Lecture 8

Laminar Diffusion Flames:

Diffusion Flamelet Theory

Systems, where fuel and oxidizer enter separately into the combustion chamber.
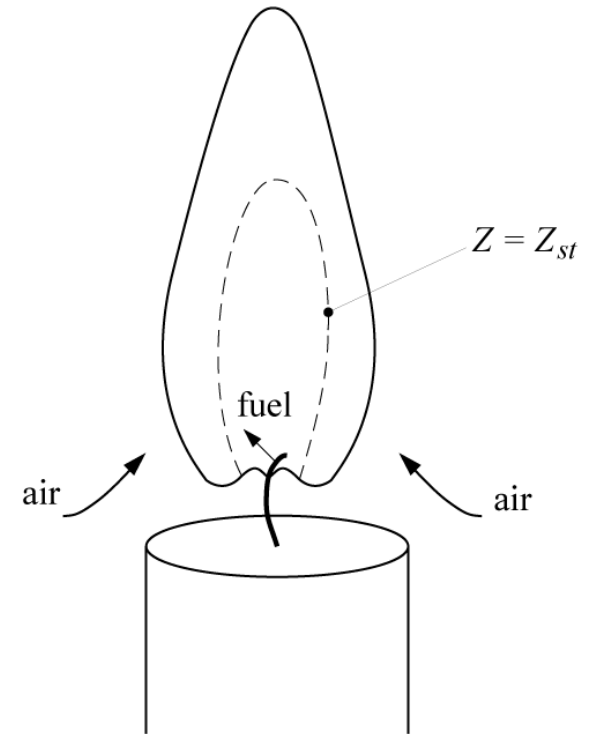
Mixing takes place by convection and diffusion.

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.

$Z = Z_{st}$

fuel

air   air

Candle flame:
A classical example of a
diffusion 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.

$Z = Z_{st}$

fuel

air

air
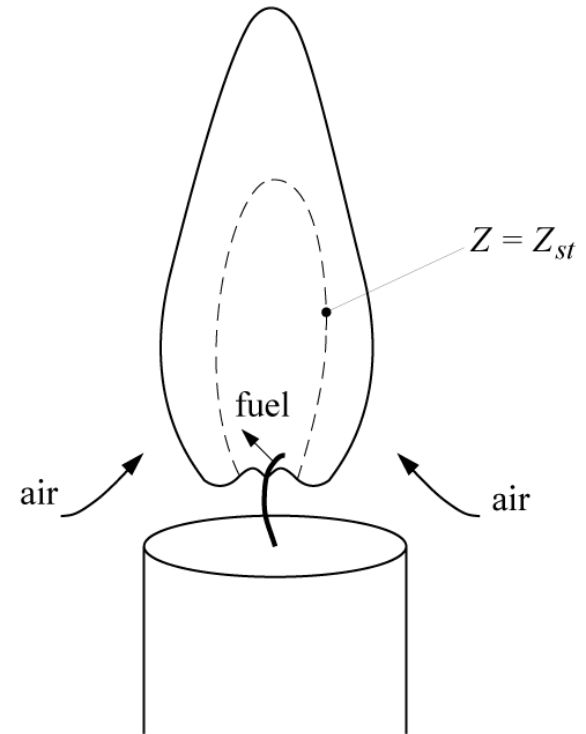
To leading order one obtains the adiabatic flame temperature which is a function of mixture fraction only.

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

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

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

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

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

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

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

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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 from

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

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
of stoichiometric mixture.

oxidizer

$Z = 0$

fuel
$Z = 1$

x_1, Z

x_2 $Z(\boldsymbol{x}, t) = Z_{st}$

$Z = 0$
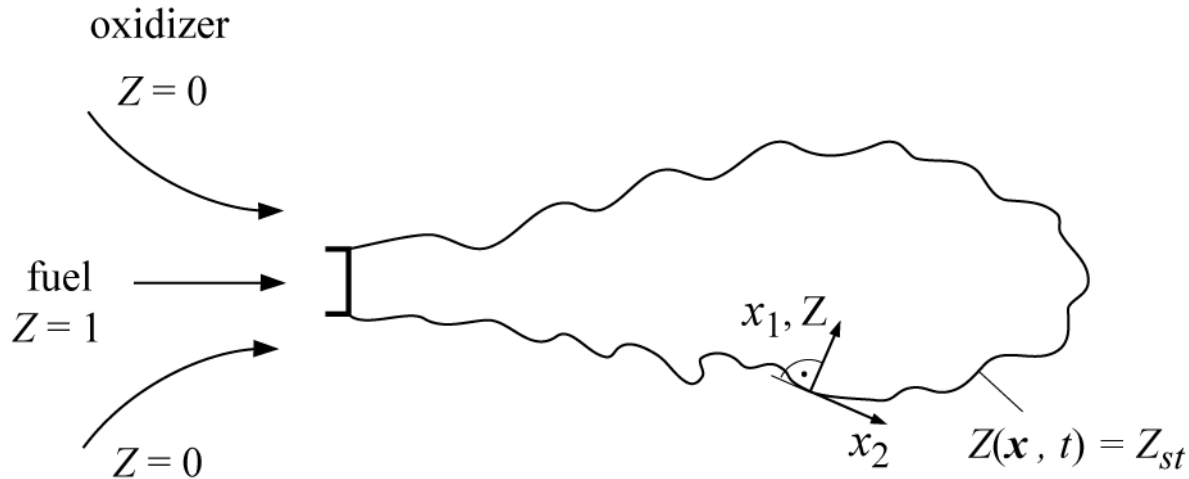
x_1 points normal to the surface Z_{st}, $\quad x_2$ and x_3 lie within the surface.

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.

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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 the stoichiometric mixture. With the transformation rules

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

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

we obtain the temperature equation in the form

$$\rho\frac{\partial T}{\partial \tau} + \rho v_2\frac{\partial T}{\partial Z_2} + \rho v_3\frac{\partial T}{\partial Z_3} - \frac{\partial(\rho D)}{\partial x_2}\frac{\partial T}{\partial Z_2} - \frac{\partial(\rho D)}{\partial x_3}\frac{\partial T}{\partial Z_3} +$$

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

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.

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

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

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

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

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

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

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.

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, we will analyze here the planar counterflow diffusion flame.

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.
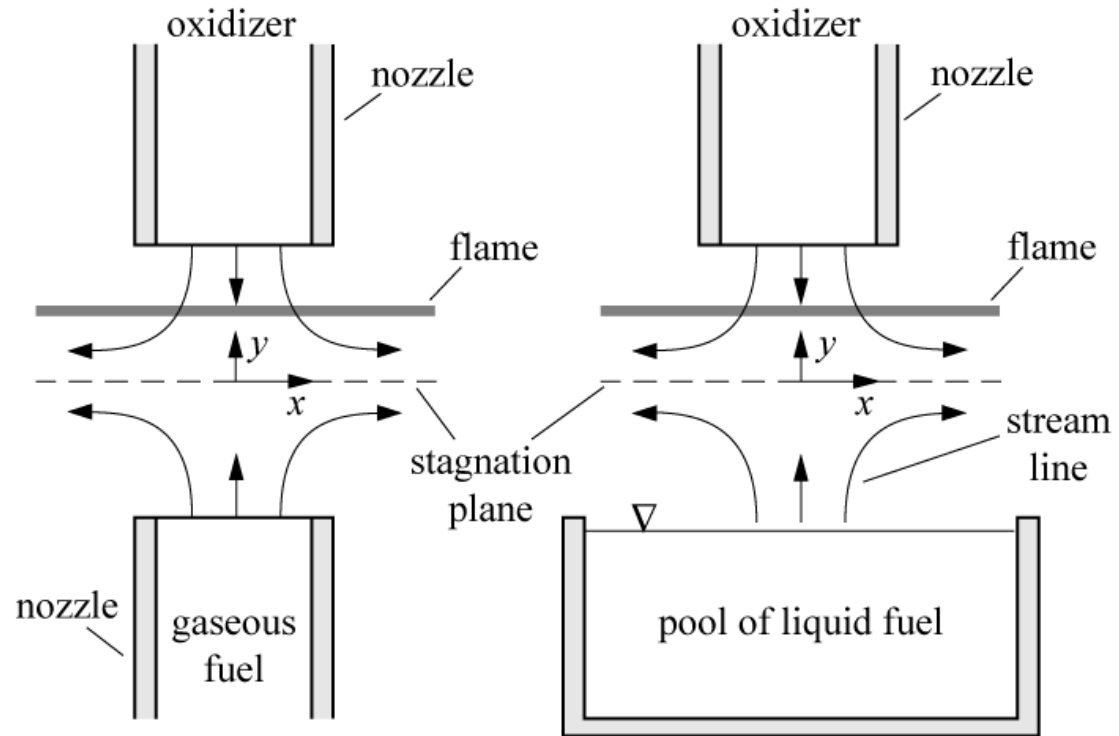
Prescribing the potential flow velocity gradient in the oxidizer stream

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

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

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

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

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

Introducing the similarity transformation

$$\eta = \left(\frac{a}{(\rho\mu)_\infty}\right)^{1/2} \int_0^y \rho\,\mathrm{d}y, \quad \xi = x$$

one obtains the system of ordinary differential equations

$$f = \int_0^\eta f'\mathrm{d}\eta$$

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

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

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-Rubesin parameter C and the Schmidt number Sc are defined

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

The boundary equations are

$$\eta = +\infty: \quad f' = 1, \ Z = 0$$
$$\eta = -\infty: \quad f' = \sqrt{\rho_\infty/\rho_{-\infty}}, \ Z = 1$$

An integral of the Z-equation is obtained as

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

where the integral $I(\eta)$ is defined as

$$I(\eta) = \int\limits_0^\eta \frac{\mathsf{Sc}}{C} \exp\left\{-\int\limits_0^\eta f\,\mathsf{Sc}/C\mathsf{d}\eta\right\}\mathsf{d}\eta$$

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

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

The instantaneous scalar dissipation rate is here

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

where

$$\eta = \left(\frac{a}{(\rho\mu)_\infty}\right)^{1/2}\int\limits_0^y \rho\,\mathsf{d}y, \quad \xi = x \quad \text{and} \quad C = \frac{\rho\mu}{(\rho\mu)_\infty}, \quad \mathsf{Sc} = \frac{\mu}{\rho D}. \quad \text{have been used.}$$

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

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

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

$$\frac{\text{d}Z}{\text{d}\eta} = -\frac{1}{2}\frac{\text{d}I}{\text{d}\eta}\frac{1}{I(\infty)} = \frac{\text{d}I}{\text{d}\eta}\frac{Z}{I(\infty) - I(\eta)} = -\frac{\text{Sc}}{C}fZ.$$

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

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

showing that χ increases as Z^2 for small Z.

Steady State Combustion and Quenching of Diffusion Flames with One-Step Chemistry

If the unsteady term is neglected

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

we obtain an ordinary differential equation that describes the structure of a steady state flamelet normal to the surface of stoichiometric mixture.

It can be solved for general reaction rates either numerically or by asymptotic analysis.

In the following we will express the chemistry by a one-step reaction with a large activation energy, assume constant pressure and the radiative heat loss to be negligible.

$$-\rho\frac{\chi_{st}}{2}\frac{\partial^2 T}{\partial Z^2} = \frac{Q}{c_p}\omega$$

We will analyze the upper branch of the S-shaped curve.

We will introduce an asymptotic analysis for large Damköhler numbers and large activation energies.

In the limit of large Damköhler numbers which corresponds to complete combustion infinitely thin sheet around $Z = Z_{st}$.
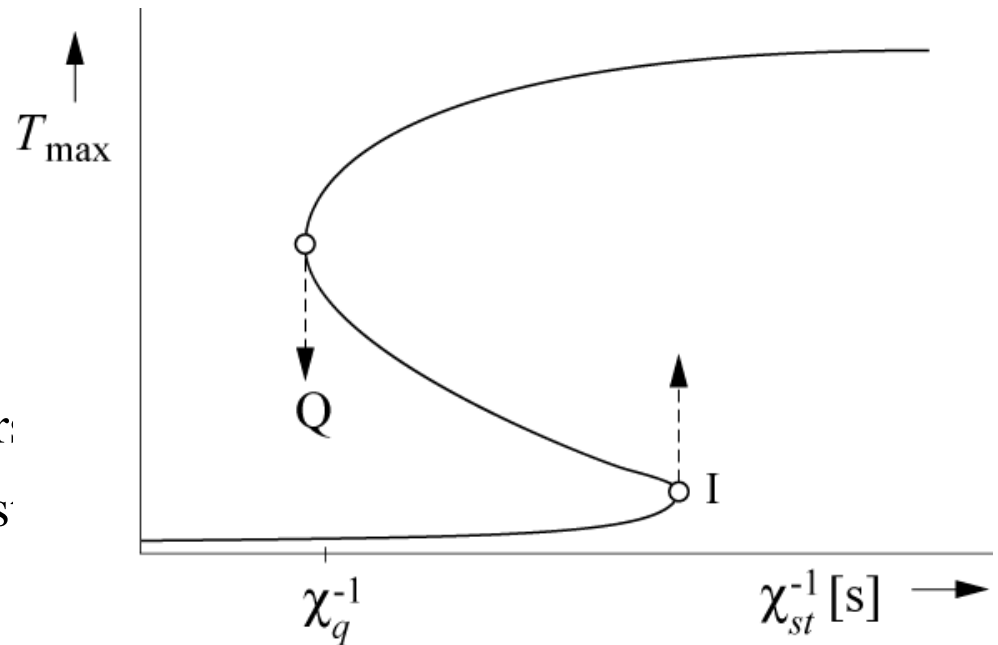
Assuming constant c_p the temperature and the fuel, oxidizer, and product mass fraction profiles are piecewise linear functions of Z.
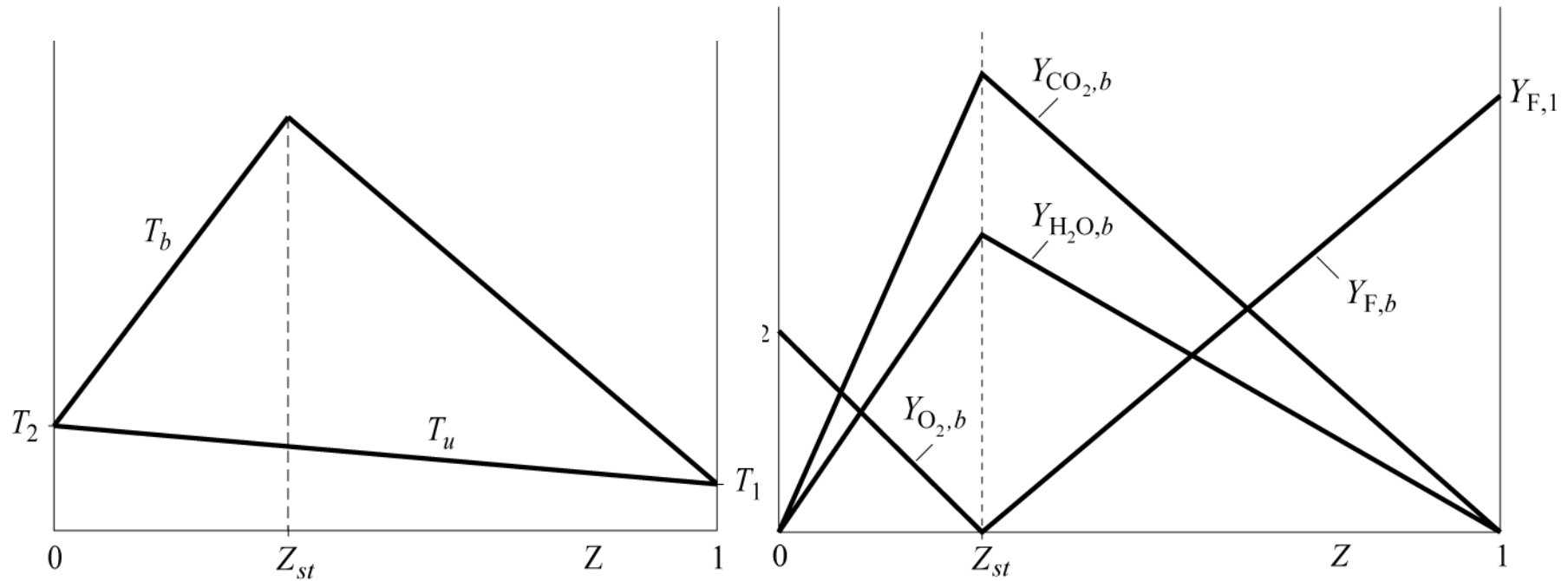
This is called the Burke-Schumann solution.
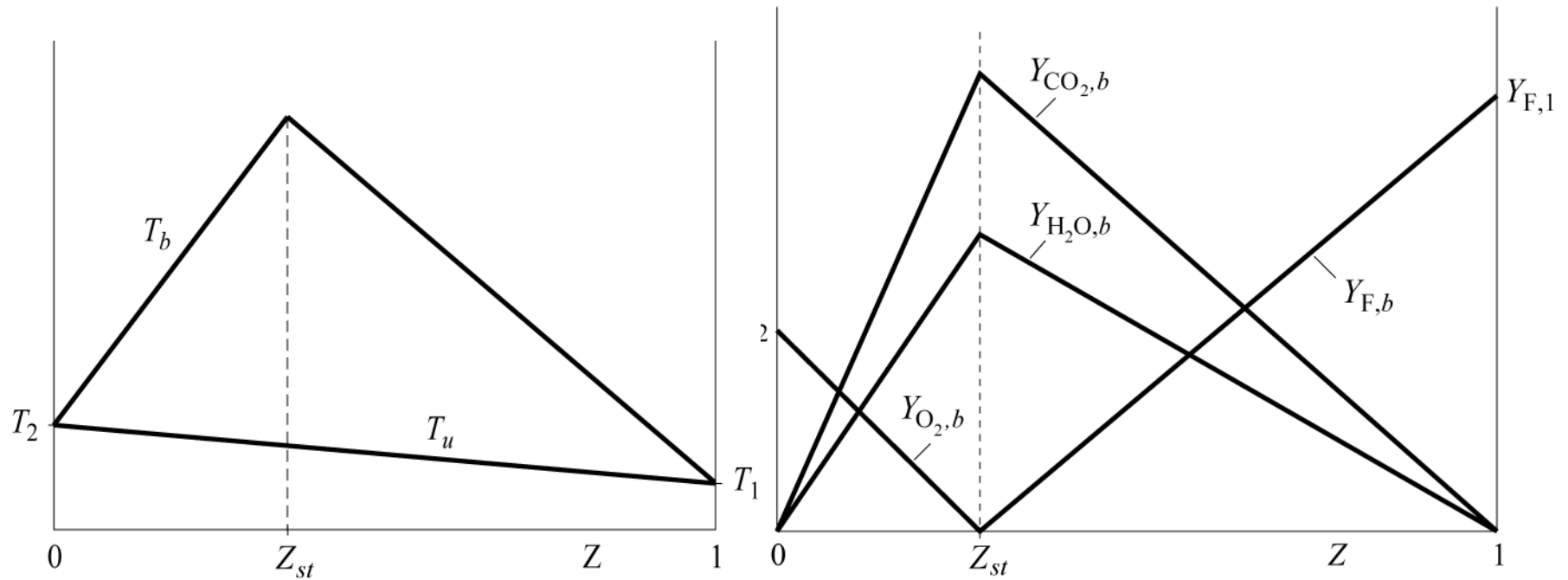
lean mixture, $Z \leq Z_{st}$:
$$T(Z) = T_u(Z) + \frac{QY_{F,1}}{c_p \nu'_F W_F} Z, \quad Y_F = 0, Y_{O_2} = Y_{O_2,2}\left(1 - \frac{Z}{Z_{st}}\right),$$

rich mixture, $Z \geq Z_{st}$:
$$T(Z) = T_u(Z) + \frac{QY_{O_2,2}}{c_p \nu'_{O_2} W_{O_2}}(1 - Z), \quad Y_{O_2} = 0, Y_F = Y_{F,1}\left(\frac{Z - Z_{st}}{1 - Z_{st}}\right)$$

where

$$T_u(Z) = T_2 + Z(T_1 - T_2)$$

We define the reaction rate as

$$\omega = B \frac{\rho Y_\mathsf{F}}{W_\mathsf{F}} \frac{\rho Y_{\mathsf{O}_2}}{W_{\mathsf{O}_2}} \exp\left(\frac{-E}{\mathcal{R}T}\right)$$

to show that

$$-\rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \frac{Q}{c_p}\omega$$

is able to describe diffusion flame quenching.

For simplicity we will assume $T_1 = T_2 = T_u$.

Then, for one reaction with

$$\frac{Q}{c_p} = \frac{(T_{st} - T_u)\nu_\mathsf{F}' W_\mathsf{F}}{Y_{\mathsf{F},1} Z_{st}}$$

$$\frac{\mathsf{d}^2 T}{\mathsf{d}Z^2} = -\frac{2B\nu_\mathsf{F}'\rho(T_{st} - T_u)}{\chi Y_{F,1} Z_{st} W_{\mathsf{O}_2}} Y_F Y_{\mathsf{O}_2} \exp\left(\frac{-E}{\mathcal{R}T}\right).$$

We define the reaction rate as

$$\omega = B \frac{\rho Y_F}{W_F} \frac{\rho Y_{O_2}}{W_{O_2}} \exp\left(\frac{-E}{\mathcal{R}T}\right) \qquad \text{and} \qquad \frac{Q}{c_p} = \frac{(T_{st} - T_u)\nu_F' W_F}{Y_{F,1} Z_{st}}$$

to show that

$$-\rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \frac{Q}{c_p}\omega$$

is able to describe diffusion flame quenching.

For simplicity we will assume $T_1 = T_2 = T_u$.

We obtain the differential equation

$$\frac{d^2 T}{dZ^2} = -\frac{2B\nu_F'\rho(T_{st} - T_u)}{\chi Y_{F,1} Z_{st} W_{O_2}} Y_F Y_{O_2} \exp\left(\frac{-E}{\mathcal{R}T}\right)$$

The temperature and the fuel and oxygen mass fraction are expanded around Z_{st} as

$$T = T_{st} - \varepsilon(T_{st} - T_u)y$$

$$Y_{\mathsf{F}} = Y_{\mathsf{F},1}\varepsilon(Z_{st}y + \xi)$$

$$Y_{\mathsf{O_2}} = Y_{\mathsf{O_2},2}\varepsilon((1 - Z_{st})y - \xi)$$

where ε is a small parameter to be defined during the analyses.

The exponential term in the reaction rate may be expanded as

$$\mathsf{exp}\left(\frac{-E}{\mathcal{R}T}\right) = \mathsf{exp}\left(\frac{-E}{\mathcal{R}T_{st}}\right) = \mathsf{exp}(-\mathsf{Ze}\varepsilon y)$$

where the Zeldovich number is defined as

$$\mathsf{Ze} = \frac{E(T_{st} - T_u)}{\mathcal{R}T_{st}^2}$$

If all other quantities in

$$\frac{\mathrm{d}^2 T}{\mathrm{d}Z^2} = -\frac{2B\nu'_\mathsf{F}\rho(T_{st} - T_u)}{\chi Y_{F,1}Z_{st}W_{\mathsf{O}_2}}Y_F Y_{\mathsf{O}_2}\exp\left(\frac{-E}{\mathcal{R}T}\right)$$

are expanded around their value at the stoichiometric flame temperature one obtains

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\xi^2} = 2\mathsf{Da}\,\varepsilon^3\,(Z_{st}y+\xi)((1-Z_{st})y-\xi)\exp(-\mathsf{Ze}\,\varepsilon\,y),$$

where

$$\mathsf{Da} = \frac{B\rho_{st}\nu'_{\mathsf{O}_2}Y_{\mathsf{F},1}}{\chi_{st}W_\mathsf{F}(1-Z_{st})}\exp\left(\frac{-E}{\mathcal{R}T}\right)$$

is the Damköhler number.

The differential equation

$$\frac{\mathrm{d}^2 y}{\mathrm{d}\xi^2} = 2\mathsf{Da}\,\varepsilon^3\,(Z_{st}y+\xi)((1-Z_{st})y-\xi)\exp(-\mathsf{Ze}\,\varepsilon\,y),$$

is cast into the same form as the one that governs Liñán's diffusion flame regime by using the further transformation

$$z = 2y(1-Z_{st})Z_{st} - \gamma\xi$$

$$\gamma = 2Z_{st} - 1$$

to yield

$$\beta = \mathsf{Ze}/[2Z_{st}(1-Z_{st})]$$

$$\frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2} = \mathsf{Da}\varepsilon^3(z^2 - \xi^2)\exp[-\beta\varepsilon(z+\gamma\xi)]$$

There are evidently two ways to define the expansion parameter ε.

Either by setting
$$\beta\varepsilon = 1$$

or by setting
$$\mathsf{Da}\varepsilon^3 = 1$$

The first one would be called a large activation energy expansion and the second one a large Damköhler number expansion.

Both formulations are interrelated if we introduce the distinguished limit, where the rescaled Damköhler number

$$\delta = \mathsf{Da}/\beta^3 \overset{!}{=} \mathcal{O}(1)$$

is assumed to be of order one.

Thus a definite relation between the Damköhler number and the activation energy is assumed as $\varepsilon \to 0$.

We set

$$\varepsilon = \mathsf{Da}^{-1/3} = \delta^{-1/3}/\beta$$

to obtain Liñán's equation for the diffusion flame regime

$$\frac{\mathrm{d}^2 z}{\mathrm{d}\xi^2} = (z^2 - \xi^2)\exp[-\delta^{-1/3}(z + \gamma\xi)].$$

The boundary conditions are obtained by matching to the outer flow solution

$$\frac{\mathrm{d}z}{\mathrm{d}\xi} = 1 \qquad \text{for} \quad \xi \to \infty,$$

$$\frac{\mathrm{d}z}{\mathrm{d}\xi} = -1 \qquad \text{for} \quad \xi \to -\infty$$

The essential property of this equation, as compared to the large Damköhler number limit $\delta \to \infty$ is that the exponential term remains, since δ was assumed to be finite.
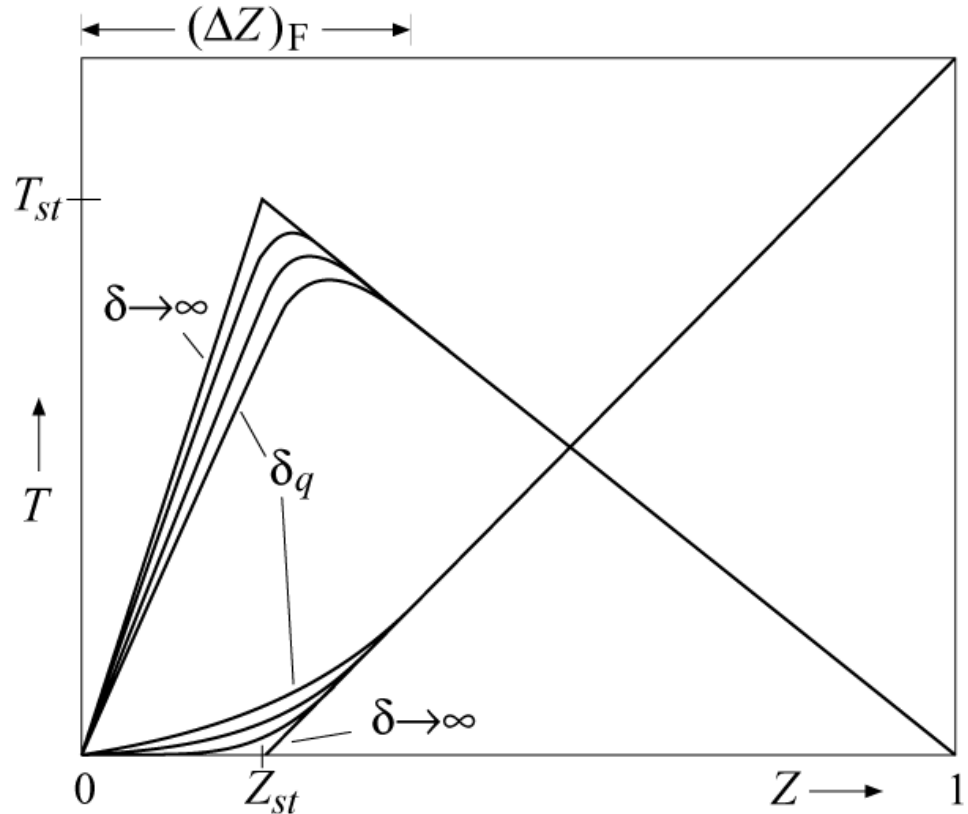
This allows extinction to occur if the parameter δ decreases below a critical value δ_q.

Liñán gives an approximation of δ_q in terms of $|\gamma|$.

For small values of Z_{st} extinction occurs at the transition to the premixed-flame regime. He obtains

$$\delta_q = e(1 - |\gamma|)$$

Characteristic profiles for the temperature over Z with δ as a parameter.

There is a limiting profile $T_q(Z)$ corresponding to δ_q.

Any solution below this profile is unstable, and the flamelet would be extinguished.

The extinction condition $\delta = \delta_q$ defines with

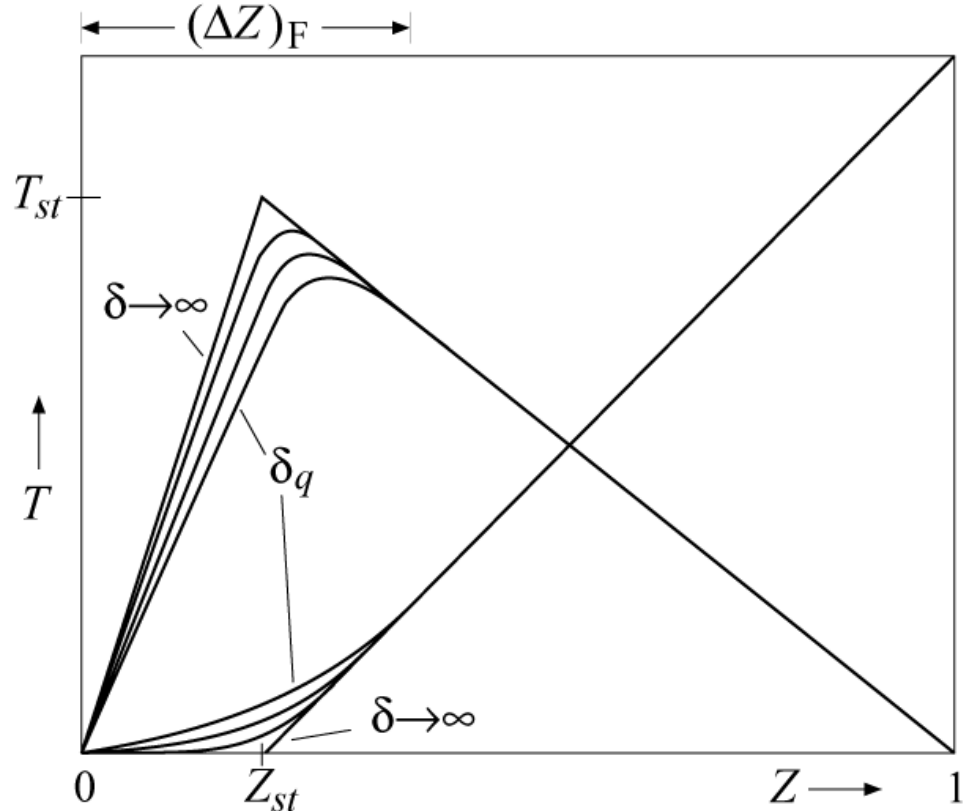$$\delta = \mathsf{Da}/\beta^3$$

and

$$\mathsf{Da} = \frac{B\rho_{st}\nu'_{\mathsf{O}_2}Y_{\mathsf{F},1}}{\chi_{st}W_{\mathsf{F}}(1 - Z_{st})}\exp\left(\frac{-E}{\mathcal{R}T}\right)$$

a maximum dissipation rate χ_q at the surface of stoichiometric mixture for a flamelet to be burning, namely
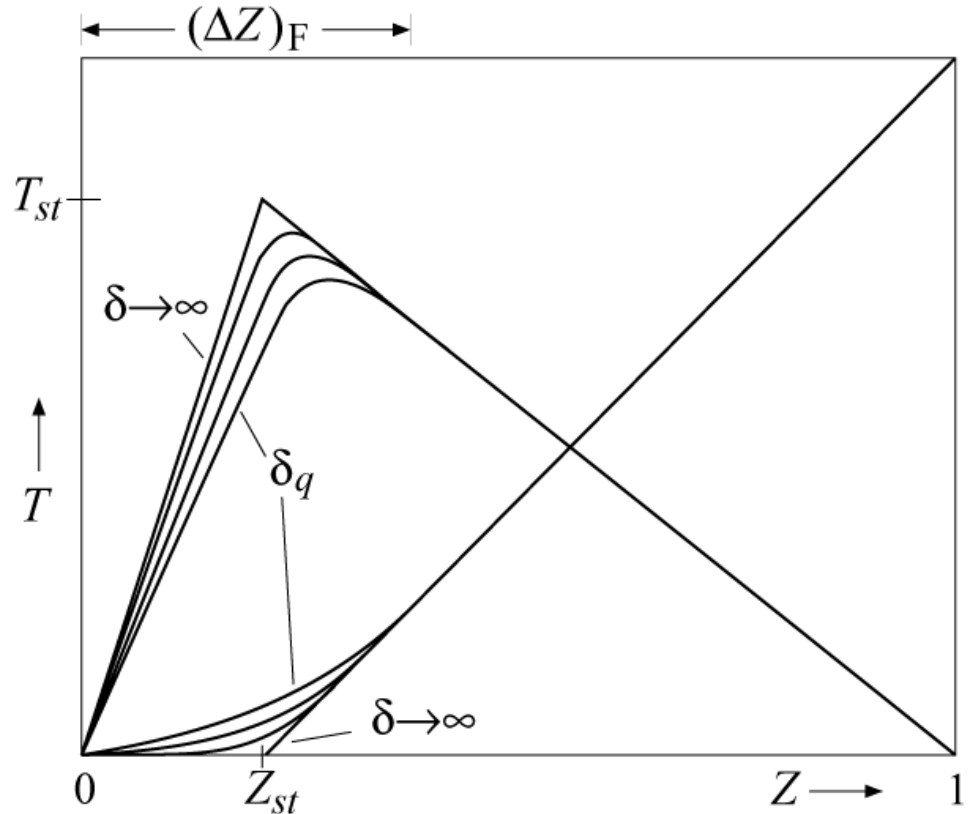

$$\chi_q = \frac{8B\rho_{st}\nu'_{\mathsf{O}_2}Y_{F,1}Z_{st}^3(1 - Z_{st})^2}{W_{\mathsf{F}}\delta_q\mathsf{Ze}^3}\exp\left(\frac{-E}{\mathcal{R}T_{st}}\right)$$

We may interpret χ_{st} as the inverse of a characteristic diffusion time.

If χ_{st} is large, heat will be conducted to both sides of the flamelet at a rate that is not balanced by the heat production due to chemical reaction.

Thus the maximum temperature will decrease until the flamelet is quenched at a value of $\chi_{st} = \chi_q$.

Burning of the flamelet corresponds 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.

T_{max}

Q

Quenching

I

χ_q^{-1}

χ_{st}^{-1} [s]
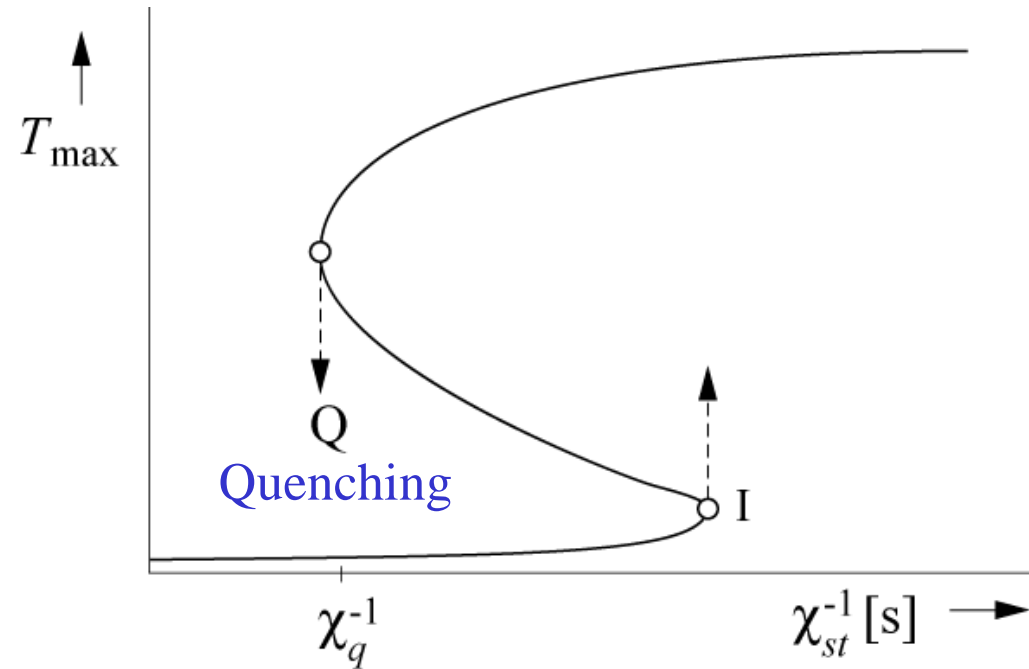
The transition from the point Q to the lower state corresponds to the unsteady transition.

Auto-ignition, which would correspond to an unsteady transition from the point I to the upper curve, is unlikely to occur in open diffusion flames, since the required very large residence times (very small values of χ_{st}) are not reached.

An example for auto-ignition in non-premixed systems is the combustion in a Diesel engine.

Here interdiffusion of the fuel from the Diesel spray with the surrounding hot air leads to continuously decreasing mixture fraction gradients and therefore to decreasing scalar dissipation rates.

This corresponds to a shift on the lower branch of the S-shaped curve up to the point I where ignition occurs.
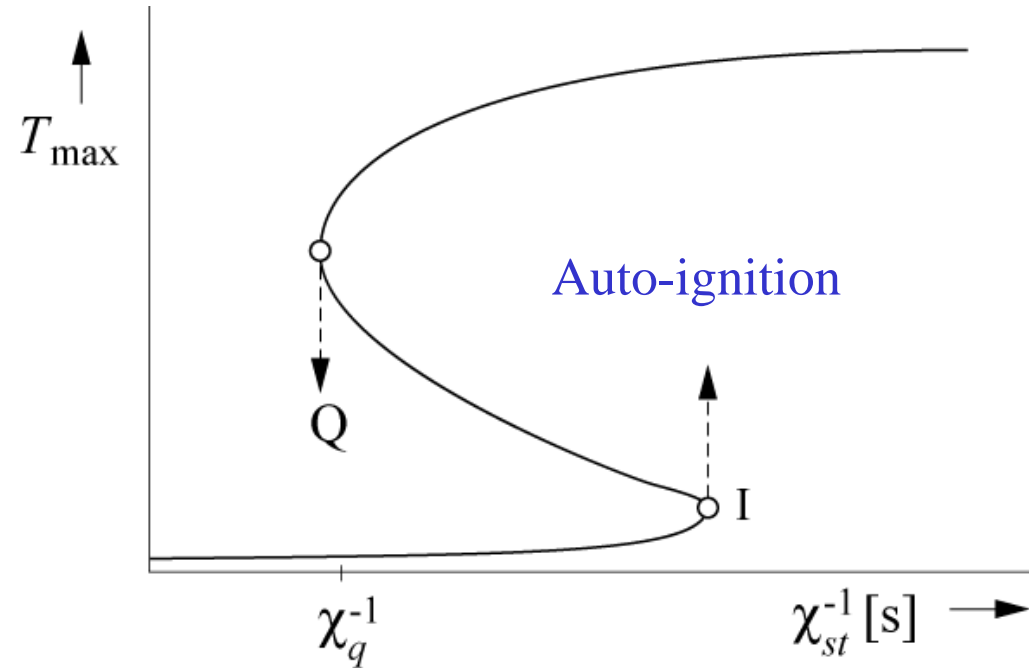
Time and Length Scales in Diffusion Flames

We will define the chemical time scale at extinction as

$$t_c = Z_{st}^2 (1 - Z_{st})^2 / \chi_q.$$

This definition is motivated by expression

$$\chi_q = \frac{8 B \rho_{st} \nu'_{O_2} Y_{F,1} Z_{st}^3 (1 - Z_{st})^2}{W_F \delta_q \mathsf{Ze}^3} \exp\left(\frac{-E}{\mathcal{R} T_{st}}\right)$$

By comparing this with the time scale of a premixed flame with the same chemical source term one obtains

$$t_c = \frac{\delta_q (\rho \lambda / c_p)_{st}}{2 (\rho_u s_L)_{st}^2}$$

Here $\rho_u\, s_L$ has been calculated from

$$\rho_u s_L = \sqrt{2\frac{B\rho_b^2\lambda_b\mathcal{R}^2 T_b^4}{c_p(T_b - T_u)^2 E^2}\exp\left(-\frac{E}{\mathcal{R}T_b}\right)S}$$

$$S \quad = \frac{\nu_\mathsf{F}' Y_{\mathsf{O}_2,b}}{M_{\mathsf{O}_2}} + \frac{\nu_{\mathsf{O}_2}' Y_{\mathsf{F},b}}{M_\mathsf{F}} + \frac{2\,\nu_{\mathsf{O}_2}'\nu_\mathsf{F}' c_p \mathcal{R} T_b^2}{(-\Delta H)E}.$$

and

$$S = \begin{cases} \dfrac{\nu_\mathsf{F}' Y_{\mathsf{O}_2,b}}{M_{\mathsf{O}_2}} & \text{for} \quad \phi \ll 1, \\[2em] \dfrac{2\,\nu_{\mathsf{O}_2}'\nu_\mathsf{F}' c_p \mathcal{R} T_b^2}{(-\Delta H)E} & \text{for} \quad \phi = 1, \\[2em] \dfrac{\nu_{\mathsf{O}_2}' Y_{\mathsf{F},b}}{M_\mathsf{F}} & \text{for} \quad \phi \gg 1. \end{cases}$$

for a stoichiometric premixed flame.

This indicates that there is a fundamental relation between a premixed flame and a diffusion flame at extinction:

In a diffusion flame at extinction the heat conduction out of the reaction zone towards the lean and the rich side just balances the heat generation by the reaction.

In a premixed flame the heat conduction towards the unburnt mixture is such that it balances the heat generation by the reaction for a particular burning velocity.

These two processes are equivalent.

A diffusion flame, however, can exist at lower scalar dissipation rates and therefore at lower characteristic flow times.

The flow time in a premixed flow is fixed by the burning velocity, which is an eigenvalue of the problem.

Therefore combustion in diffusion flame offers an additional degree of freedom: that of choosing the ratio of the convective to the reactive time, represented by the Damköhler number defined in

$$\mathsf{Da} = \frac{B\rho_{st}\nu'_{\mathsf{O}_2}Y_{\mathsf{F},1}}{\chi_{st}W_{\mathsf{F}}(1-Z_{st})}\exp\left(\frac{-E}{\mathcal{R}T}\right)$$

as long as $\chi_{st} < \chi_q$.

This makes non-premixed combustion to be better controllable and diffusion flames more stable.

It is also one of the reasons why combustion in Diesel engines which operate in the non-premixed regime is more robust and less fuel quality dependent than that in spark ignition engines where fuel and air are premixed before ignition.

Equations

$$t_c = Z_{st}^2(1 - Z_{st})^2 / \chi_q.$$

and

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

may now be used to calculate chemical time scales for diffusion flames:

$$\text{erfc}^{-1}(2Z_{st}) = \begin{cases} 1.34 & \text{for hydrogen-air flames with } Z_{st} = 0.0284 \\ 1.13 & \text{for methane-air flames with } Z_{st} = 0.055 \end{cases}$$

Extinction of the hydrogen-air diffusion flame occurs at a strain rate a_q =14260/s and that of the methane-air flame at 420/s.

$$\Rightarrow \quad t_c = \begin{cases} 0.64 \cdot 10^{-5} & \text{for hydrogen-air flames} \\ 0.29 \cdot 10^{-3} & \text{for methane-air flames} \end{cases}$$

The latter estimate is of the same order of magnitude as t_c for stoichiometric premixed methane flames.

In diffusion flames, in contrast to premixed flames, there is no velocity scale, such as the burning velocity, by which a characteristic length scale such as the premixed flame thickness could be defined.

There is, however, the velocity gradient a, the inverse of which may be interpreted as a flow time.

Based on this flow time one may define an appropriate diffusive length scale.

Based on this flow time $1/a$ one may define an appropriate diffusive length scale.

Dimensional analysis leads to a diffusive flame thickness

$$\ell_F = \sqrt{\frac{D_{\mathrm{ref}}}{a}}.$$

Here the diffusion coeffcient D should be evaluated at a suitable reference condition, conveniently chosen at stoichiometric mixture.

Assuming a one-dimensional mixture fraction profile in y-direction as for the insteady mixing layer the flame thickness in mixture fraction space may be defined

$$(\Delta Z)_F = \left(\frac{\partial Z}{\partial y}\right)_F \ell_F$$

Here $\left(\dfrac{\partial Z}{\partial y}\right)_F$ is the mixture fraction gradient normal to the flamelet.

This flamelet thickness contains the reaction zone and the surrounding diffusive layers.

The equation

$$(\triangle Z)_F = \left(\frac{\partial Z}{\partial y}\right)_F \ell_F$$

leads with

$$\ell_F = \sqrt{\frac{D_{\mathsf{ref}}}{a}}. \qquad \text{and} \qquad \chi_{st} = 2D\left(\frac{\partial Z}{\partial x_\alpha}\right)^2$$

to

$$(\triangle Z)_F = \sqrt{\frac{\chi_{\mathsf{ref}}}{2a}}$$

where χ_{ref} represents the scalar dissipation rate at the reference condition.

If χ_{ref} is evaluated at Z_{st} and $\chi = 2af^2Z^2(\mathrm{Sc}/C)$ is used, it is seen that ΔZ_F is of the order of Z_{st}, if Z_{st} is small.

With an estimate $\Delta Z_F = 2\,Z_{st}$ the flame thickness would cover the reaction zone and the surrounding diffusive layers in a plot of the flamelet structure in mixture fraction space.

Diffusion Flame Structure of Methane-Air Flames

The 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.
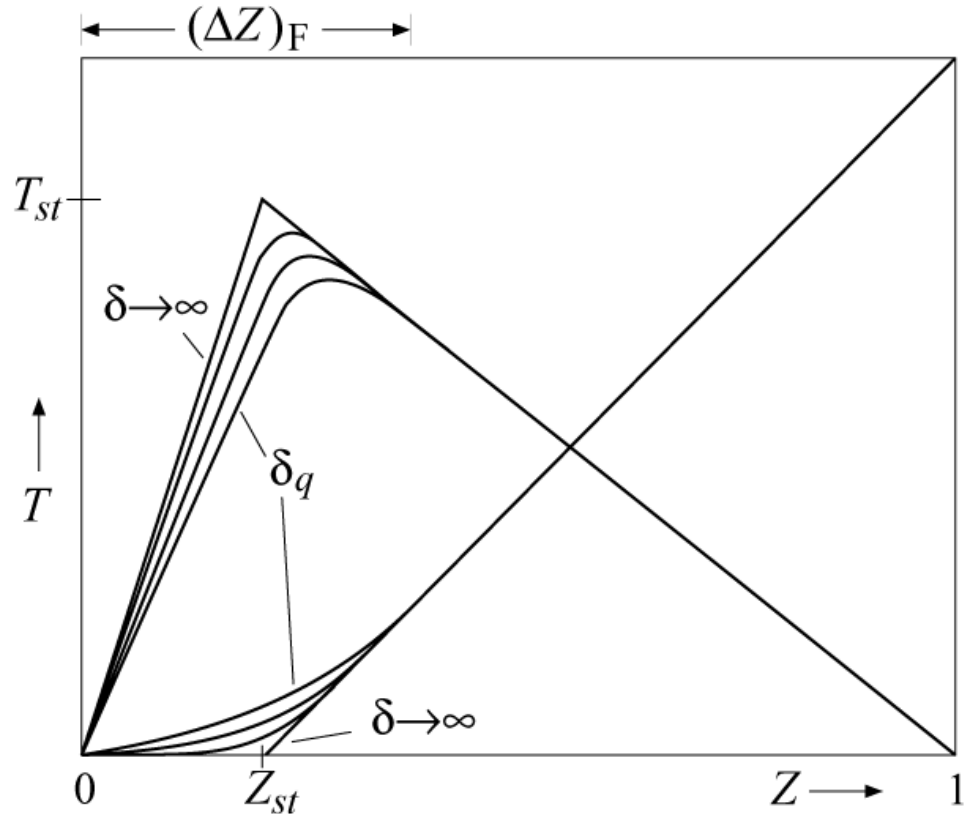
Experiments of methane flames, on the contrary, show leakage of oxygen rather
than of fuel through the reaction zone.

A numerical calculation with the four-step reduced mechanism

$$CH_4 + 2H + H_2O = CO + 4H_2$$

$$CO + H_2O = CO_2 + H_2$$

$$H + H + M = H_2 + M$$

$$O_2 + 3H_2 = 2H + 2H_2O$$

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.
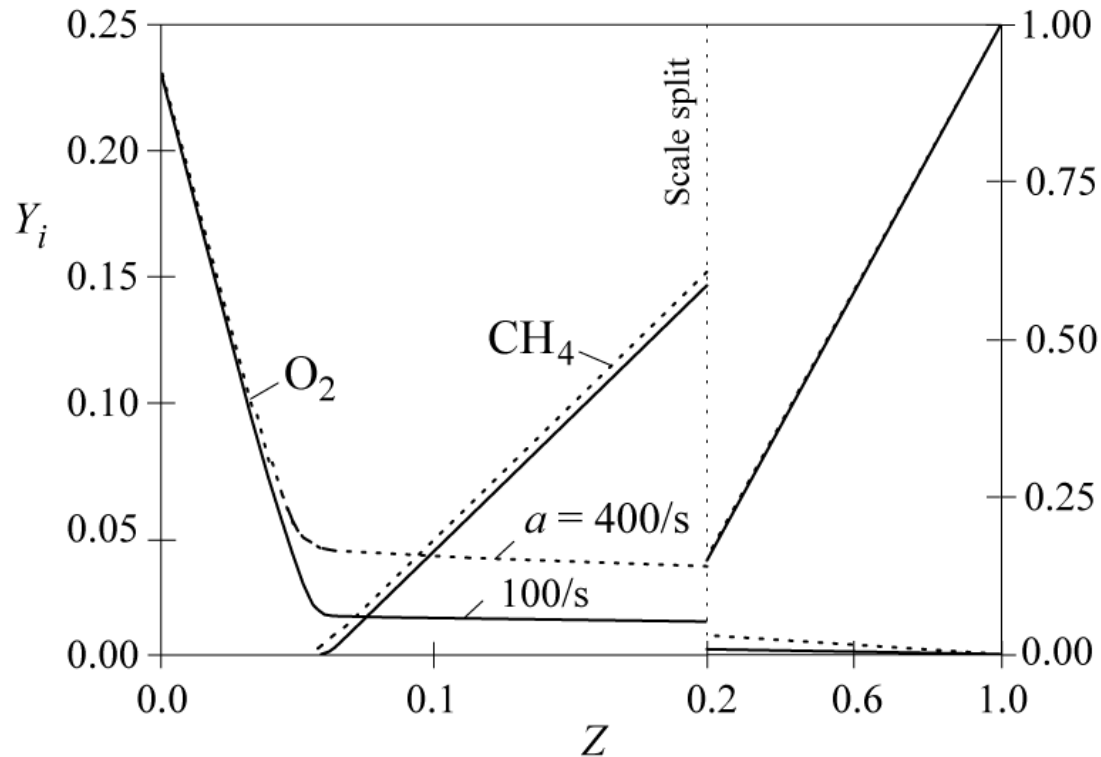
Temperature profiles for methane-air flames
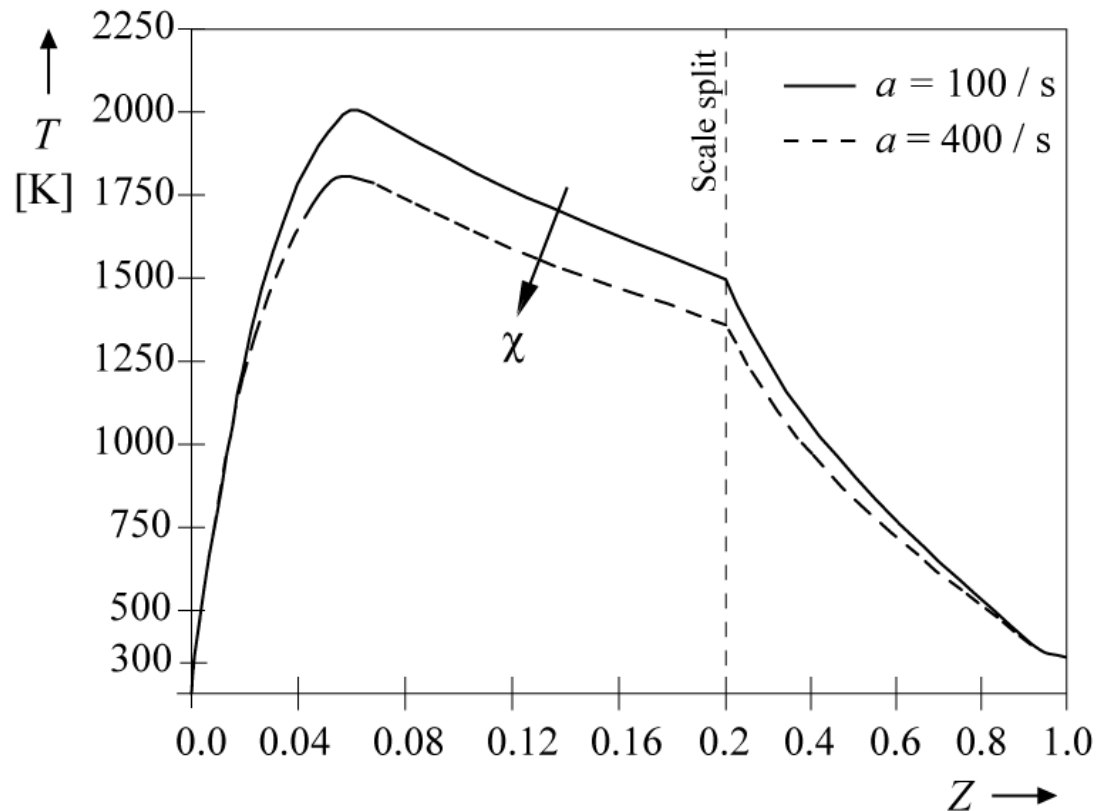
The second value of the strain rate corresponds to a condition close to extinction.

It is seen that the temperature in the reaction zone decreases

Fuel and oxygen mass fractions 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.
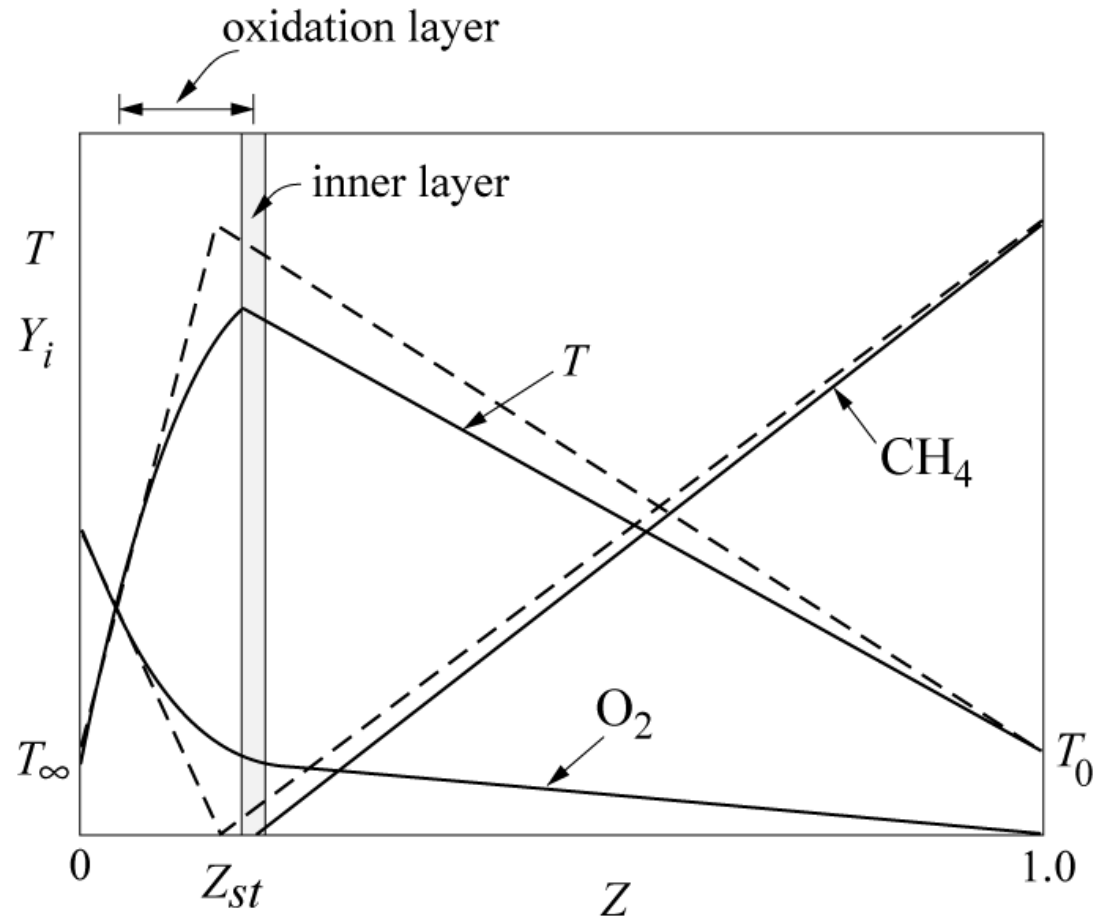
The outer structure of the diffusion flame is the classical Burke-Schumann structure governed by the overall one-step reaction

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$
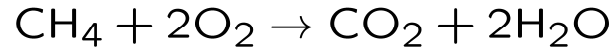
with the flame sheet positioned at $Z = Z_{st}$.

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 the rich part of the diffusion flame corresponds to the upstream preheat zone of the premixed flame while its lean part corresponds to the downstream oxidation layer.

The maximum temperature corresponds to the inner layer temperature of the asymptotic structure.

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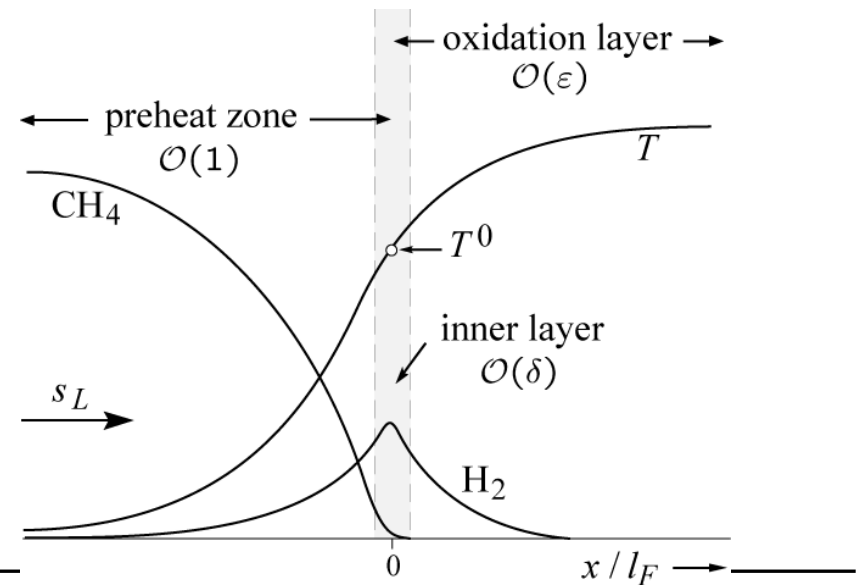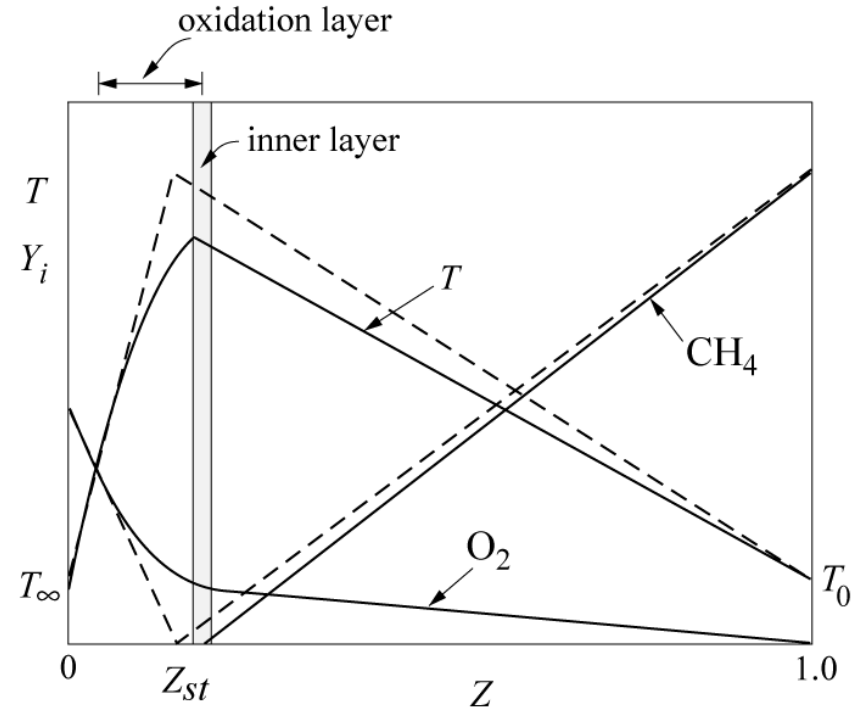
The plot of the maximum temperature also corresponds to the upper branch of the S-shaped curve.

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