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

\[ \text{Le}_i = \frac{\lambda}{(c_p \rho D_i)} = 1, \quad i = 1, 2, \ldots, k \implies D = \frac{\lambda}{(\rho c_p)} \]

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

\[
\begin{align*}
\rho \frac{\partial Z}{\partial t} + \rho v_\alpha \frac{\partial Z}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left( \rho D \frac{\partial Z}{\partial x_\alpha} \right) &= 0 \\
\rho \frac{\partial T}{\partial t} + \rho v_\alpha \frac{\partial T}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left( \rho D \frac{\partial T}{\partial x_\alpha} \right) &= \sum_{i=1}^{k} \dot{m}_i \frac{h_i}{c_p} + \dot{q}_R \frac{1}{c_p} \frac{\partial p}{\partial t} \\
\rho \frac{\partial Y_i}{\partial t} + \rho v_\alpha \frac{\partial Y_i}{\partial x_\alpha} - \frac{\partial}{\partial x_\alpha} \left( \rho D \frac{\partial Y_i}{\partial x_\alpha} \right) &= \dot{m}_i \quad i = 1, 2, \ldots, k
\end{align*}
\]

- 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 $Y_i$, 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

\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t} \frac{\partial}{\partial Z}, \quad \frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1} + \frac{\partial}{\partial Z} \frac{\partial}{\partial x_1} \frac{\partial}{\partial Z} \quad (\alpha = 2, 3)
\]

we obtain the temperature equation in the form

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

• 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

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

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

- 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 \( \xi \) and the fast time scale \( \sigma \):
  \[
  \xi = (Z - Z_{st}) / \varepsilon, \quad \sigma = \tau / \varepsilon^2
  \]

- \( \varepsilon \) 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

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

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

• Here

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

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 \( \chi_{st} \to 0 \), 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 \( \chi_{st} \) is increased, the curve is traversed to the left until \( \chi_q \) 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

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

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

\[ y \to \infty : \quad v_\infty = -ay, \quad u_\infty = ax, \quad Z = 0 \]

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

\[ y \to -\infty : \quad v_{-\infty} = -\sqrt{\frac{\rho_\infty}{\rho_{-\infty}}} ay, \quad u_{-\infty} = \sqrt{\frac{\rho_\infty}{\rho_{-\infty}}} ax, \quad Z = 1. \]
• 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

\[
\begin{align*}
\frac{\partial}{\partial \eta} \left( C \frac{\partial f'}{\partial \eta} \right) &+ f \frac{\partial f'}{\partial \eta} + \frac{\rho_\infty}{\rho} f'^2 = 0 \\
\frac{\partial}{\partial \eta} \left( \frac{C}{Sc} \frac{\partial Z}{\partial \eta} \right) &+ f \frac{\partial Z}{\partial \eta} = 0
\end{align*}
\]

in terms of the non-dimensional stream function

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

and the normalized tangential velocity

\[
f' = \frac{u}{a x}
\]
• Furthermore the Chapman-Rubesin 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

\[
\eta = +\infty : \quad f' = 1, \quad Z = 0
\]
\[
\eta = -\infty : \quad f' = \sqrt{\frac{\rho_\infty}{\rho_{-\infty}}}, \quad Z = 1
\]

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

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

\[
I(\eta) = \int_0^\eta \frac{Sc}{C} \exp \left\{ - \int_0^\eta f Sc/C d\eta \right\} d\eta
\]
• 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

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

• 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

$$\eta = \left( \frac{a}{(\rho \mu)_{\infty}} \right)^{1/2} \int_0^y \rho \, dy, \quad \xi = x \quad \text{and} \quad C = \frac{\rho \mu}{(\rho \mu)_{\infty}}, \quad Sc = \frac{\mu}{\rho D}.$$
• When the scalar dissipation rate is evaluated with the assumptions that led to

\[ Z = \frac{1}{2} \text{erfc}\left(\frac{\eta}{\sqrt{2}}\right). \]

one obtains

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

• For small \( Z \) one obtains with l’Hospital's rule

\[
\frac{dZ}{d\eta} = -\frac{1}{2} \frac{dI}{d\eta} I(\infty) = \frac{dI}{d\eta} \frac{Z}{I(\infty) - I(\eta)} = \frac{\text{Sc}}{C^f} fZ.
\]

• Therefore, in terms of the velocity gradient \( a \) the scalar dissipation rate becomes

\[ \chi = 2af^2Z^2(\text{Sc}/C) \]

showing that \( \chi \) 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

\[
\begin{align*}
\text{CH}_4 + 2\text{H} + \text{H}_2\text{O} & = \text{CO} + 4\text{H}_2 \\
\text{CO} + \text{H}_2\text{O} & = \text{CO}_2 + \text{H}_2 \\
\text{H} + \text{H} + \text{M} & = \text{H}_2 + \text{M} \\
\text{O}_2 + 3\text{H}_2 & = 2\text{H} + 2\text{H}_2\text{O}
\end{align*}
\]

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

![Graph showing 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

\[ \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O} \]

with the flame sheet positioned at \( Z = Z_{st} \)

• The inner structure consists of a thin \( \text{H}_2 - \text{CO} \) oxidation layer of thickness of order \( \varepsilon \) toward the lean side and a thin inner layer of thickness of order \( \delta \) 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 $\chi^{-1}_{st}$ which corresponds to extinction