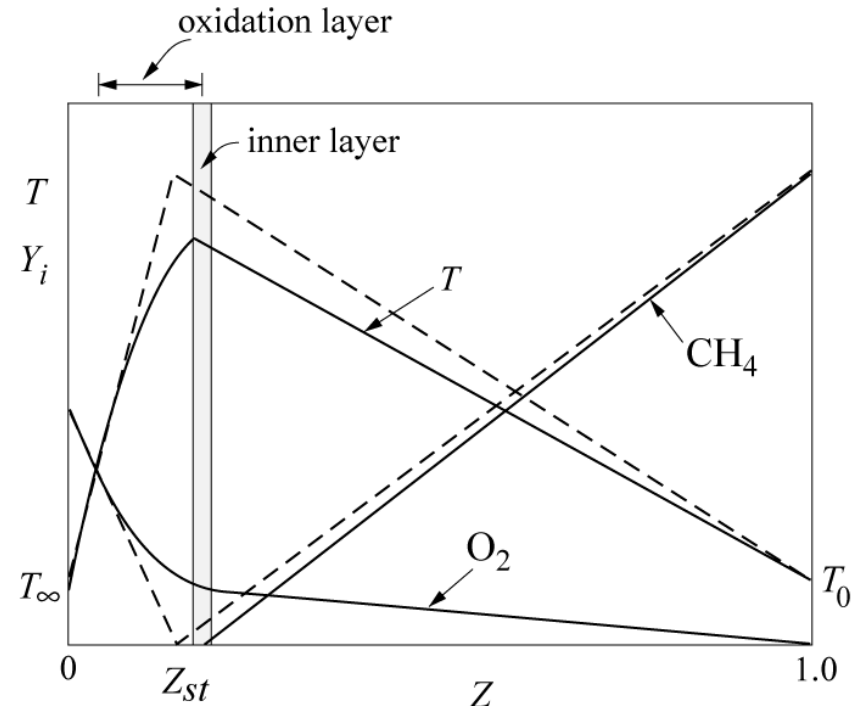
- The outer structure of the diffusion flame is the **classical Burke-Schumann structure** governed by the overall one-step reaction



with the flame sheet positioned at $Z = Z_{st}$

- The inner structure consists of a thin H_2 - CO **oxidation layer** of thickness of **order ε** toward the lean side and a **thin inner layer** of thickness of order **δ** slightly toward the rich side of $Z = Z_{st}$
- Beyond this layer, the rich side is chemically inert, because all radicals are consumed by the fuel

- The comparison of the diffusion flame structure with that of a premixed flame shows that
 - Rich part of the diffusion flame corresponds to the upstream preheat zone of the premixed flame
 - Lean part corresponds to the downstream oxidation layer
- The maximum temperature corresponds to the inner layer temperature of the asymptotic structure



- The plot of the maximum temperature also corresponds to the upper branch of the S-shaped curve

- The calculations agree well with numerical and experimental data and they also show the vertical slope of T^0 versus χ_{st}^{-1} which corresponds to extinction

