Laminar Diffusion Flames

CEFRC Combustion Summer School

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Course Overview

Part I: Fundamentals and Laminar Flames

- Introduction
- Fundamentals and mass balances of combustion systems
- Thermodynamics, flame temperature, and equilibrium
- Governing equations
- Laminar premixed flames: Kinematics and Burning Velocity
- Laminar premixed flames: Flame structure
- Laminar diffusion flames

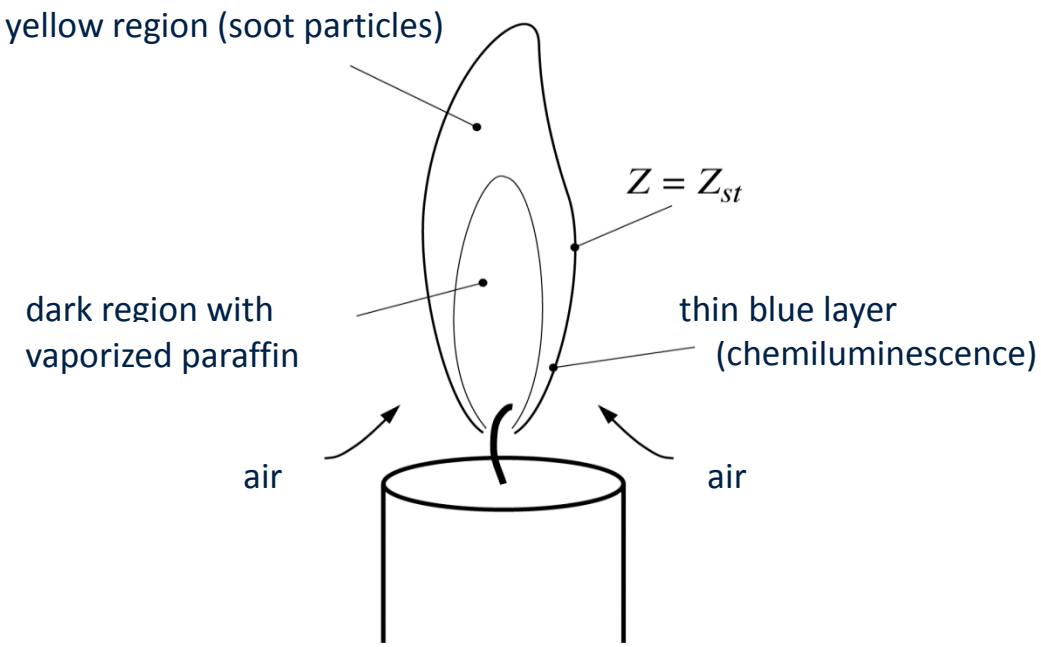
- Introduction
- Counterflow diffusion flame
- Flamelet structure of diffusion flames
- FlameMaster flame calculator
- Single droplet combustion

Laminar diffusion flames

- Seperate feeding of fuel and oxidizer into the combustion chamber
  - Diesel engine
  - Jet engine
- In the combustion chamber:
  - Mixing
  - Subsequently combustion
- Mixing: Convection and diffusion
  - On a molecular level
    → (locally) stoichiometric mixture
- Simple example for a diffusion flame: Candle flame
  - Paraffin vaporizes at the wick
    → diffuses into the surrounding air
- Simultaneously: Air flows towards the flame due to free convection and forms a mixture with the vaporized paraffin

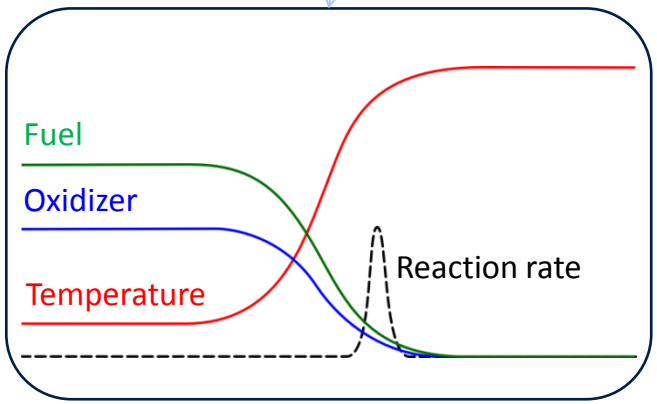
Injection and combustion in a diesel engine

Candle flame

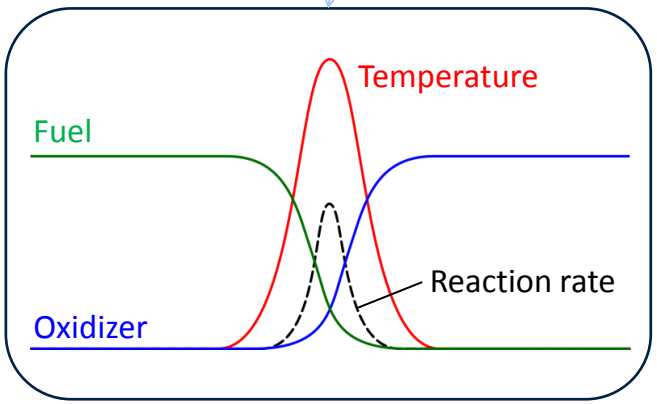


- In a first approximation, combustion takes place at locations, where the concentrations of oxygen and fuel prevail in stoichiometric conditions.

Comparison of laminar premixed and diffusion flames



Structure of a premixed flame (schematic)



Structure of a diffusion flame (schematic)

Soot in candle flames

- Soot particles
  - Formation in fuel rich regions of the flame
  - Transported to lean regions through the surface of stoichiometric mixture
  - In the oxygen containing ambient: Combustion of the soot particles

- Sooting flame: Residence time of the soot particles in the region of oxidizing ambient and high temperatures too short to burn all particles

Timescales

- Considering the relative times required for
  - Convection and diffusion
  - Proceeding reactions

- For technical combustion processes in diffusion flames:
  - Characteristic times of convection and diffusion are approximately of same order of magnitude
  - Characteristic times of chemical reactions much smaller
- Limit of fast chemical reactions

➢ Mixing is the slowest and therefore rate determining process

→ “mixed = burnt”

The mixture fraction

- Mixture fraction: $$Z = \frac{\nu Y_{\mathrm{B}} - Y_{\mathrm{O_2}} + Y_{\mathrm{O_2},2}}{\nu Y_{\mathrm{B},1} + Y_{\mathrm{O_2},2}}$$

- Stoichiometric mixture fraction:

$$Z_{st} = \frac{Y_{\mathrm{O_2},2}}{\nu Y_{\mathrm{F},1} + Y_{\mathrm{O_2},2}}$$

- Relation with equivalence ratio

$$\phi = \frac{Z}{1 - Z} \frac{(1 - Z_{st})}{Z_{st}}$$

  - Pure oxidizer ($\phi = 0$): $Z = 0$
  - Pure fuel ($\phi = \infty$): $Z = 1$

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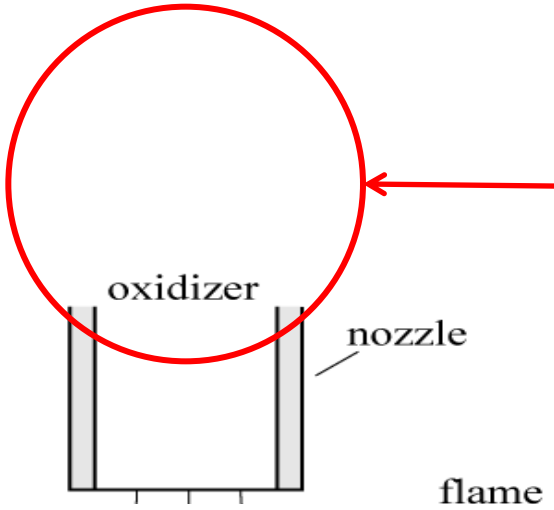
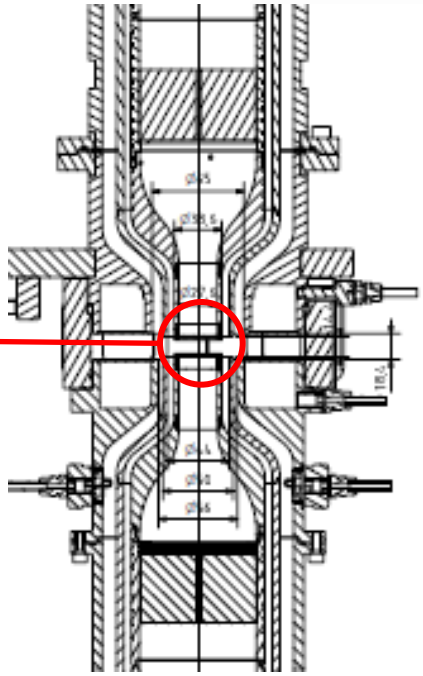
Counterflow Diffusion flame

- One-dimensional similarity solution
- Strain appears as parameter → Da
- Used for
  - Studying flame structure
  - Studying chemistry in diffusion flames
  - Study interaction of flow and chemistry





Counterflow diffusion flame: Governing Equations

- Continuity

$$\frac{\partial}{\partial v}(\rho V) + \frac{1}{x}\frac{\partial}{\partial x}(\rho x U) = 0$$

- X – Momentum

$$\rho U\frac{\partial U}{\partial x} + \rho V\frac{\partial U}{\partial y} = -\frac{\partial P}{\partial x} + \frac{1}{x}\frac{\partial}{\partial x}\left(x\mu\frac{\partial U}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu\frac{\partial U}{\partial y}\right) - \mu\frac{U}{x^2} + \frac{\partial U}{\partial x}\frac{\partial \mu}{\partial x} + \frac{\partial V}{\partial x}\frac{\partial \mu}{\partial y}$$

- Energy

$$\rho U c_p\frac{dT}{dx} + \rho V c_p\frac{dT}{dy} = \frac{1}{x}\frac{\partial}{\partial x}\left(x\lambda\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right) - \sum_{i=1}^{N} h_i \dot{m}_i - \sum_{i=1}^{N} c_{p,i} j_{i,y}\frac{dT}{dy} - \sum_{i=1}^{N} c_{p,i} j_{i,x}\frac{dT}{dx}.$$

Counterflow diffusion flame: Similarity solution

- Three assumptions reduce systems of equation to 1D

1. Similarity assumption for velocity

$$U = G(y)x$$

2. Similarity assumption

$$P = P_0 - \frac{1}{2}\left(P'x^2\right) + F(y)$$

3. Mass fractions and temperature have no radial dependence close to centerline

Counterflow diffusion flame: Similarity solution

- This results in

$$\frac{\partial}{\partial y}(\rho V) + 2\rho G = 0$$

$$\rho G^2 + \rho V \frac{dG}{dy} = P' + \frac{d}{dy}\left(\mu \frac{dG}{dy}\right)$$

$$\rho V c_p \frac{dT}{dy} = \frac{d}{dy}\left(\lambda \frac{dT}{dy}\right) - \sum_{i=1}^{N} h_i \dot{m}_i - \sum_{i=1}^{N} c_{p,i} j_{i,y} \frac{dT}{dy}$$

- with boundary conditions

$$y \to 0 : V = V_{\text{nozzle}},\ G = (dU/dx)_{x=0,\ y=0},\ T = T_{\text{u}}$$

$$y \to L : V = -V_{\text{nozzle}},\ G = (dU/dx)_{x=0,\ y=L},\ T = T_{\text{u}}$$

Counterflow diffusion flame: Similarity solution

- Alternatively, potential flow boundary conditions can be used at $y \rightarrow \pm\infty$ instead of nozzles
- With definition of strain rate

$$a = \frac{du_\infty}{dx}$$

the similarity coordinate η

$$\eta = \left[\frac{a}{(\rho\mu)_{\text{ref}}}\right]^{1/2} \int_0^y \rho \, dy$$

the non-dimensional stream function f defined by

$$\rho u = \sqrt{(\rho\mu)_{\text{ref}} a}\, x \frac{\partial f}{\partial y} \qquad \rho v = -\sqrt{(\rho\mu)_{\text{ref}} a}\, \frac{\partial x f}{\partial x}$$

and the Chapman-Rubesin parameter

$$C = \frac{\rho\mu}{(\rho\mu)_{\text{ref}}}$$

the 1D similarity solution can be derived

Counterflow diffusion flame: Similarity solution

- Potential flow similarity solution

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

$$f\frac{\mathrm{d}Y_i}{\mathrm{d}\eta}-\frac{1}{\sqrt{(\rho\mu)_{\mathrm{ref}}a}}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\rho Y_i V_{iy}\right)+\frac{\dot{m}_i}{\rho a}=0\,,\qquad i=1,2,...,n$$

$$f\frac{\mathrm{d}T}{\mathrm{d}\eta}+\frac{1}{c_p(\rho\mu)_{\mathrm{ref}}}\frac{\mathrm{d}}{\mathrm{d}\eta}\left(\rho\lambda\frac{\mathrm{d}T}{\mathrm{d}\eta}\right)-\frac{1}{\sqrt{(\rho\mu)_{\mathrm{ref}}a}}\frac{\mathrm{d}T}{\mathrm{d}\eta}\sum_{i=1}^{n}\frac{c_{pi}}{c_p}\rho Y_i V_{iy}-\frac{1}{c_p\rho a}\sum_{i=1}^{n}\dot{m}_i h_i-\frac{1}{c_p\rho a}\sum_{i=1}^{n}q_{Ri}=0$$

- With Dirichlet boundary conditions for mass fractions and temperature

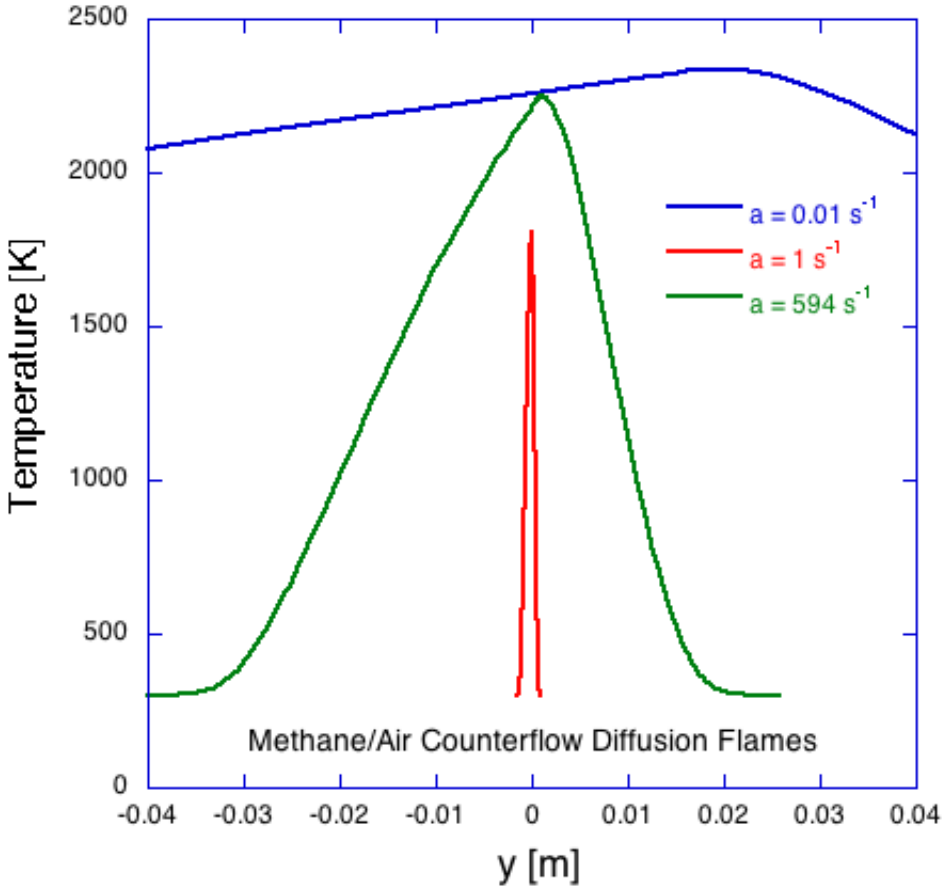
$$\eta\to-\infty:\quad \frac{\mathrm{d}f}{\mathrm{d}\eta}=\sqrt{\frac{\rho_\infty}{\rho_{-\infty}}}\qquad \eta=0:\quad f=0\qquad \eta\to\infty:\quad \frac{\mathrm{d}f}{\mathrm{d}\eta}=1$$

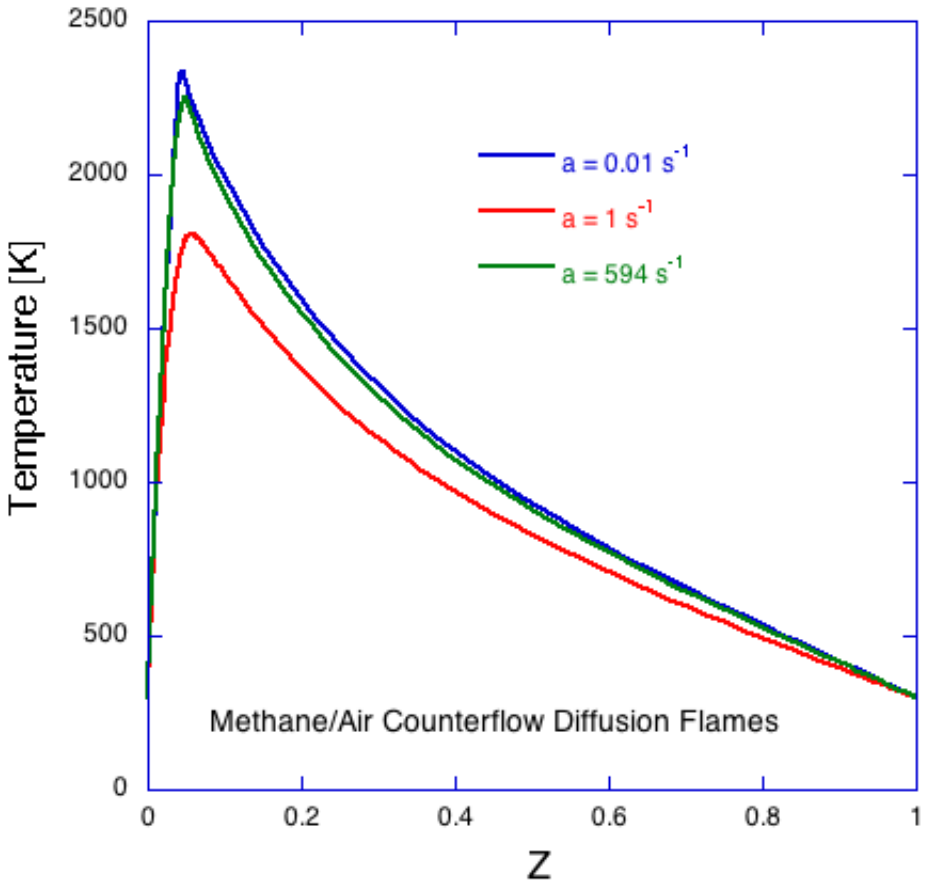
and where the velocities are obtained from

$$u=a\xi\frac{\partial f}{\partial\eta}\qquad \rho v=-\sqrt{(\rho\mu)_{\mathrm{ref}}a}\,f(\eta)$$

Structure of non-premixed laminar flames

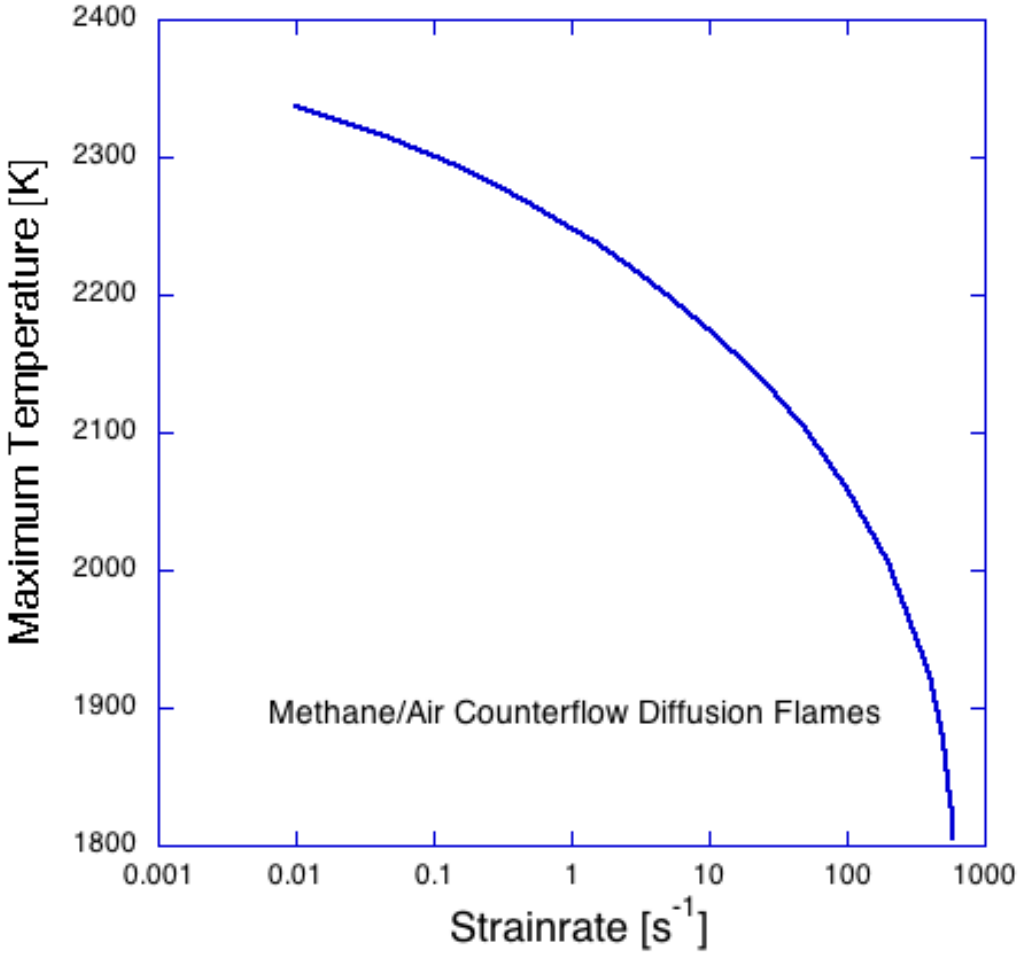
Temperature for methane/air counterflow diffusion flames





Structure of non-premixed laminar flames

Maximum flame temperature for methane/air counterflow diffusion flames



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Theoretical description of diffusion flames

- Assumption of fast chemical reactions
  - Without details of the chemical kinetics
  - Global properties, e.g. flame length

- If characteristic timescales of the flow and the reaction are of same order of magnitude:
  - Chemical reaction processes have to be considered explicitly
  - Liftoff and extinction of diffusion flames
  - Formation of pollutants

- Flamelet formulation for non-premixed combustion
  - Mixture fraction as independent coordinate for all reacting scalars,
  - Asymptotic approximation in the limit of sufficiently fast chemistry to one-dimensional equations for reaction zone

Flamelet structure of a diffusion flame

- Assumptions: Equal diffusivities of chemical species and temperature

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

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

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

- Low Mach number limit
  - Zero spatial pressure gradients
  - Temporal pressure change is retained

Flamelet structure of a diffusion flame

- Balance equation for the mixture fraction

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

- No chemical source term, since elements are conserved in chemical reactions

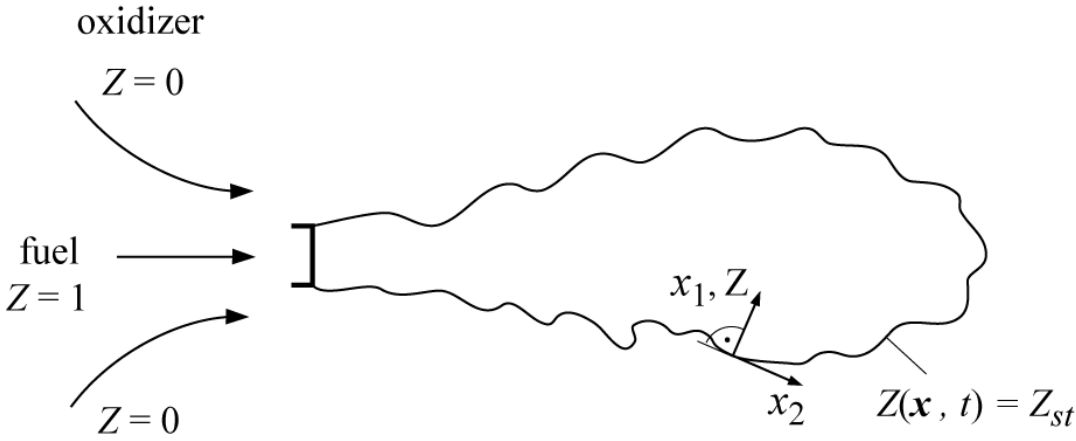
- We assume the mixture fraction Z to be given in the flow field as a function of space and time: $Z = Z(x_\alpha, t)$

Flamelet structure of a diffusion flame

- Surface of the stoichiometric mixture: $Z(x_\alpha, t) = Z_{st}$
- If local mixture fraction gradient is sufficiently high:

  → Combustion occurs in a thin layer in the vicinity of this surface

- Locally introduce an orthogonal coordinate system x_1, x_2, x_3 attached to the surface of stoichiometric mixture



- x_1 points normal to the surface Z_{st} , x_2 and x_3 lie within the surface

- Replace coordinate x_1 by mixture fraction Z

  and x_2, x_3 and t by $Z_2 = x_2$, $Z_3 = x_3$ and $t = \tau$

Flamelet structure of a diffusion flame

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

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

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

we obtain the temperature equation in the form

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

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

- Transformation of equation for mass fractions is similar

Flamelet structure of a diffusion flame

- If 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

Flamelet structure of a diffusion flame

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

- Time derivative $\partial T/\partial \tau$ important if very rapid changes occur, e.g. extinction

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

Flamelet structure of a diffusion flame

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

- Dimension 1/s → Inverse of characteristic diffusion time
- Depends on *t* and *Z* and acts as a external parameter, representing the flow and the mixture field

Flamelet structure of a diffusion flame

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

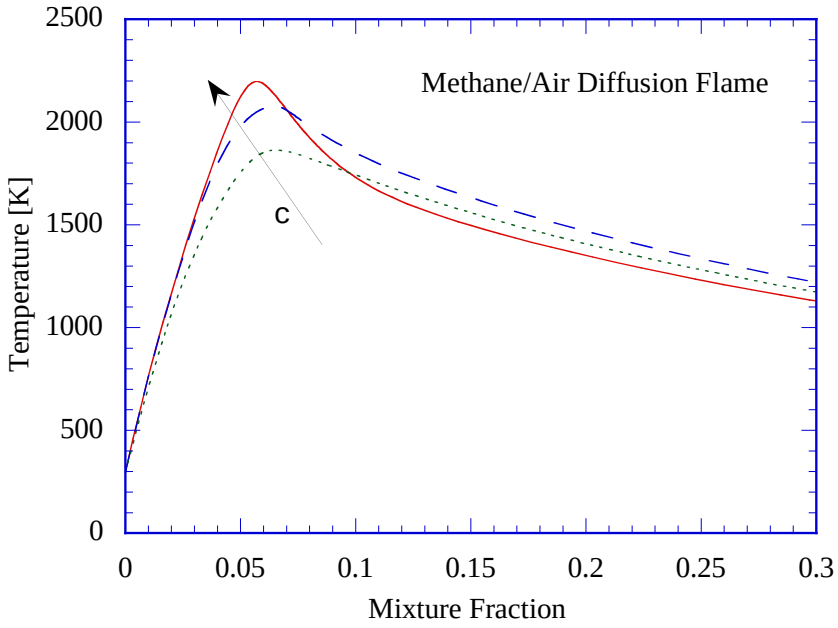
$$\chi_{st} = 2D\left(\frac{\partial Z}{\partial x_\alpha}\right)^2_{st}$$

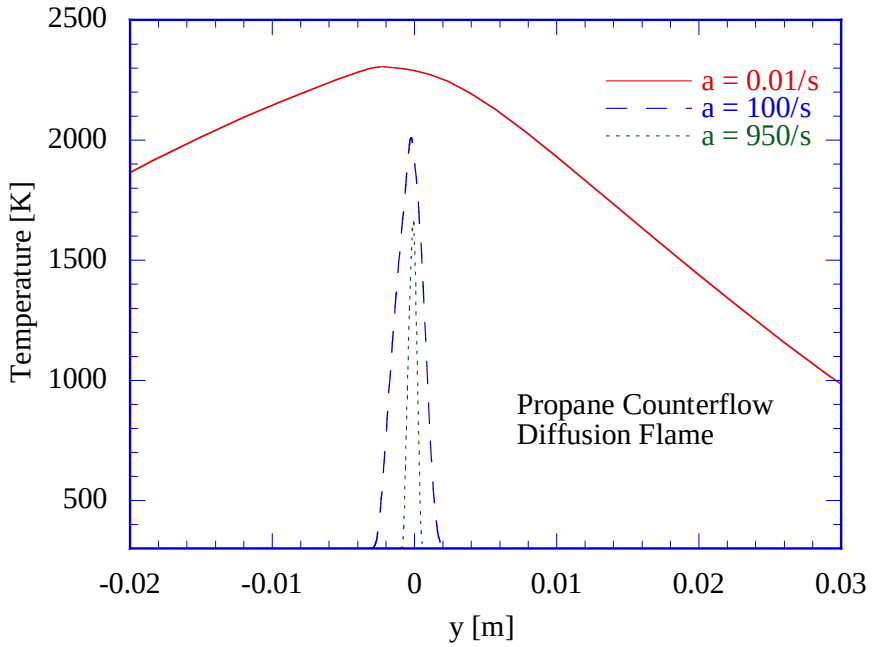
  implicitly incorporates the influence of convection and diffusion normal to the surface of the stoichiometric mixture

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

Structure of non-premixed laminar flames

Temperature and CH Profiles for Different Scalar Dissipation Rates



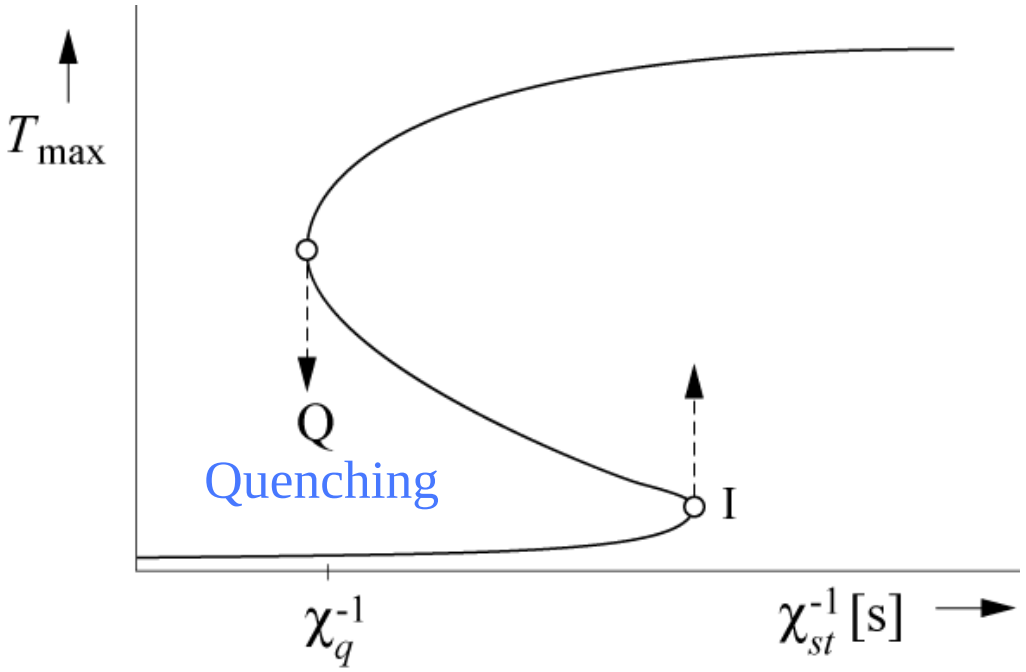


Steady solutions of the Flamelet equation: The S-Shaped Curve

- 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

Steady solutions of the Flamelet equation: The S-Shaped Curve

- The neglect of all spatial derivatives tangential to the flame front is formally only valid in the thin reaction zone around $Z = Z_{st}$

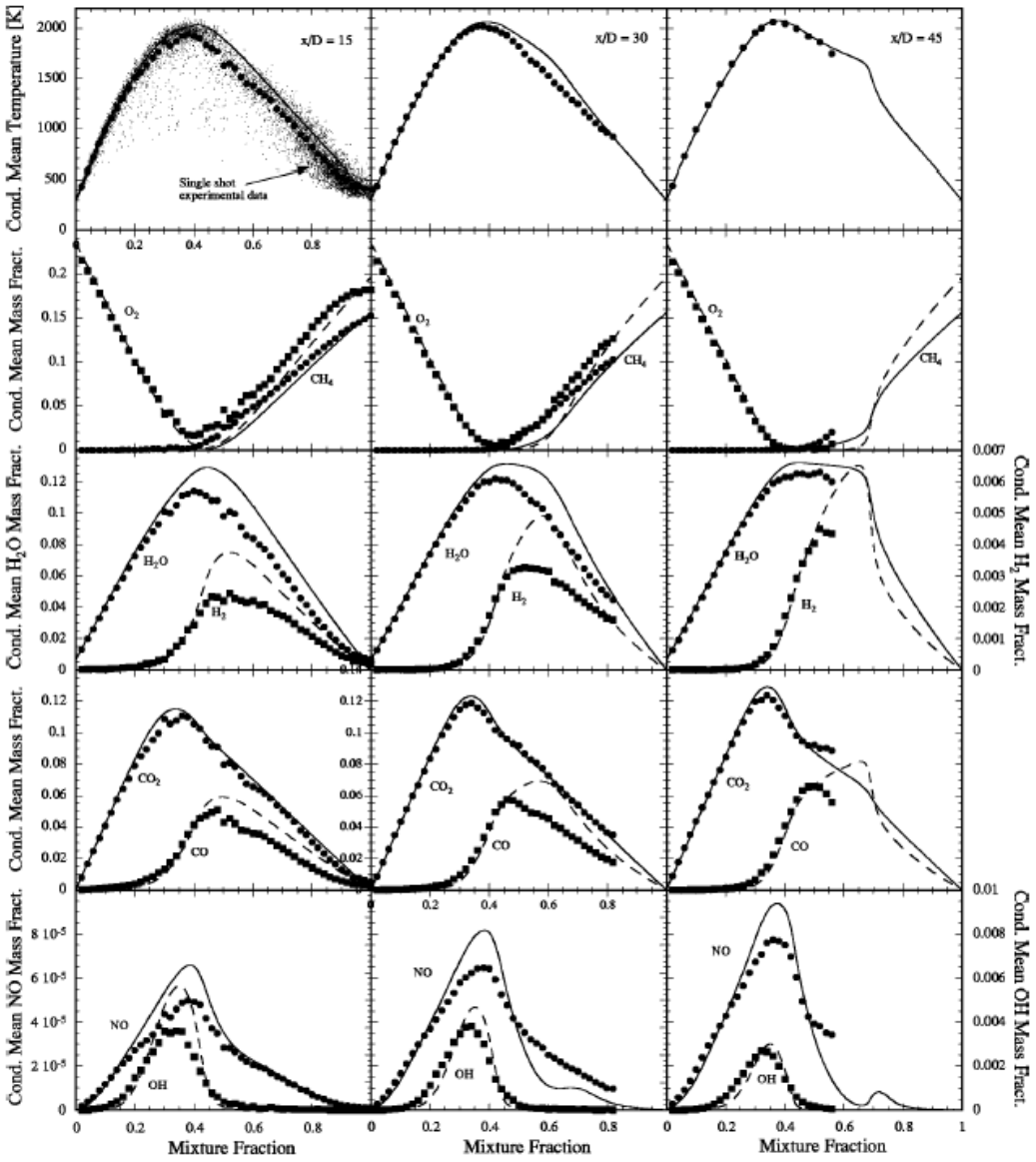
- There are, however, a number of typical flow configurations, where

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

  is valid in the entire Z-space

- As example, the analysis of a planar counterflow diffusion flame is included in the lecture notes

LES of Sandia Flame D with Lagrangian Flamelet Model

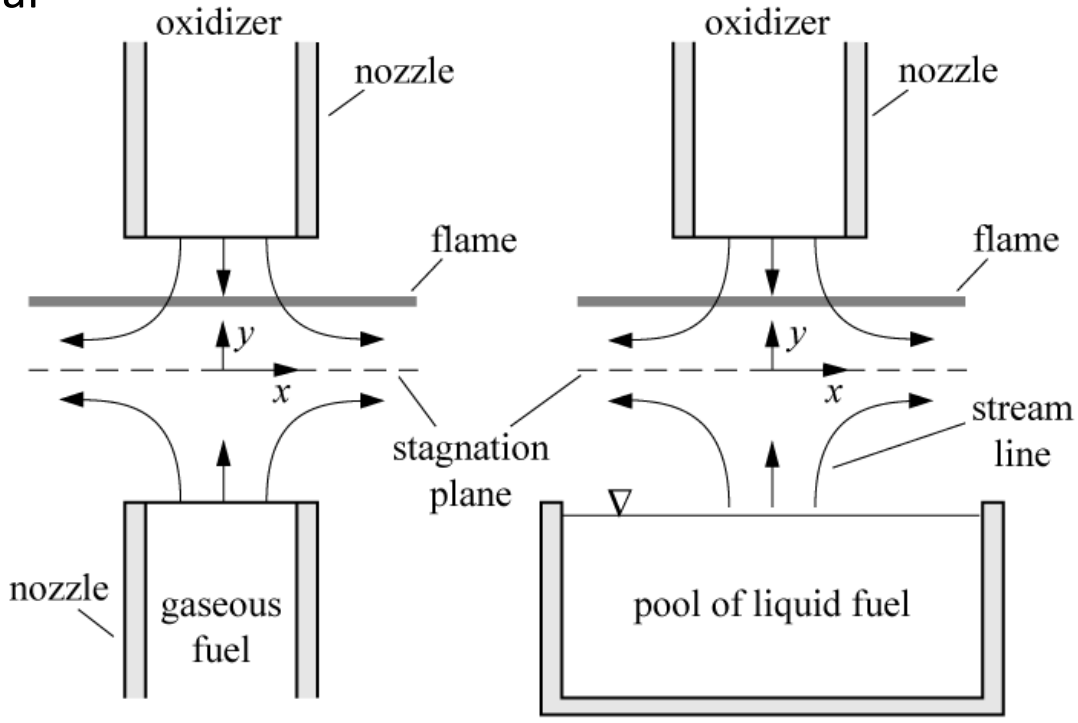


Curvature corresponds to source term!

Planar Counterflow Diffusion Flame: Analytic Solution

- Counterflow diffusion flames
  - Often used
  - Represent one-dimensional diffusion flame structure

- Flame embedded between two potential flows, if
  - Flow velocities of both streams are sufficiently large and removed from stagnation plane



The Planar Counterflow Diffusion Flame

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 Planar Counterflow Diffusion Flame

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

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

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

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

Example: Analysis of the Counterflow Diffusion Flame

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

  one obtains the system of ordinary differential equations

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

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

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

  in terms of the non-dimensional stream function

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

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

Example: Analysis of the Counterflow Diffusion Flame

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

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

- 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*(η) is defined as

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

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

Example: Analysis of the Counterflow Diffusion Flame

- 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

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

- The instantaneous scalar dissipation rate is here

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

where

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

Example: Analysis of the Counterflow Diffusion Flame

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

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

one obtains

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

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

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

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

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

showing that χ increases as Z^2 for small Z

Results of Analysis of the Counterflow Diffusion Flame

- Mixture fraction field described as

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

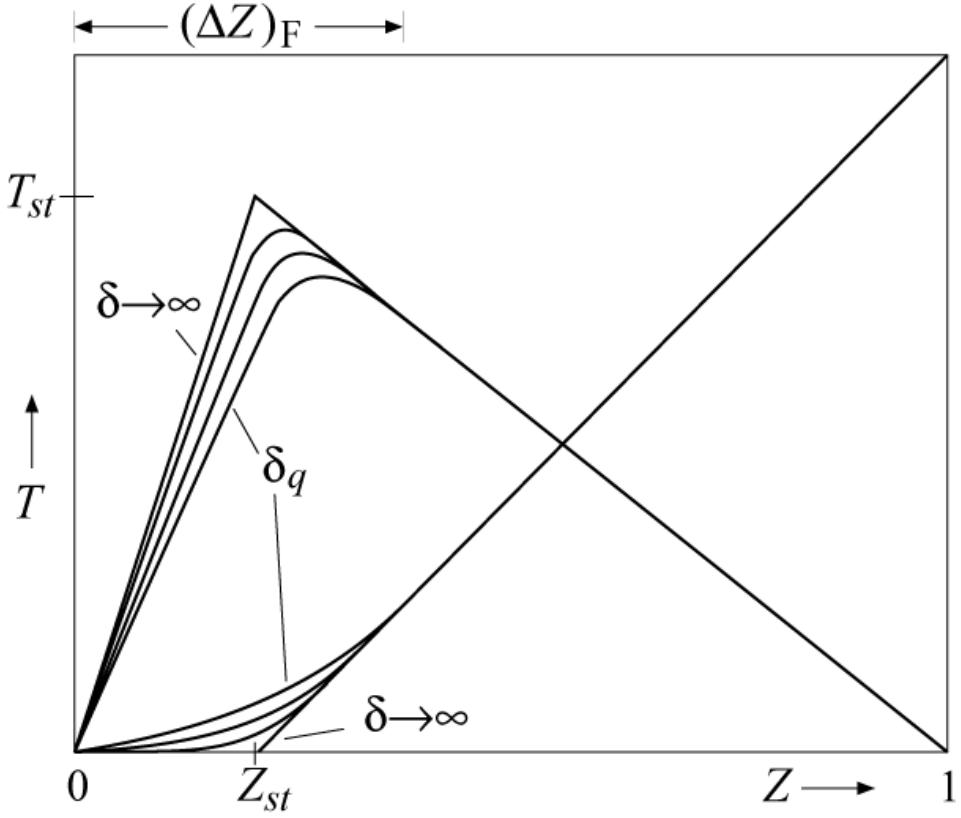
- From this follows scalar dissipation rate as

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

- This provides
  - Relation between strain rate and scalar dissipation rate
  - Mixture fraction dependence of scalar dissipation rate, often used in solving flamelet equations

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

Diffusion Flame Structure of Methane-Air Flames

- A numerical calculation with the four-step reduced mechanism

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

$$CO + H_2O = CO_2 + H_2$$

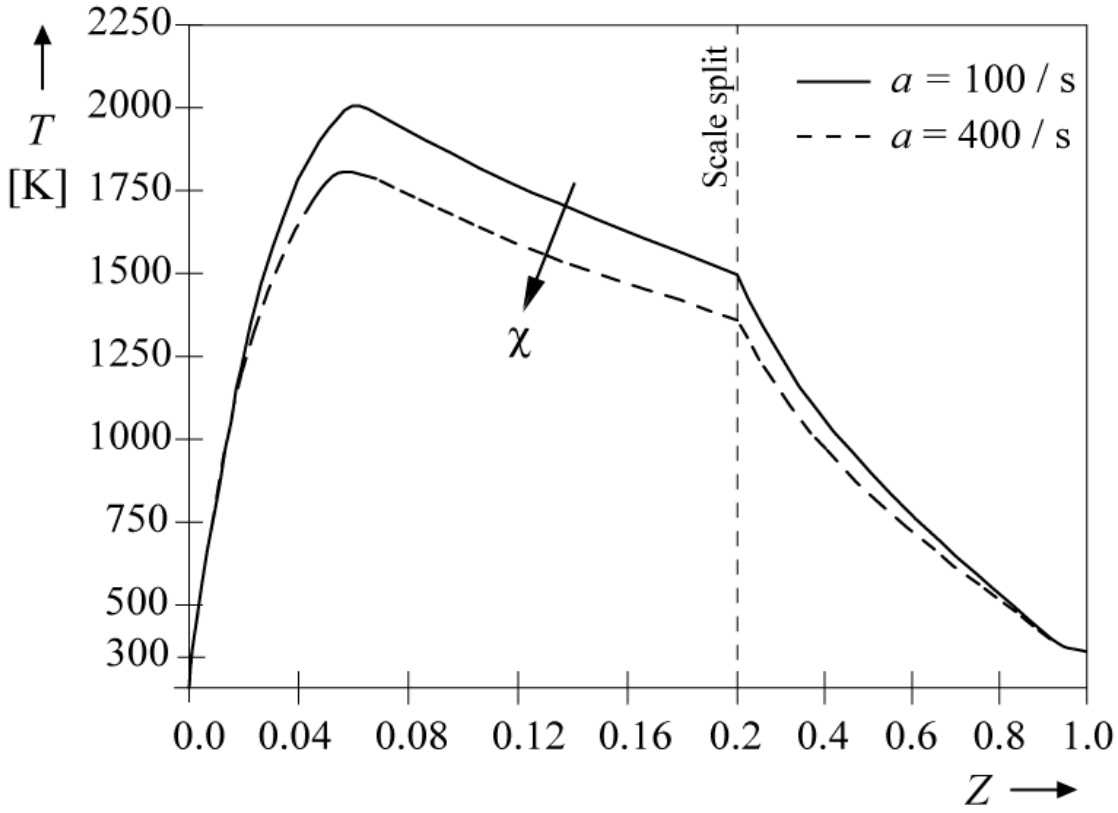
$$H + H + M = H_2 + M$$

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

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

Diffusion Flame Structure of Methane-Air Flames

- Temperature profiles for methane-air flames

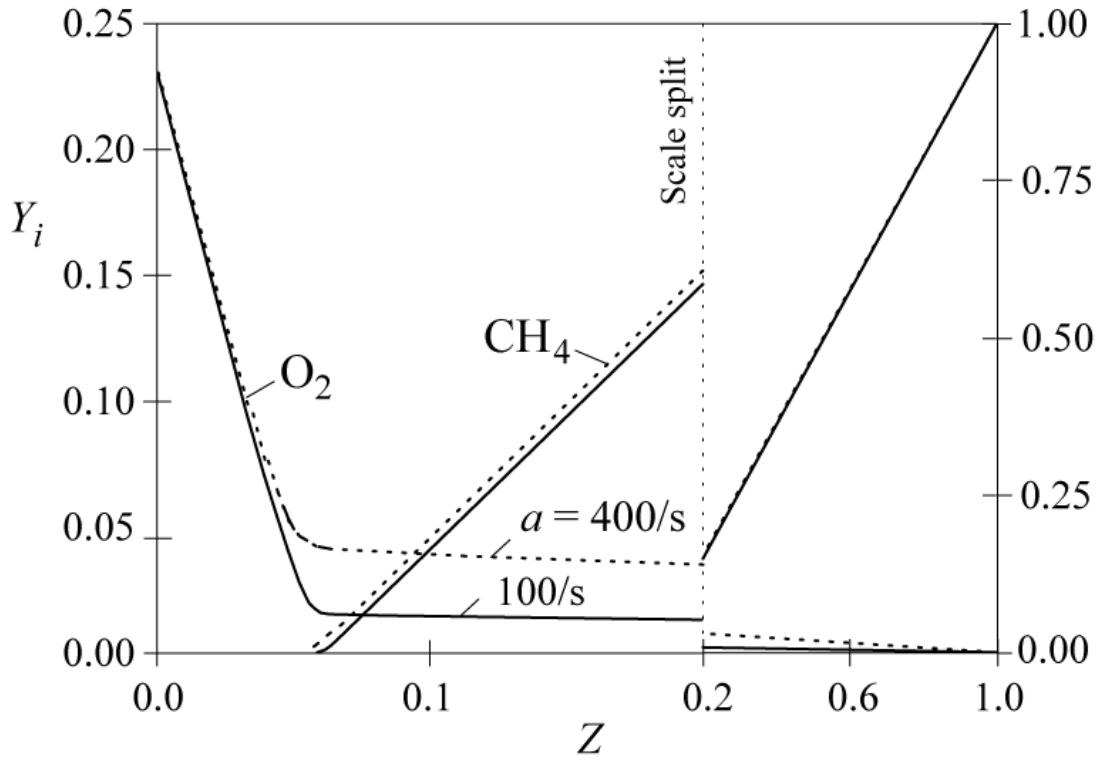


- Second value of the strain rate corresponds to a condition close to extinction

  → Temperature in the reaction zone decreases

Diffusion Flame Structure of Methane-Air Flames

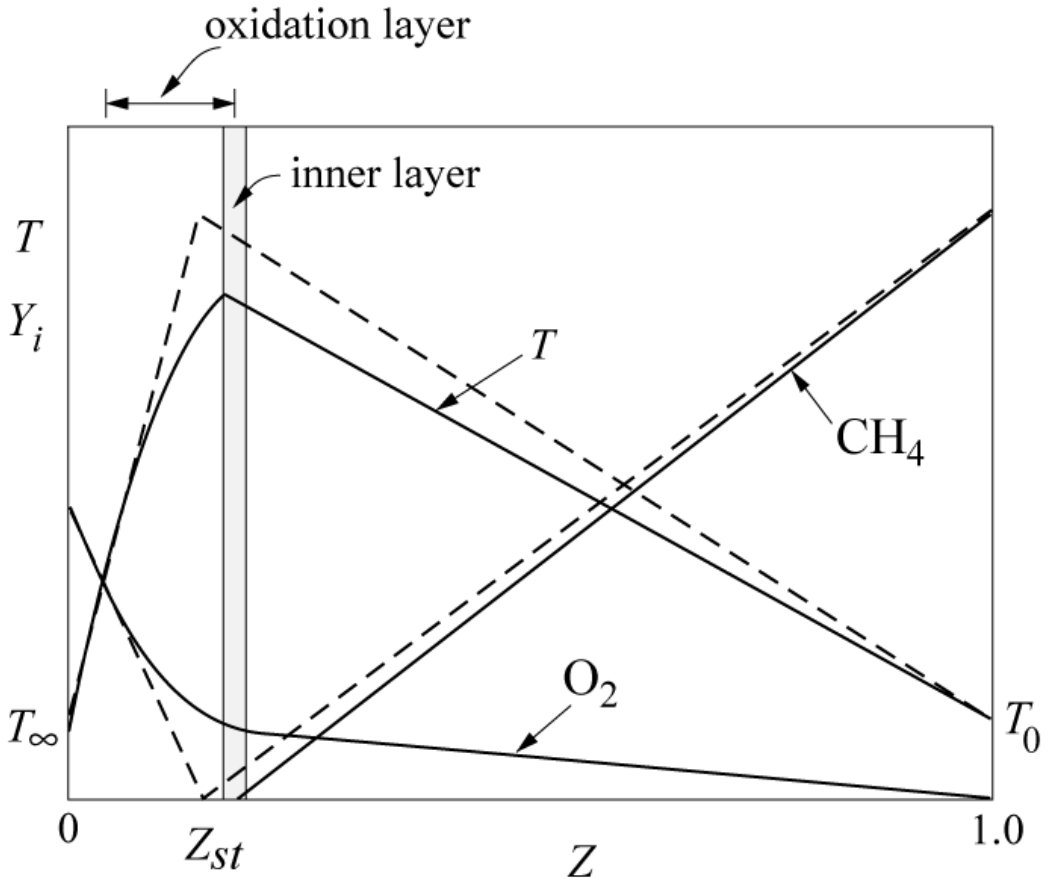
- Fuel and oxygen mass fraction profiles for methane-air flames



- The oxygen leakage increases as extinction is approached

Diffusion Flame Structure of Methane-Air Flames

- 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



Diffusion Flame Structure of Methane-Air Flames

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

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

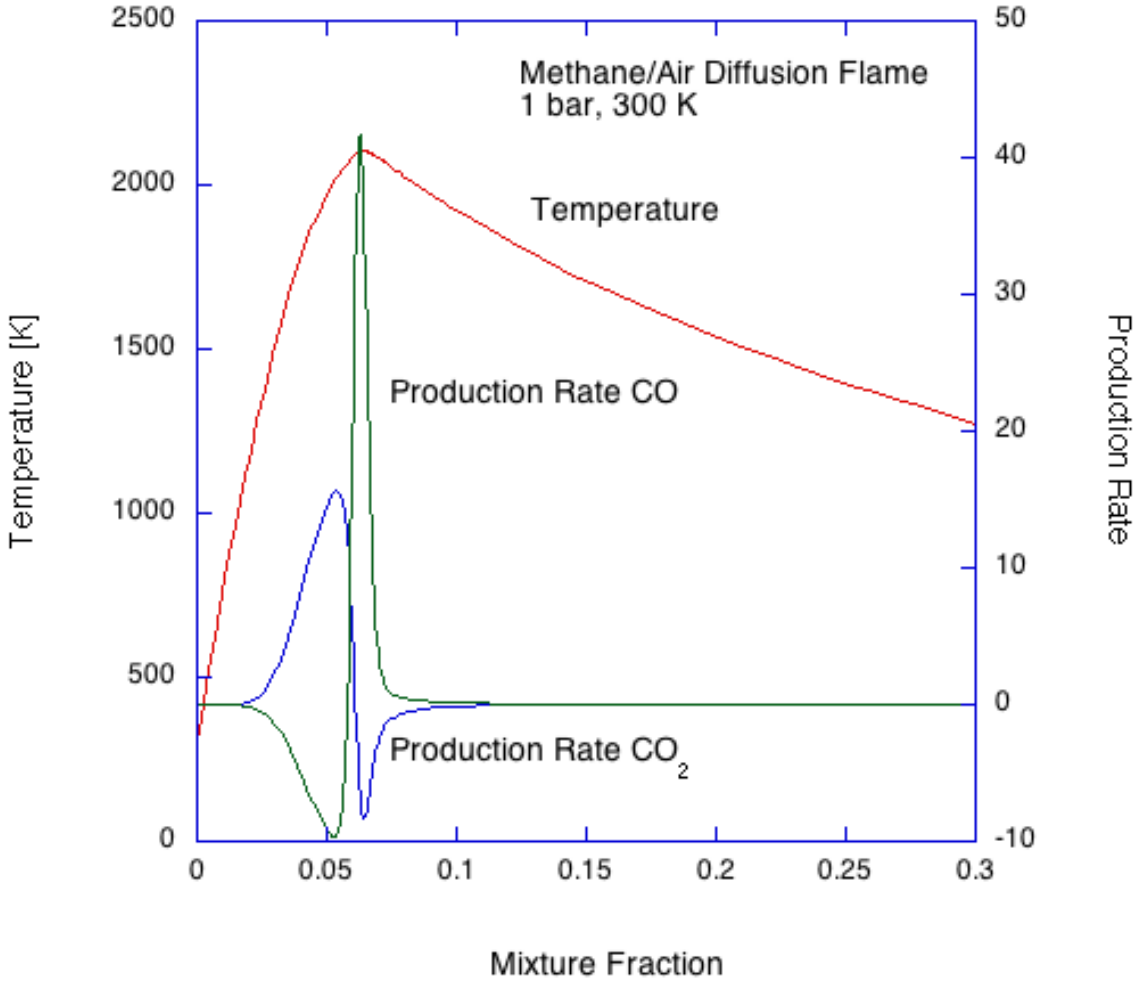
with the flame sheet positioned at $Z = Z_{st}$

- 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

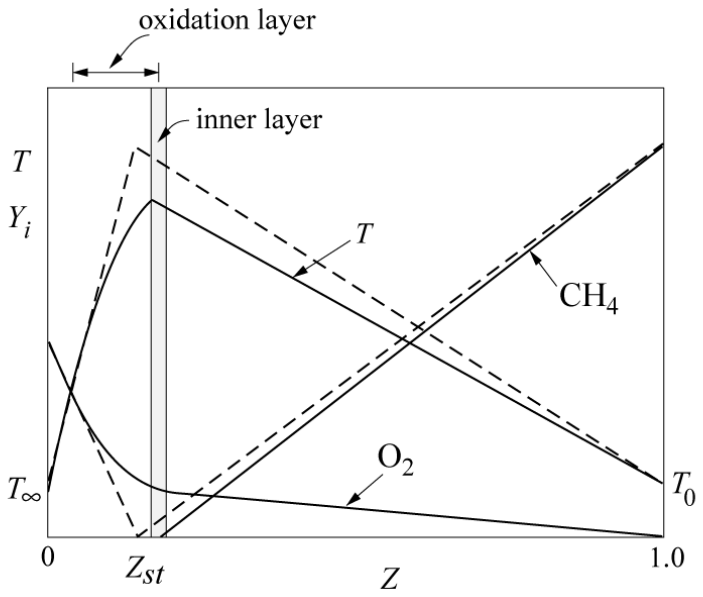
Diffusion Flame Structure of Methane-Air Flames

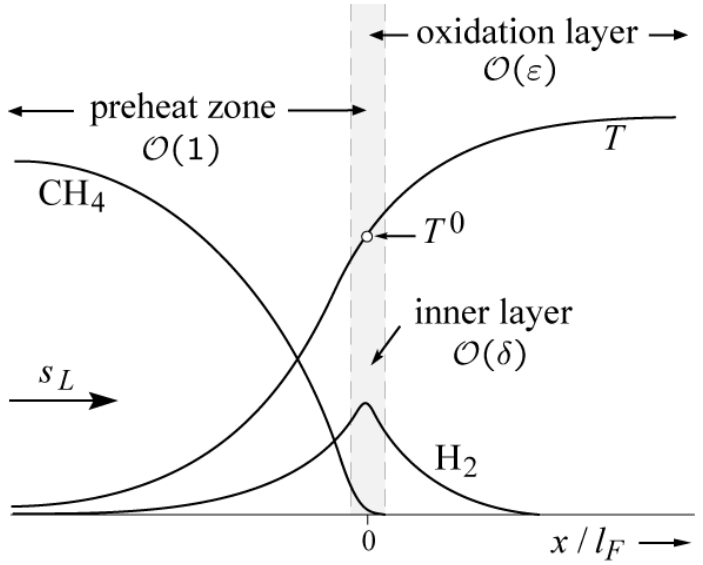
- Results from numerical Simulation of Methane/Air diffusion flame



Diffusion Flame Structure of Methane-Air Flames

- 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

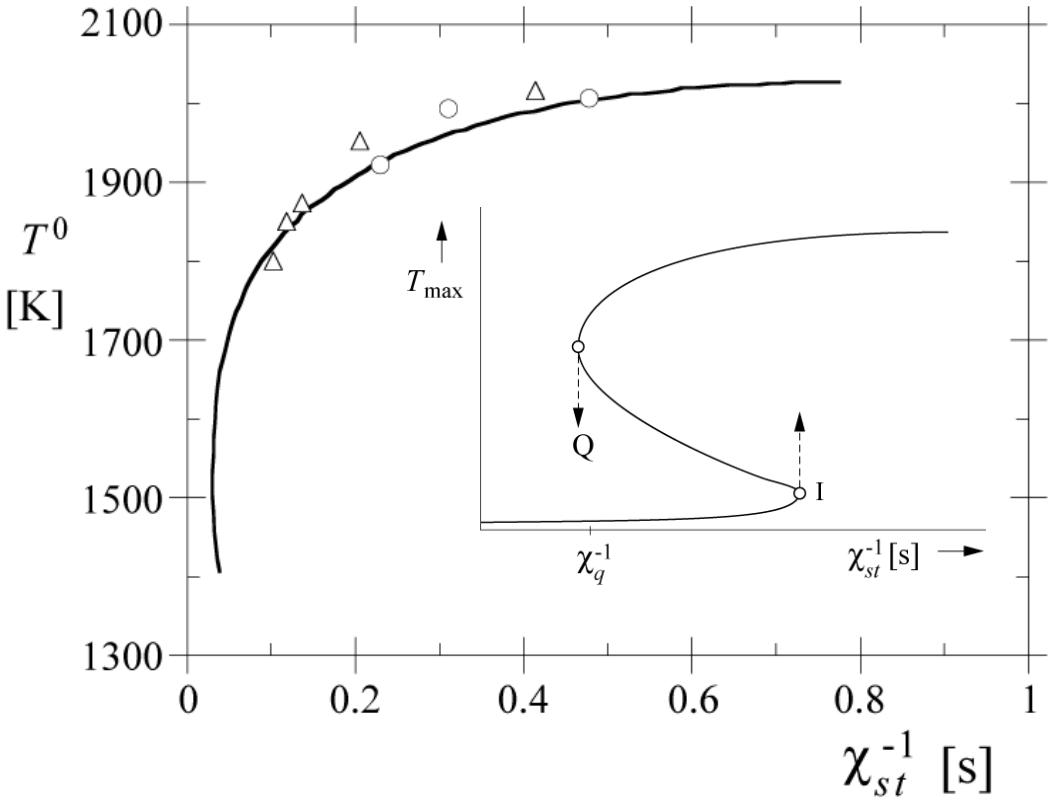




Diffusion Flame Structure of Methane-Air Flames

- 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



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- Introduction
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- Laminar premixed flames: Flame structure
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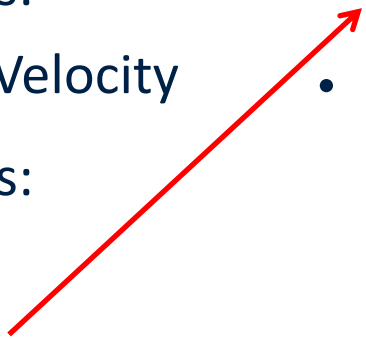

- Introduction
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FlameMaster Flame Calculator

- FlameMaster: A C++ Computer Program for 0D Combustion and 1D Laminar Flame Calculations
  - Premixed and non-premixed
  - Steady and unsteady
  - Emphasis on pre- and post-processing
    - Sensitivity analysis
    - Reaction flux analysis
- At request, available online at
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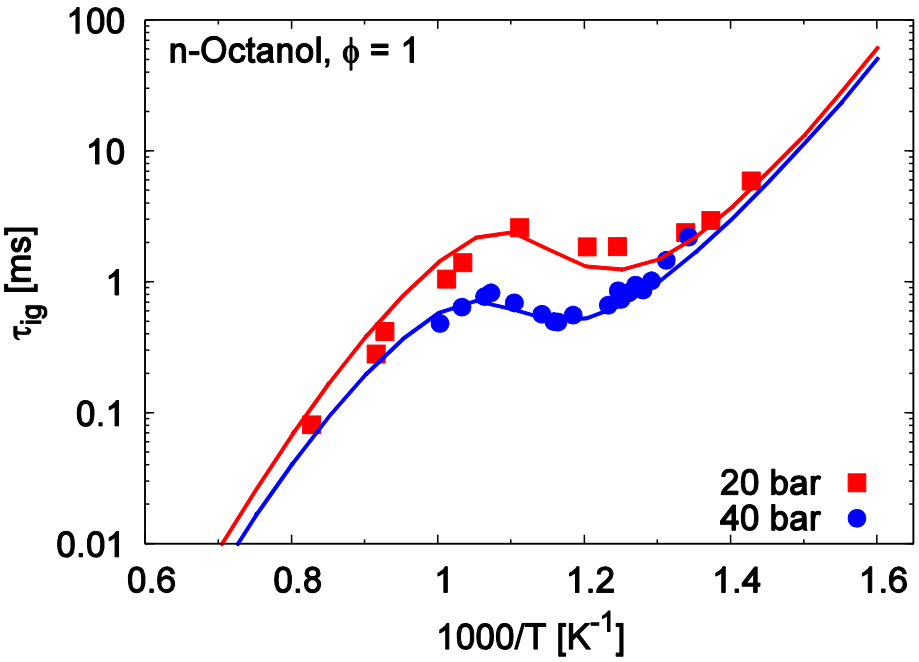
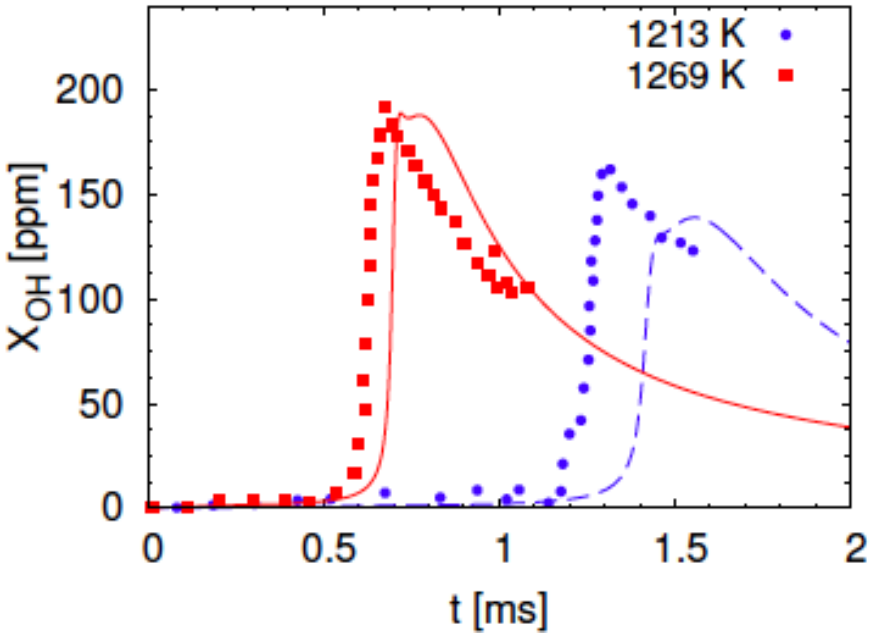
FlameMaster Flame Calculator

- Example: Shock tube, homogeneous reactor

N-Octanol Ignition Delay Times

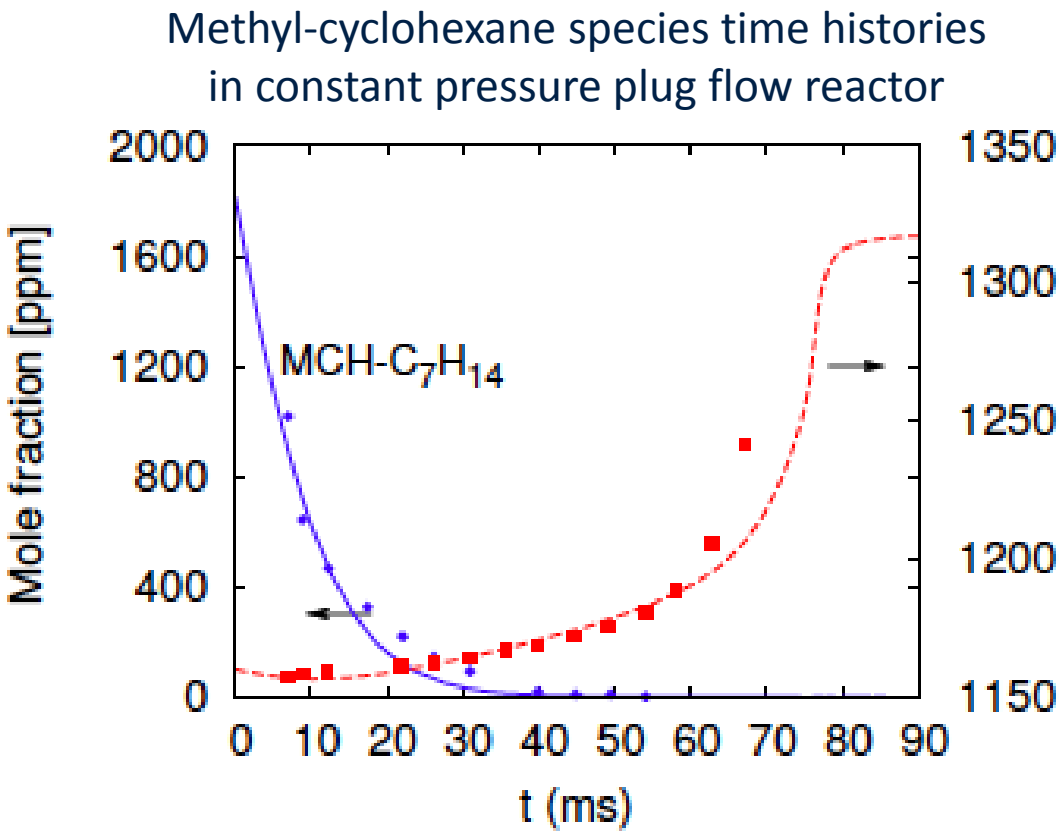


Methyl-cyclohexane species time histories in shock tube



FlameMaster Flame Calculator

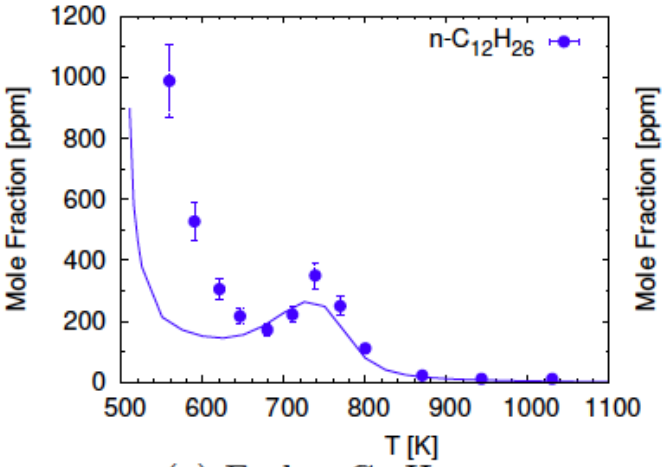
- Example: Flow reactor



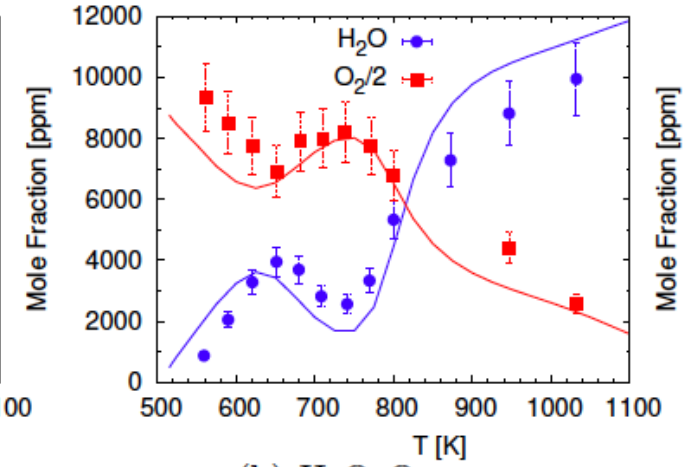
FlameMaster Flame Calculator

- Example: Jet stirred reactor

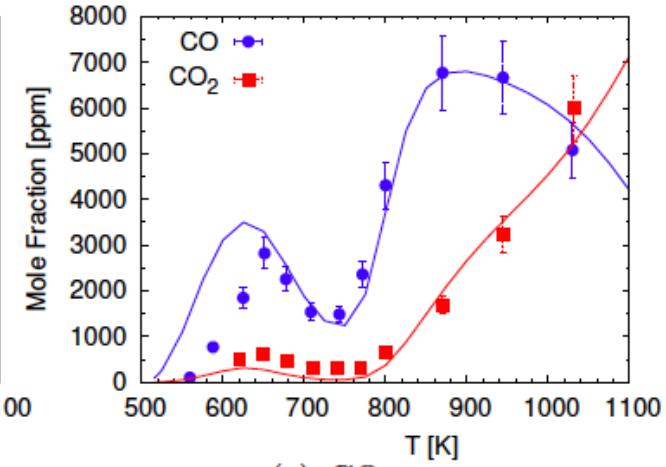
N-Dodecane oxidation in jet stirred reactor



(a) Fuel, n-$C_{12}H_{26}$



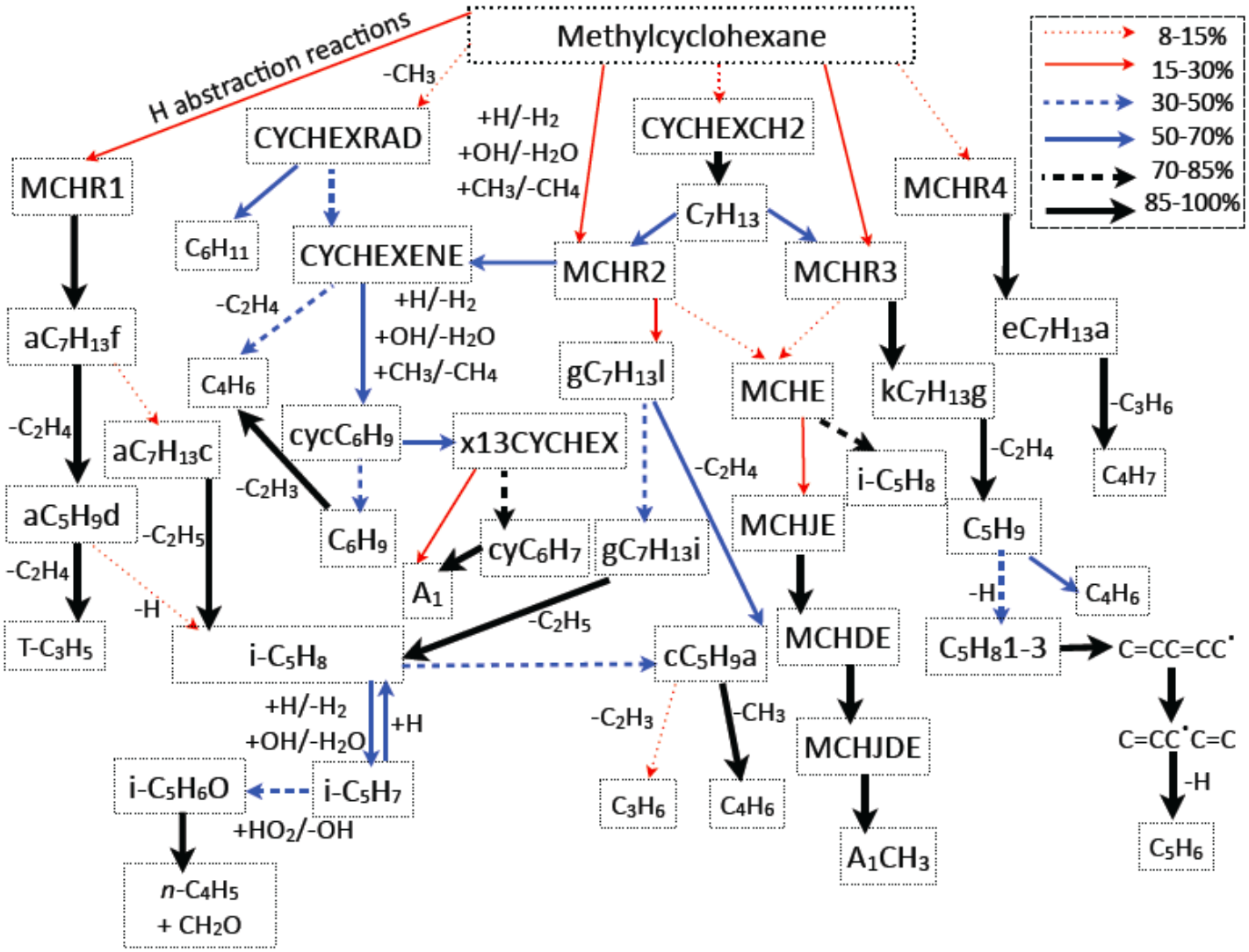
(b) H_2O, O_2



(c) CO_x

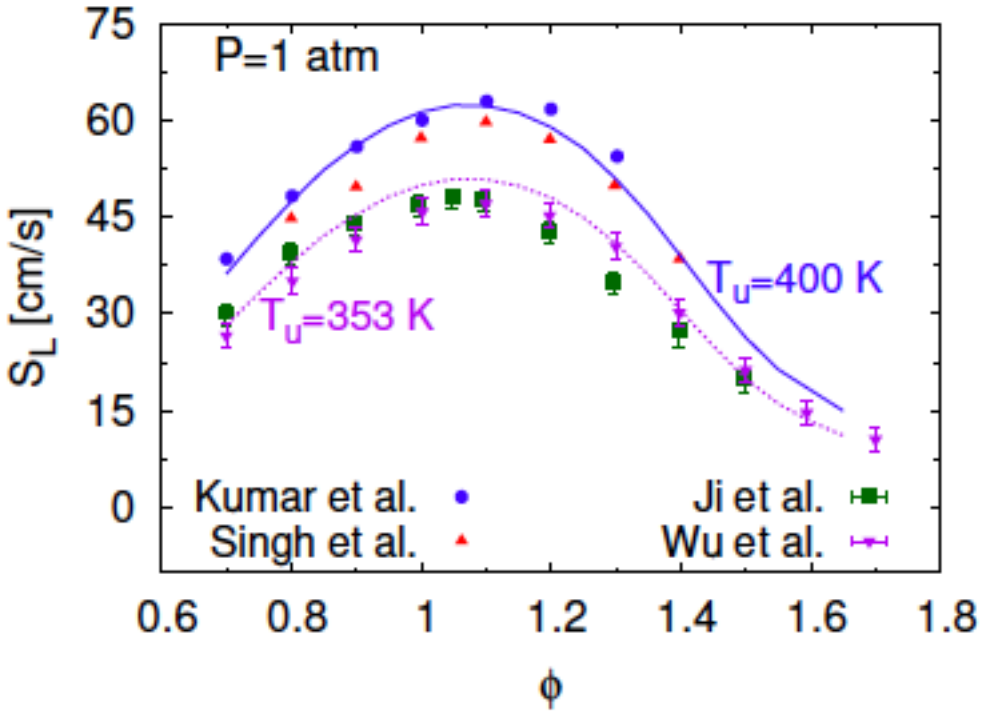
FlameMaster Flame Calculator

- Example: Reaction flux analysis



FlameMaster Flame Calculator

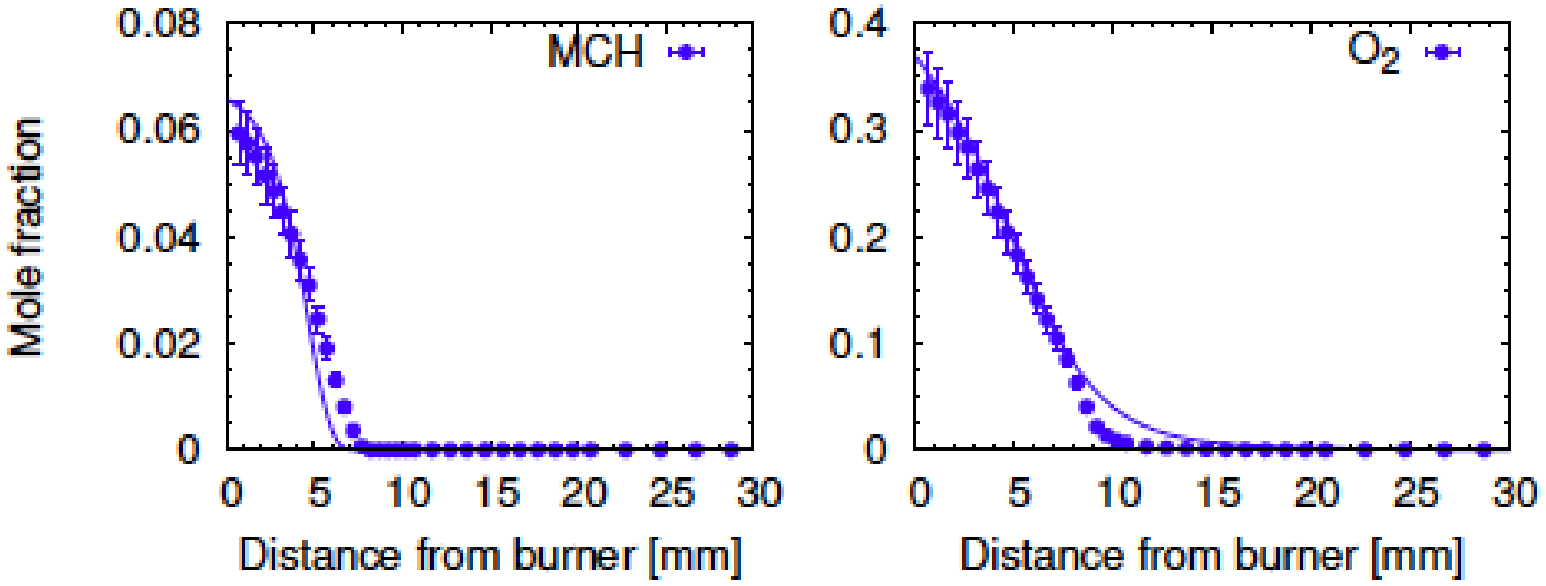
- Example: Laminar burning velocities



FlameMaster Flame Calculator

- Example: Premixed flame structure

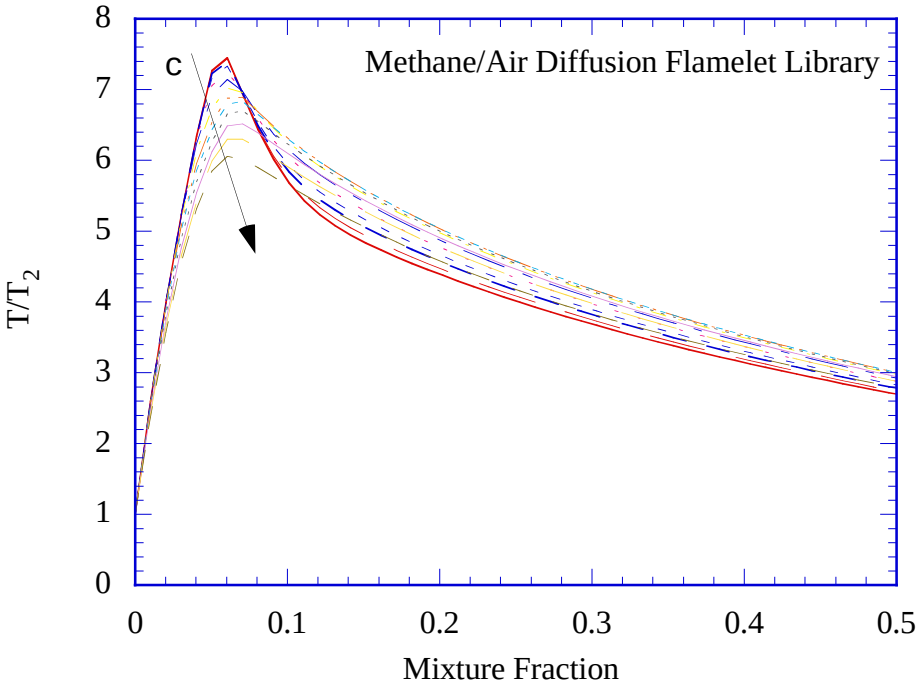
Methyl-cyclohexane species profiles in
premixed burner stabilized flame

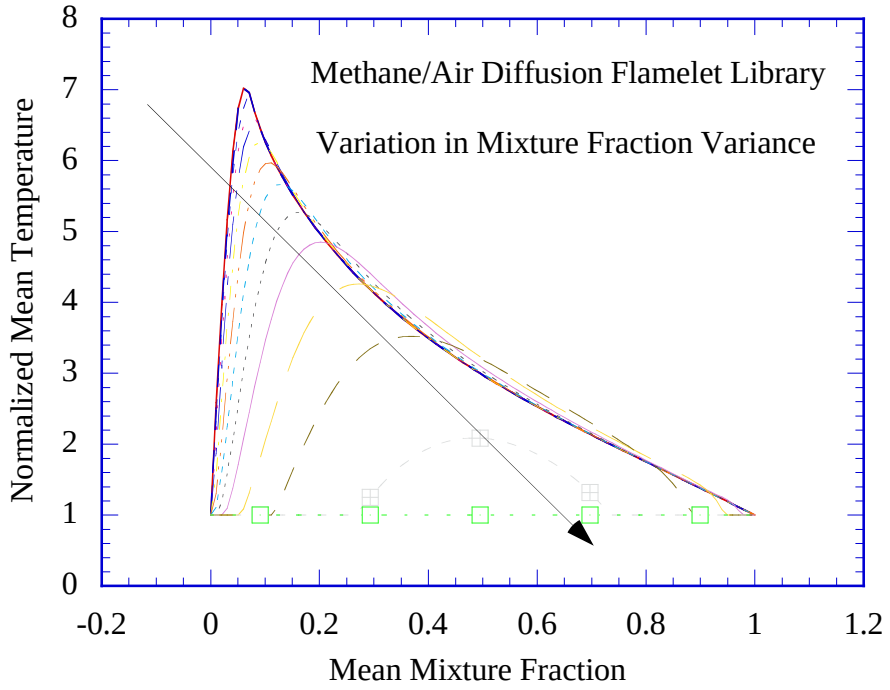


FlameMaster Flame Calculator

- Example: Flamelet libraries

Flamelet library for methane/air non-premixed combustion





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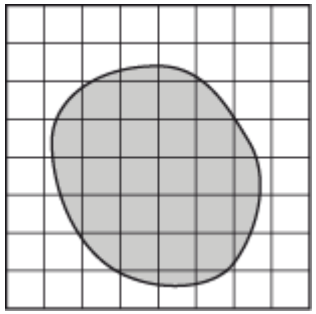
Spray Combustion: Gas Turbine Combustion Chamber

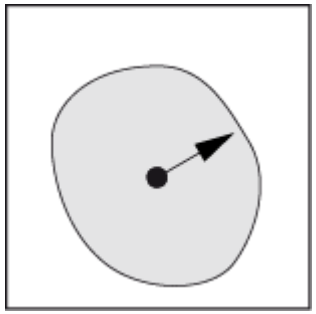
Quelle: C. Edwards, Stanford University

Modelling Multiphase Flows

- Euler-Euler Approach
  - All phases: Eulerian description
  - Conservation equation for each phase
  - One Phase per Volume element → Volume Fraction
  - Phase-phase interaction
  - Surface-tracking technique applied to a fixed Eulerian mesh

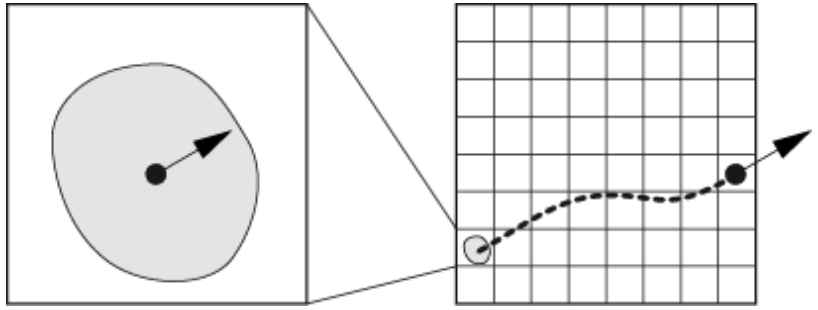


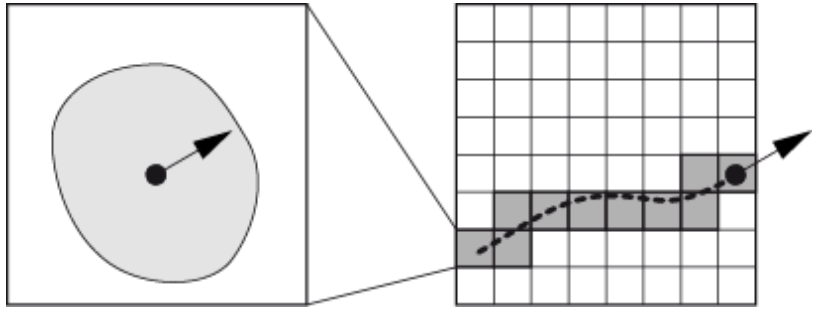
- Euler-Lagrange Approach
  - Fluid phase: continuum → Navier-Stokes Equations
  - Dispersed phase is solved by tracking a large number of particles
  - The dispersed phase can exchange momentum, mass, and energy with the fluid phase



Dispersed Phase: Droplets

- Lagrangian frame of reference
- Droplets
  - Diameter (evaporation)
  - Temperature (heat transfer)
  - Deformation (aerodynamic forces)
  - Collision, breakup, …
- Source terms along droplet trajectories
- Stochastic approaches:
  - Monte Carlo method
  - Stochastic Parcel method





Lagrangian Description: Balance equations

- Mass balance (single droplet)

$$\frac{\mathrm{D}m_{\mathrm{tr}}}{\mathrm{D}t} = -g\,\overset{f(Re,\,Sc)}{\frac{Y_{\mathrm{tr}} - Y_{\mathrm{g}}}{1 - Y_{\mathrm{tr}}}}$$

- Balance of energy (single droplet)

$$m_{\mathrm{tr}} c_p \frac{\mathrm{D}T_{\mathrm{tr}}}{\mathrm{D}t} = -A_{\mathrm{tr}}\,\overset{f(Re,\,Pr)\text{ , radiation}}{\alpha}\,(T_{\mathrm{tr}} - T_{\mathrm{g}}) + \frac{\mathrm{D}m_{\mathrm{tr}}}{\mathrm{D}t}\Delta h(T_{\mathrm{tr}})$$

- Momentum balance (single droplet)

$$\frac{\mathrm{D}}{\mathrm{D}t}\left(m_{\mathrm{tr}} u_i\right) = \sum_j F_{j,i}$$

  - $F_{\mathrm{W},i}$: Drag
  - $F_{\mathrm{G},i}$: Weight/buoyant force
  - …: Pressure/virtual/Magnus forces,…

Coupling Between the Discrete and Continuous Phases

- Mass

$$\dot{\omega}_{\mathrm{M}} = \frac{1}{V_{\mathrm{cell}}} \sum_k \dot{N} \left[m_{\mathrm{tr}}^{\mathrm{in}} - m_{\mathrm{tr}}^{\mathrm{out}} \right]$$

- Momentum

$$\dot{\omega}_{\mathrm{I}} = \frac{1}{V_{\mathrm{cell}}} \sum_k \dot{N} \left[(m_{\mathrm{tr}} u_{j,\mathrm{tr}})^{\mathrm{in}} - (m_{\mathrm{tr}} u_{j,\mathrm{tr}})^{\mathrm{out}} \right]$$

- Energy

$$\dot{\omega}_{\mathrm{E}} = \frac{1}{V_{\mathrm{cell}}} \sum_k \dot{N} \left[m_{\mathrm{tr}}^{\mathrm{in}} (h_{\mathrm{tr}} + e_{\mathrm{tr}})^{\mathrm{in}} - m_{\mathrm{tr}}^{\mathrm{out}} (h_{\mathrm{tr}} + e_{\mathrm{tr}})^{\mathrm{out}} \right]$$

Coupling Between the Discrete and Continuous Phases

- Continuous phase impacts the discrete phase (one-way coupling)
- + effect of the discrete phase trajectories on the continuum (source terms, two-way coupling)
- + interaction within the discrete phase: particle/particle (four-way coupling)

Single Droplet Combustion

- Multiphase combustion
  → phase change during combustion process:

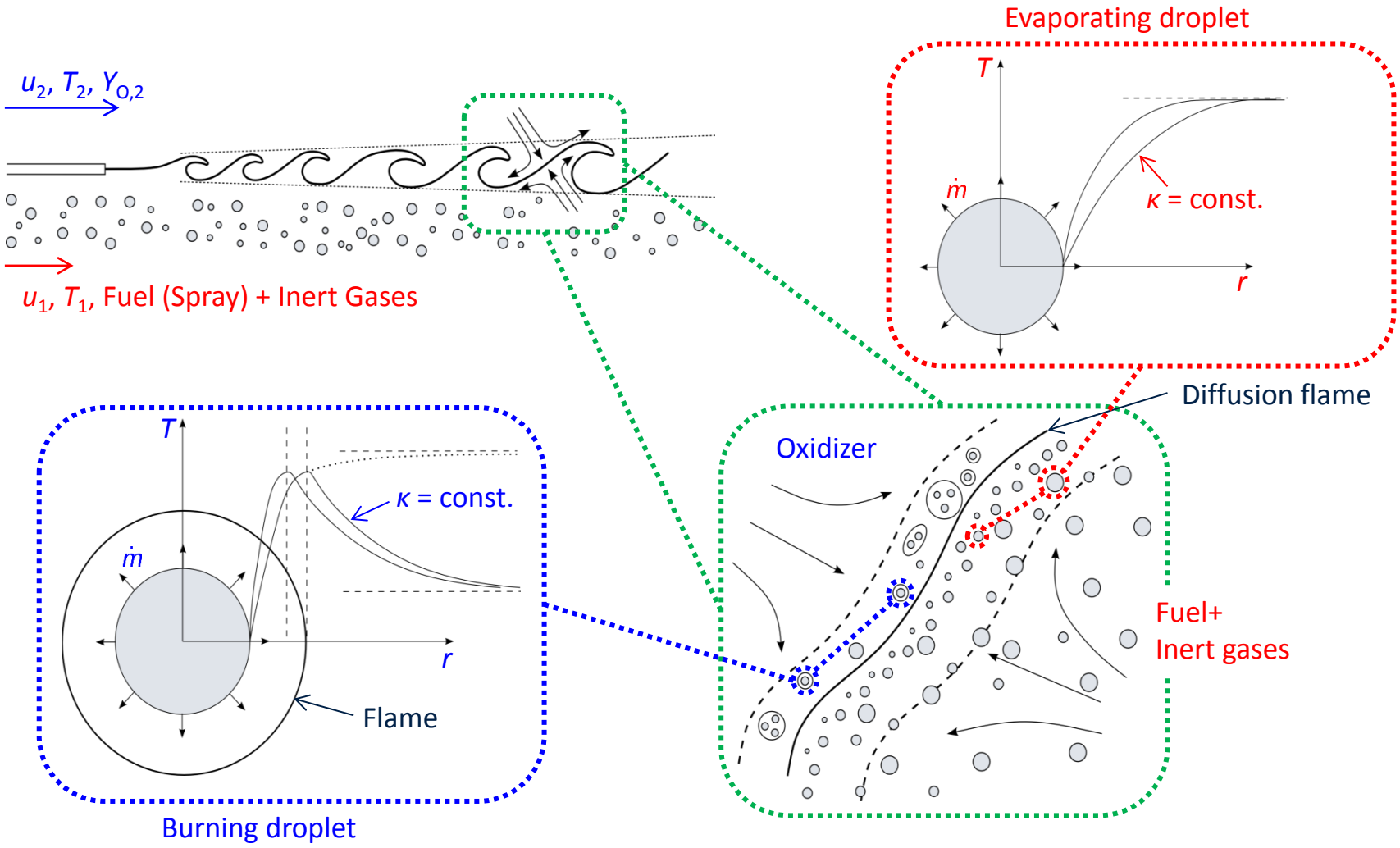
Liquid → gas phase

- Theoretical description: Single Droplet Combustion
- Aim: Mass burnig rate d*m*/d*t* as function of
  - Chemical properties of droplet and surrounding: mixture fraction *Z*
  - Thermodynamical properties: Temperature *T*, density *ρ*, pressure *p*
  - Droplet size and shape: diameter *d*

Single Droplet Combustion

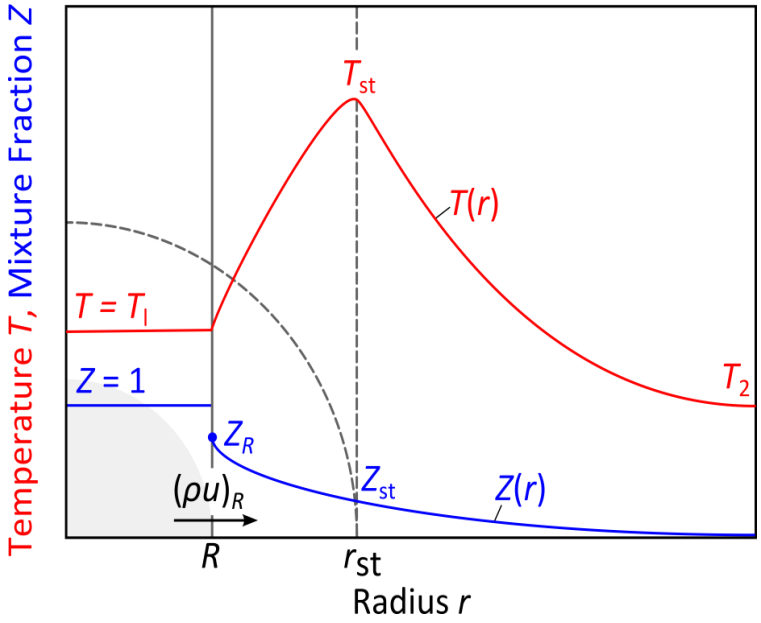
- Assumptions
  - Small droplets which follow the flow very closely
  - Velocity difference between the droplet and the surrounding fuel is zero
  - Quiescent surrounding
  - Spherically symmetric droplet
  - Neglect buoyant forces
  - Fuel and oxidizer fully separated → Combustion where the surface of stoichiometric mixture surrounds the single droplet → Diffusion flame
  - Evaporation and combustion process: quasi-steady

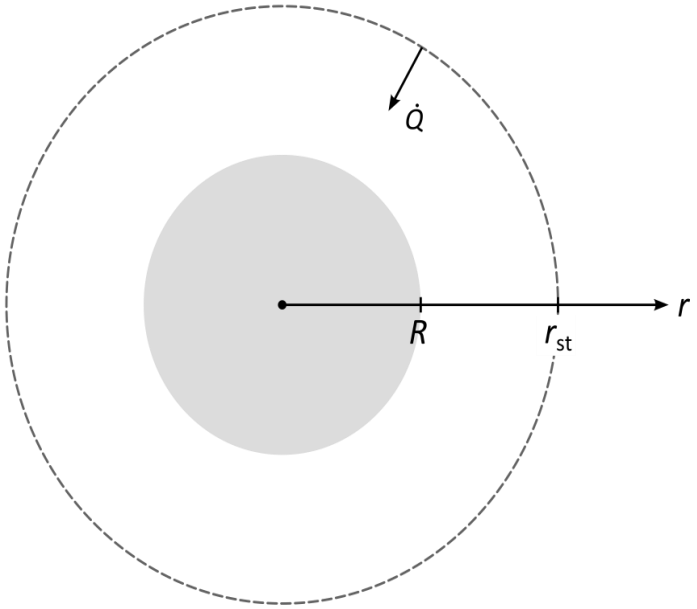
Single Droplet Combustion



Single Droplet Combustion

- Expected temperature and mixture fraction profiles:





Single Droplet Combustion

- Quasi stationary evaporation and combustion of a spherically symmetric droplet in Quiescent surrounding
  - One step reaction with fast chemistry
  - $Le = 1$

→ Balance equations:

  - Momentum equation: p = const.
  - Conservation of mass: $r^2 \rho u$ = const.
  - Temperature

$$\rho u \frac{\mathrm{d}T}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}T}{\mathrm{d}r}\right) + \frac{(-\Delta h_\mathrm{m})}{c_\mathrm{p}}\dot{\omega}$$

  - Mixture Fraction

$$\rho u \frac{\mathrm{d}Z}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Z}{\mathrm{d}r}\right)$$

Single Droplet Combustion

- Temperature boundary conditions

$$\rho u \frac{\mathrm{d}T}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}T}{\mathrm{d}r}\right) + \frac{(-\Delta h_\mathrm{m})}{c_\mathrm{p}}\dot{\omega}$$

$$\updownarrow \quad Le = \frac{\lambda}{\rho c_p D} = 1$$

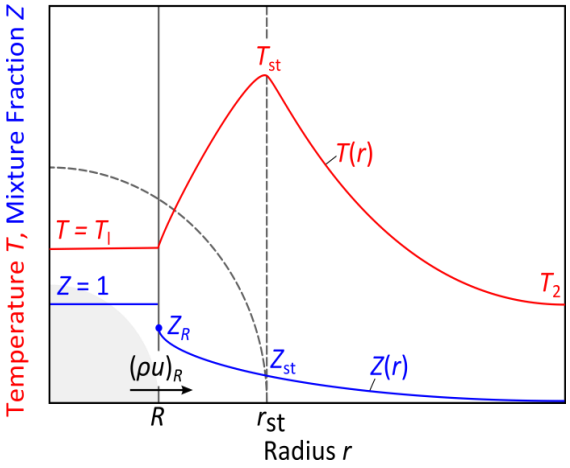
$$\rho u \underbrace{c_p \frac{\mathrm{d}T}{\mathrm{d}r}}_{\frac{\mathrm{d}h}{\mathrm{d}r}} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \lambda \frac{\mathrm{d}T}{\mathrm{d}r}\right) + (-\Delta h_\mathrm{m})\dot{\omega}$$

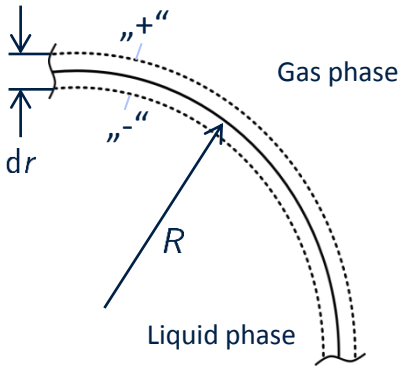
$$\updownarrow \quad r^2 \rho u = \text{const.}$$

$$r^2 \rho u \int_-^+ \frac{\mathrm{d}h}{\mathrm{d}r}\mathrm{d}r = \int_-^+ \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \lambda \frac{\mathrm{d}T}{\mathrm{d}r}\right)\mathrm{d}r + \int_-^+ (-\Delta h_\mathrm{m})\dot{\omega} r^2 \mathrm{d}r$$

$$\updownarrow$$

$$r^2 \rho u \left[\mathrm{d}h\right]_-^+ = \left[r^2 \lambda \frac{\mathrm{d}T}{\mathrm{d}r}\right]_-^+ \quad \Leftrightarrow \quad \rho u \Delta h_\mathrm{l} = \lambda \frac{\mathrm{d}T}{\mathrm{d}r}\bigg|_\mathrm{gas}$$





Single Droplet Combustion

- Mixture Fraction boundary conditions

$$\rho u \frac{\mathrm{d}Z}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Z}{\mathrm{d}r}\right)$$

$$\Updownarrow$$

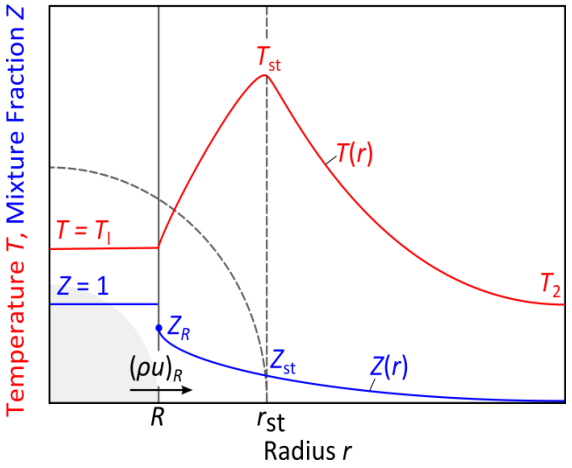
$$r^2 \rho u \frac{\mathrm{d}Z}{\mathrm{d}r} = \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Z}{\mathrm{d}r}\right)$$

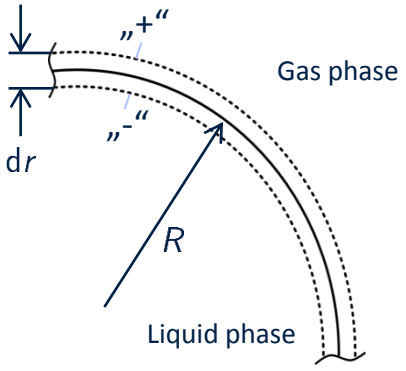
$$\Updownarrow \quad r^2 \rho u = \text{const.}$$

$$r^2 \rho u \int_-^+ \frac{\mathrm{d}Z}{\mathrm{d}r}\mathrm{d}r = \int_-^+ \frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Z}{\mathrm{d}r}\right)\mathrm{d}r$$

$$\Updownarrow$$

$$r^2 \rho u \left[\mathrm{d}Z\right]_-^+ = \left[r^2 \lambda \frac{\mathrm{d}Z}{\mathrm{d}r}\right]_-^+ \quad \Leftrightarrow \quad (\rho u)_R (Z_R - 1) = \rho D \left.\frac{\mathrm{d}Z}{\mathrm{d}r}\right|_R$$

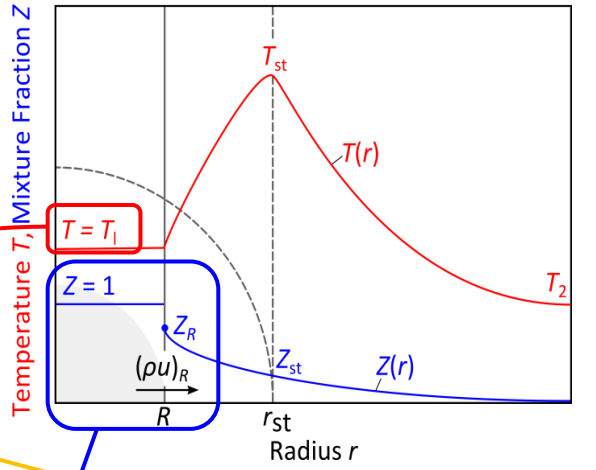




Single Droplet Combustion

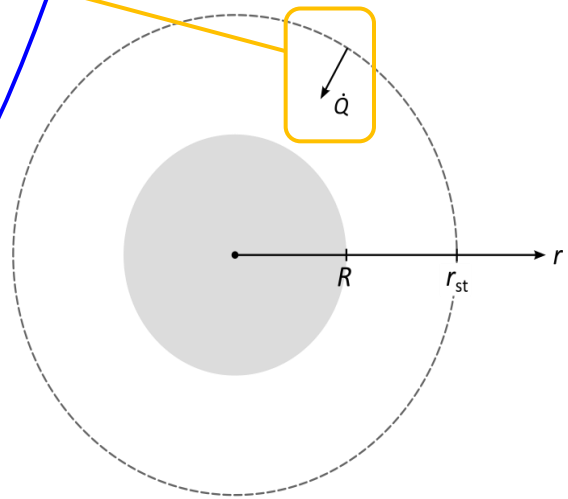
- Temperature BCS:
  - Enthalpy of evaporation h_l
  - Temperature within the droplet T_l = const.
  - T_L is boiling temperature $T_l = T_s(p)$

$$r = R: \quad \lambda \left.\frac{\mathrm{d}T}{\mathrm{d}r}\right|_R = (\rho u)_R h_l, \qquad T_R = T_l$$



- Mixture Fraction BCS:
  - Difference between the mixture fraction within the droplet and that in the gas phase at the droplet surface

$$r = R: \quad \rho D \left.\frac{\mathrm{d}Z}{\mathrm{d}r}\right|_R = (\rho u)_R (Z_R - 1)$$



Single Droplet Combustion

$$r = R: \quad \lambda \left.\frac{\mathrm{d}T}{\mathrm{d}r}\right|_R = (\rho u)_R h_l, \quad T_R = T_l$$

$$r = R: \quad \rho D \left.\frac{\mathrm{d}Z}{\mathrm{d}r}\right|_R = (\rho u)_R (Z_R - 1)$$

} 3 BCS

- Quasi-stationarity: R = const.
- BCS in Surrounding:

$$r \to \infty: \quad T = T_2, \quad Z = 0$$

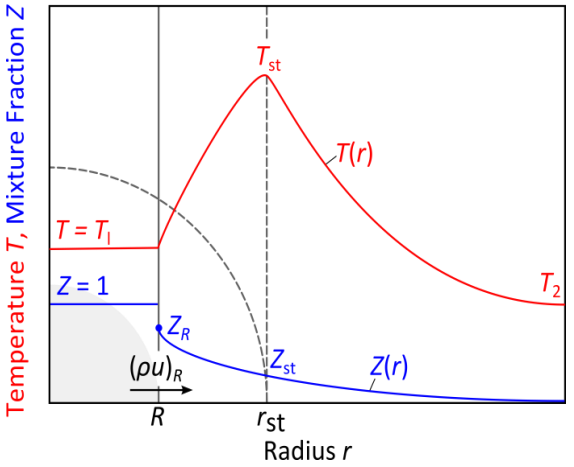
} 2 BCS

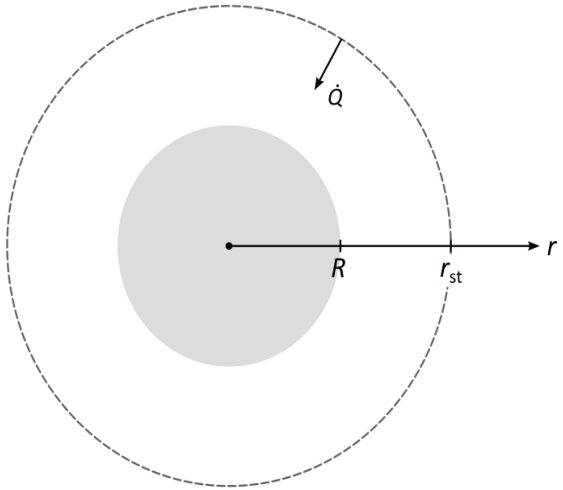
- Integration of the continuity equation leads to

$$\dot{m} = 4\pi r^2 \rho u = 4\pi R^2 (\rho u)_R$$

Eigenvalue

- Mass flux at r equals mass flux at $r + \mathrm{d}r$ and at $r = R$





Single Droplet Combustion

- Coordinate transformation:

$$\zeta = \int_r^\infty \frac{u}{D} \mathrm{d}r = \frac{\dot{m}}{4\pi} \int_r^\infty (\rho D r^2)^{-1} \mathrm{d}r$$

$$\eta = \int_r^\infty \frac{u}{D} \exp(-\zeta) \mathrm{d}r$$

- Relation between η und ζ:

$$\frac{\mathrm{d}\eta}{\mathrm{d}\zeta} = \frac{\mathrm{d}\eta/\mathrm{d}r}{\mathrm{d}\zeta/\mathrm{d}r} = \exp(-\zeta)$$

- Integration and BC $\zeta = 0$ at $\eta = 0 \rightarrow \eta = 1 - \exp(-\zeta)$
- At $r = R \rightarrow \eta_R = 1 - \exp(-\zeta_R)$ and therefore $\zeta_R = -\ln(1 - \eta_R)$

Single Droplet Combustion

- From the equations for temperature and mixture fraction it follows in transformed coordinates:

$$\rho u \frac{\mathrm{d}T}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}T}{\mathrm{d}r}\right) + \frac{(-\Delta h_\mathrm{m})}{c_p}\dot{\omega}$$

$$\rho u \frac{\mathrm{d}Z}{\mathrm{d}r} = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \rho D \frac{\mathrm{d}Z}{\mathrm{d}r}\right)$$

$\rightarrow$

$$\rho D \left(\frac{\mathrm{d}\eta}{\mathrm{d}r}\right)^2 \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2} = -\frac{(-\Delta h_\mathrm{m})}{c_p}\dot{\omega}$$

$$\frac{\mathrm{d}^2 Z}{\mathrm{d}\eta^2} = 0$$

- Transformed BCS

$$\eta = \eta_R: \qquad (\eta_R - 1)\frac{\mathrm{d}T}{\mathrm{d}\eta} = \frac{h_\mathrm{l}}{c_p}, \quad T_R = T_\mathrm{l} \quad \text{and} \quad (\eta_R - 1)\frac{\mathrm{d}Z}{\mathrm{d}\eta} = Z_R - 1$$

$$\eta = 0: \qquad T = T_2 \quad \text{and} \quad Z = 0$$

- Solution of the mixture fraction

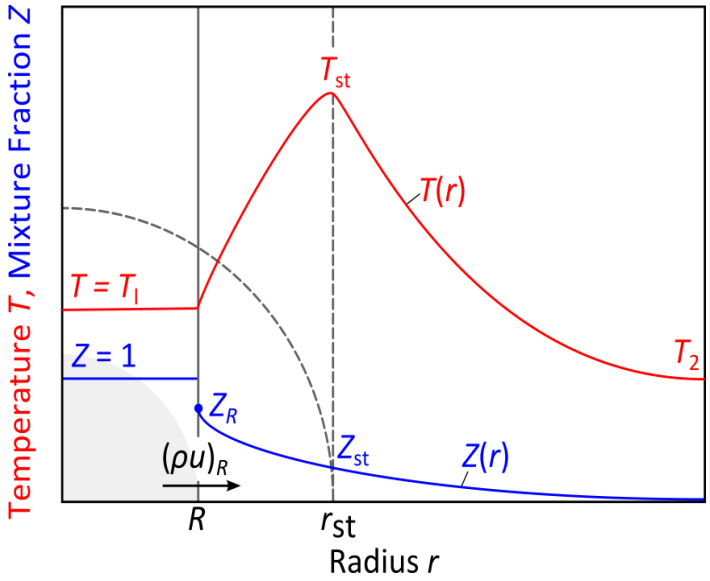
$$Z = \eta$$

Single Droplet Combustion

- Temperature solution where $Z = \eta$

$$\rho D\left(\frac{\mathrm{d}\eta}{\mathrm{d}r}\right)^2 \frac{\mathrm{d}^2 T}{\mathrm{d}\eta^2} = -\frac{(-\Delta h_m)}{c_p}\dot{\omega} \quad \xrightarrow{\eta = Z \text{ and } \frac{\chi}{2} = \rho D\left(\frac{\mathrm{d}Z}{\mathrm{d}r}\right)^2} \quad \boxed{\frac{\chi}{2}\frac{\mathrm{d}^2 T}{\mathrm{d}Z^2} = -\frac{(-\Delta h_m)}{c_p}\dot{\omega}}$$

- Known Structure→ Compares to the flamelet equations
- We consider the Burke-Schumann-solution
  - T_2: Temperature in the surrounding
  - T_l: Temperature at droplet surface



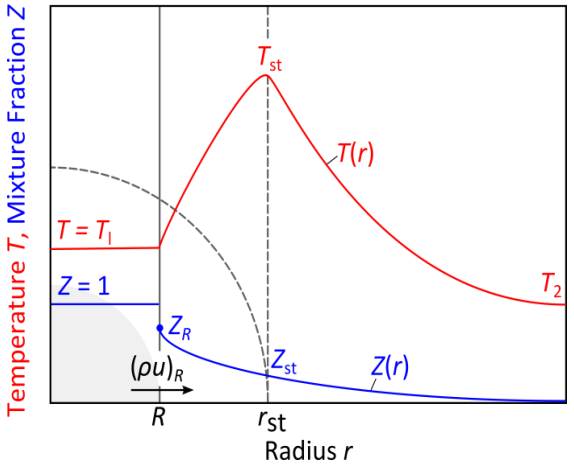
Single Droplet Combustion

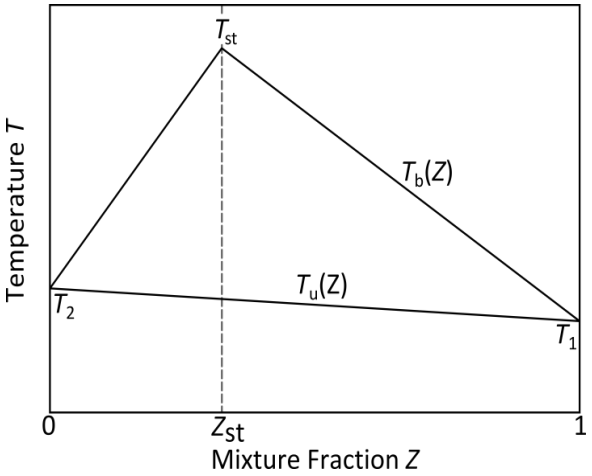
- At fuel rich side

$$T_b(Z) = T_u(Z) + \frac{(-\Delta h_m) Y_{O_2,2}}{c_p \nu'_{O_2} M_{O_2}} (1 - Z)$$

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

- Problem:
  - Temperature T_1 not known
  - Needed to determine $T_u(Z)$ in the unburnt mixture





Single Droplet Combustion

- From BC

$$(\eta_R - 1)\left.\frac{\mathrm{d}T}{\mathrm{d}\eta}\right|_R = \frac{h_\mathrm{l}}{c_p} \quad \xrightarrow{\eta=Z} \quad (Z_R - 1)\left.\frac{\mathrm{d}T}{\mathrm{d}Z}\right|_R = \frac{h_\mathrm{l}}{c_p}$$

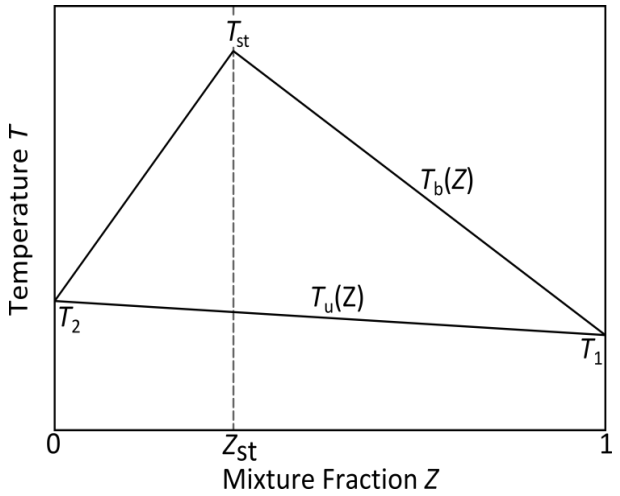
and

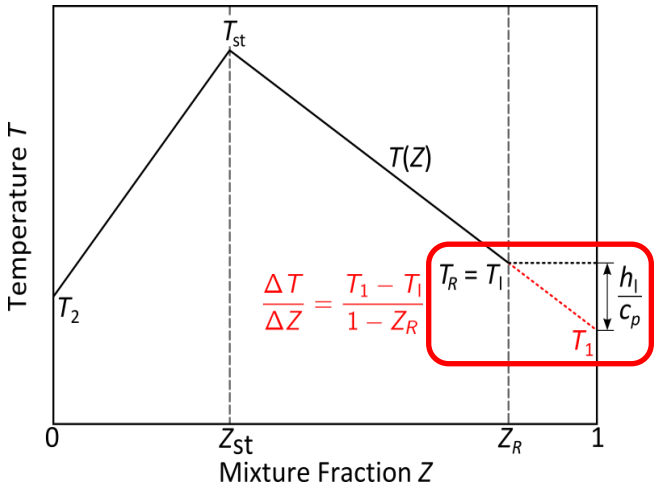
$$T(Z) = \underbrace{T_2 + (T_1 - T_2)Z}_{T_\mathrm{u}(Z)} + \frac{(-\Delta h_m) Y_{\mathrm{O}_2,2}}{c_p \nu'_{\mathrm{O}_2} M_{\mathrm{O}_2}}(1 - Z)$$

it follows

$$T_1 = T_\mathrm{l} - \frac{h_\mathrm{l}}{c_p}$$

- T_1 is a hypothetical temperature corresponding to the fuel if one considers the droplet as a point source of gaseous fuel





Single Droplet Combustion

- Result: Non-dimensional mass burning rate using $\zeta_R = -\ln(1-\eta_R)$:

$$\zeta_R = \ln\left(1 + \frac{c_p(T_2 - T_l) + Y_{O_2,2}(-\Delta h_m)/\nu'_{O_2} M_{O_2}}{h_l}\right)$$

- RHS is not a function of the droplet radius
- Mass burning rate

$$\zeta = \int_r^\infty \frac{u}{D}\mathrm{d}r = \frac{\dot{m}}{4\pi}\int_r^\infty (\rho D r^2)^{-1}\mathrm{d}r$$

Single Droplet Combustion

$$\zeta = \int_r^\infty \frac{u}{D} \mathrm{d}r = \frac{\dot{m}}{4\pi} \int_r^\infty (\rho D r^2)^{-1} \mathrm{d}r$$

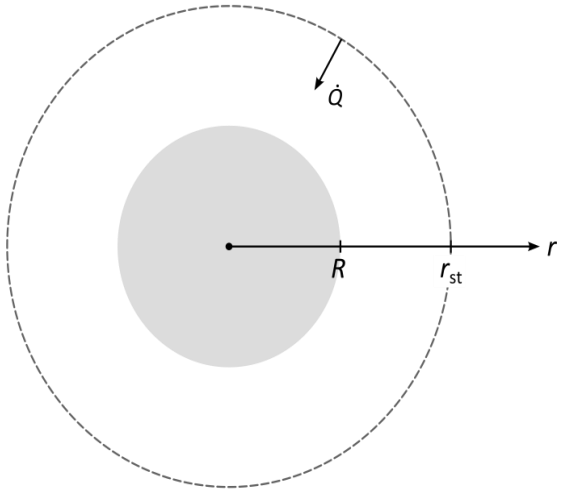
- Approximately: $\rho D \approx (\rho D)_{\mathrm{ref}} \approx$ const. →

$$\dot{m} = 4\pi (\rho D)_{\mathrm{ref}} \zeta_R R$$

→ Mass burning rate is proportional to R

→ Assumptions:

- Quasi stationary diffusion flame surrounding the droplet
- Constant temperature T_l within the droplet



Burnout time

→ It is possible to determine the time needed to burn a droplet with initial radius *R*

$$\dot{m} = -\frac{\mathrm{d}m}{\mathrm{d}t} = -\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{4}{3}\pi R^3 \rho_\mathrm{l}\right) = -\rho_\mathrm{l} 4\pi R^2 \frac{\mathrm{d}R}{\mathrm{d}t}$$

$$\int_0^{t_a} \mathrm{d}t = -\frac{\rho_L}{\zeta_R (\rho D)_\mathrm{ref}} \int_{d/2}^{0} R\mathrm{d}R$$

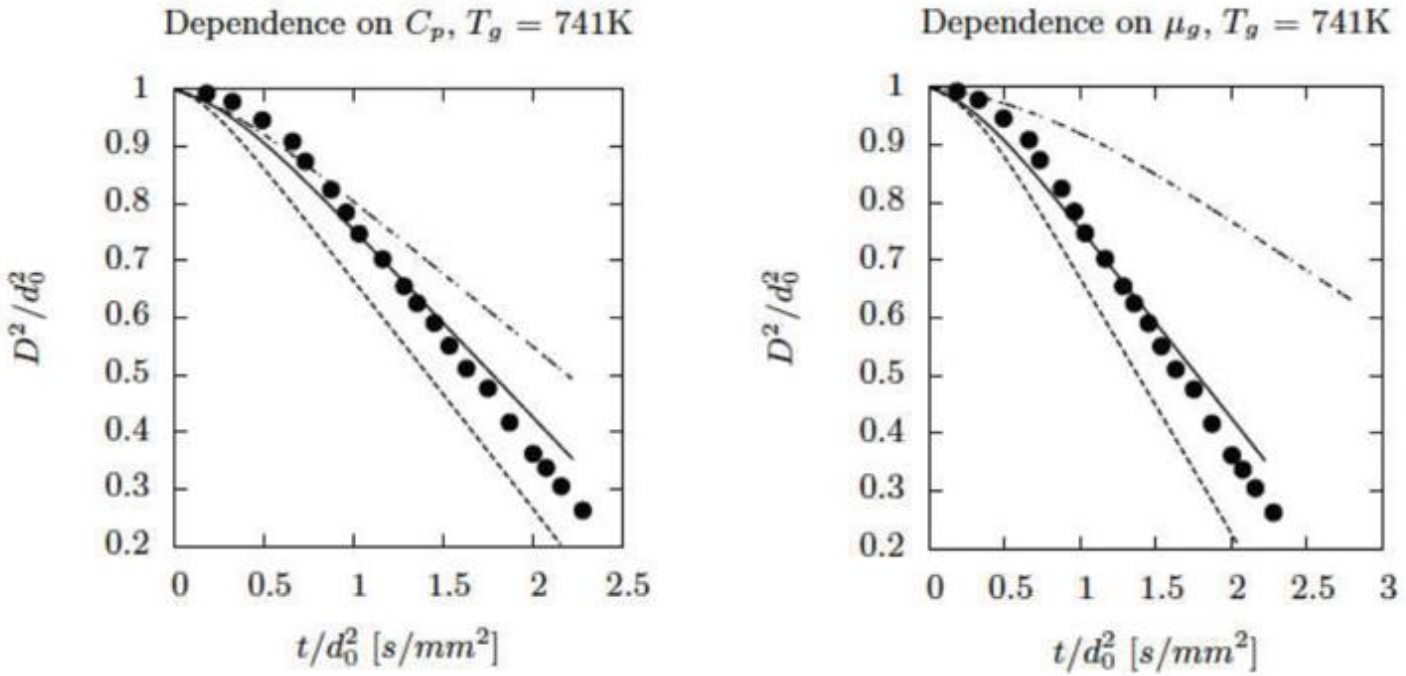
- Burnout time:

$$t_\mathrm{a} = \frac{\rho_L}{8\zeta_R (\rho D)_\mathrm{ref}} d^2$$

- This is called d^2-law of droplet combustion
- It represents a very good first approximation for the droplet combustion time and has often be confirmed by experiments.

Single Droplet Evaporation

Heptane drop in 741 K ambient air



$$C_p = (Y_{ref})C_{p,f} + (1 - Y_{ref})C_{p,g},$$

similar rule for viscosity

dots: experiments
solid: $Y_{ref} = 2/3\,Y_f + 1/3\,Y_g$
dashed: $Y_{ref} = 0$
dot dash: $Y_{ref} = 1$

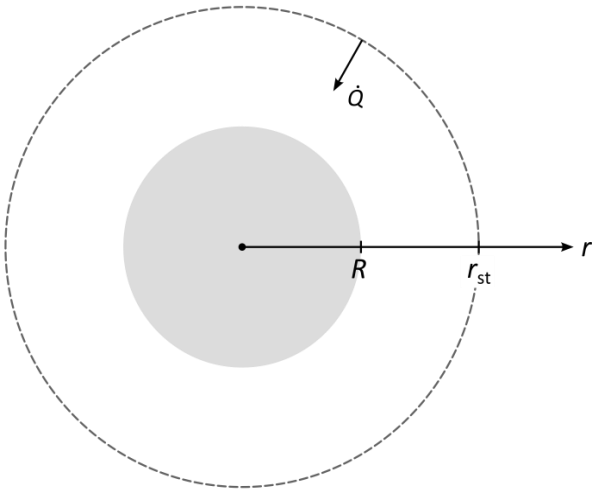
Radius of the surrounding diffusion flame

- We want to calculate the radial position of the surrounding flame:
  - From $\rho D \approx (\rho D)_{ref} \approx$ const. →

$$\zeta = \int_r^\infty \frac{u}{D} \mathrm{d}r = \frac{\dot{m}}{4\pi} \int_r^\infty (\rho D r^2)^{-1} \mathrm{d}r \quad \rightarrow \quad \zeta_{st} = \frac{\dot{m}}{4\pi (\rho D)_{ref} r_{st}} = \zeta_R \frac{R}{r_{st}}$$

  - With $\eta = 1 - \exp(-\zeta)$ and $Z = \eta$
  - $1 - Z_{st} = \exp(-\zeta_{st})$ →

$$\frac{r_{st}}{R} = \frac{\zeta_R}{\ln(1/(1 - Z_{st}))}$$



→ Flame radius

→ For sufficiently small values of Z_{st} the denominator may be approximated by Z_{st} itself showing that ratio r_{st}/R may take quite large values.

Summary

Part I: Fundamentals and Laminar Flames

- Introduction
- Fundamentals and mass balances of combustion systems
- Thermodynamics, flame temperature, and equilibrium
- Governing equations
- Laminar premixed flames: Kinematics and Burning Velocity
- Laminar premixed flames: Flame structure
- Laminar diffusion flames
  - Introduction
  - Counterflow diffusion flame
  - Flamelet structure of diffusion flames
  - FlameMaster flame calculator
  - Single droplet combustion