Aerospace Combustion

Lecture 11:

Combustion Modeling

Modelling Combustion

Characterization of Combustion Processes

There are many ways combustion processes can be characterized. Generally, people distinguish between

- premixed,
- non-premixed,
- and partially premixed combustion

However, there are many applications where heterogeneous processes are involved such as

- spray combustion in internal combustion engines, gas turbines or rocket engines
- or combustion in coal-fired power plants or in solid rocket motors.

The heat release may occur in a

- deflagration mode with flame velocities ranging from *cm/s - m/s*
- or detonation mode with flame velocities in the *km/s* range. Propagation is faster in liquid and solids than in gases.

Combustion Modelling

Although Fluid Mechanics seems already complicated enough, things turn even worse in case of chemical reactions in particular of reactions with hydrocarbons.

Chemical reactions mean

- Steep gradients in temperature, density, concentrations and thus in thermo-physical properties such as heat capacity, viscosity, thermal conductivity
- Local heat addition generally generates local pressure peaks and thus expansion
- Species are consumed and generated or exist only in an intermediate phase during the reaction processes, number of moles may change
- Only number of atoms remains constant

- Numerical treatment requires source and sink terms for mass, energy and species

Modelling Combustion

Basic Equations (1)

Let's start with the conservation of momentum

τ_{ik}, shear stress in the *i*-th direction on a surface whose normal is in the *k*-th direction

g_i body force in *i*-th direction

$$\frac{\partial}{\partial t}\rho u_i + \frac{\partial}{\partial x_k}\left(\rho u_k u_i\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_k}\tau_{ik} + g_k;$$

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\frac{\partial u_k}{\partial x_k}\delta_{ij}\right);$$

When bulk viscosity is neglected.

Continuity (supplemented by species conservation)

J_{ki}, mass molecular flux of species *k* in the *i*-th coordinate direction

$\dot{w}_k$ mass rate of creation of species k

$$\frac{\partial \rho}{\partial t}Y_k + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = -\frac{\partial}{\partial x_i}J_{ki} + \dot{w}_k;$$ Eqn (1)

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Basic Equations (2)

- To reduce complexity, J_{ki} is often simplified although this may cause erroneous results with molecules which are more agile than others such as hydrogen or in areas where turbulent mixing isn't dominant such as in boundary layers;

$$J_{ki} = -\rho D_k \frac{\partial Y_k}{\partial x_i};$$ Eqn (2)

- In air-breathing combustion, nitrogen is often considered as background fluid and the individual diffusion coefficients D_k will become the binary diffusion coefficient of nitrogen and the species of interest

→ and then the continuity equation becomes a simpler form

$$\frac{\partial \rho}{\partial t} Y_k + \frac{\partial}{\partial x_i}\left(\rho u_i Y_k\right) = \frac{\partial}{\partial x_i} \rho D_k \frac{\partial Y_k}{\partial x_i} + \dot{w}_k;$$

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Basic Equations (3)

Implementing the mass fraction μ_{ik} of element *i* in species *k* with $Z_i = \sum_{i=1}^{N} \mu_{ik} Y_k$ and $\sum_{i=1}^{M} Z_i = 1$ yields finally the conservation equation of elements

$$\frac{\partial \rho}{\partial t} \rho Z_k + \frac{\partial}{\partial x_i}\left(\rho u_i Z_k\right) = \frac{\partial}{\partial x_i} \sum_{l=1}^{N} \rho \mu_{il} D_l \frac{\partial Y_l}{\partial x_i};$$

Generally, this equation is too complicated due to the species diffusion coefficients and therefore it is assumed that diffusion can be described sufficiently by a single coefficient D

$$\frac{\partial \rho}{\partial t} \rho Z_k + \frac{\partial}{\partial x_i}\left(\rho u_i Z_k\right) = \frac{\partial}{\partial x_i} \rho D \frac{\partial Z_k}{\partial x_i};$$

Eqn (3)

This conservation of element formulation is useful for laminar flows and simple chemical systems. If *M* is the number of elements and *N* the number of species, we have to take into account *M-1* times Eqn (3) and N-M times Eqn (2) and this approach isn't feasible anymore and the species conservation form Eqn (1) is applied.

Modelling Combustion

Basic Equations (4)

Energy (various formulations depending on application)

Low speed turbulent flow (M<<1)

$$\frac{\partial \rho}{\partial t}\rho h + \frac{\partial}{\partial x_i}\left(\rho u_i h\right) = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}\left[\frac{\mu}{\sigma}\frac{\partial h}{\partial x_i} + \mu\sum_{l=1}^{N}\left(\frac{1}{Sc_k} - \frac{1}{Pr}\right)h_k \frac{\partial Y_l}{\partial x_i}\right];$$

*Radiation is neglected here

h, static enthalpy of the mixture and h_i that of species *i* ; *σ*, Prandtl number of the mixture and Sc_i, Schmidt number of species *i*.

with the definition $Sc_i = \frac{\eta}{\rho D_i}$ the importance of the single diffusion coefficient $D \approx D_i$ becomes obvious.

→ $Sc_i = Sc$ and $Sc = Pr$

and then

$$\frac{\partial \rho}{\partial t}\rho h + \frac{\partial}{\partial x_i}\left(\rho u_i h\right) = \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i}\frac{\mu}{Pr}\frac{\partial h}{\partial x_i};$$

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Basic Equations (5)

Hence, this energy equation has the form of a standard convection-diffusion one except the pressure term $\frac{\partial p}{\partial t}$.

Look at the two time derivate terms $\frac{\partial \rho}{\partial t}\rho h$ and $\frac{\partial p}{\partial t}$ and argue that a velocity fluctuation *u'* is associated with a pressure fluctuation $\rho u'^2$ and an enthalpy fluctuation $c_p T'$, then we can show that the ratio of pressure and enthalpy terms is similar to the square of Mach number fluctuation $\frac{u'^2}{c_p T'} \approx M'^2$ and with M << 1 we can neglect the pressure term.

Equation of State

For combustion studies it is often sufficient to assume an ideal gas (this isn't applicable if propellant injection is included where you have to deal with liquids and in case of rocket engines the liquids may be at cryogenic temperatures and even at trans-critical conditions).

$$p = \rho \frac{R_0 T}{W} = \rho R_0 T \sum_{k=1}^{N} \frac{Y_k}{W_k};$$

with *W,* the mixture molecular weight and W_i that of the species *i.*

For many applications it is acceptable to assume *p = const.,* except high speed flows and rocket engines.

Modelling Combustion

Basic Equations (6)

Thermo-physical Properties

$h = \sum_{k=1}^{N} Y_k h_k$; with $h_i = h_i(T)$ for turbulent flows the accuracy of $h_i = c_{p_i} T + \Delta_i$ is usually sufficient.

c_{p_i} and Δ_i are chosen such that this equation accurately predicts the static enthalpy for the desired range of temperature.

$$h = c_p T + \sum_{k=1}^{N} Y_k \Delta_k; \quad \text{with} \quad c_p = \sum_{k=1}^{N} c_{p_k} Y_k$$

and now we have a relation to predict the temperature.

c_p is the mixture heat capacity at constant pressure (Prandtl number)

$$T = \frac{h - \sum_{k=1}^{N} Y_k \Delta_k}{c_p}$$

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Basic Equations (7)

Chemical Source Terms

Let's consider *N* species are destroyed and generated in *R* elementary reactions

$$\sum_{k=1}^{N} \nu'_{ij} M_i \underset{k_{bj}}{\overset{k_{fj}}{\rightleftharpoons}} \sum_{k=1}^{N} \nu''_{ij} M_i$$

M_i is the symbol for the *i*-th species, ν'_i and ν''_i are the stoichiometric coefficients for species *i* in reaction *j*.

The chemical source term $\dot{w}_i$ accounts for generation and consumption of species *i* due to each reaction step.

$$\dot{w}_i = \sum_{J=1}^{R} \dot{w}_{ij}; \quad \text{with } \dot{w}_{ij} = 0 \text{ if species } i \text{ doesn't participate in reaction step } j.$$

$$\dot{w}_{ij} = \left(\nu''_{ij} - \nu'_{ij}\right) k_{fj} \rho^{m_{fj}} \frac{W_i}{W_j} \prod_{i=1}^{N} Y_i^{\nu'_{ij}} \left[1 - \frac{k_{bj}}{k_{fj}} \rho^{\left(m_{bj} - m_{fj}\right)} \prod_{i=1}^{N} Y_i^{\left(m_{bj} - m_{fj}\right)}\right] \quad \text{Eqn (4)} \qquad \text{with } W_j = \sum_{i=1}^{N} \nu'_{ij} W_i;$$

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Basic Equations (8)

Chemical Source Terms

$m_{\mathrm{f}j} \equiv \sum_{i=1}^{N} \nu'_{ij}$ and $m_{\mathrm{b}j} \equiv \sum_{i=1}^{N} \nu''_{ij}$ the forward and backward reaction rates for reaction *j*

Setting the bracket term in Eqn 4 to zero is the condition for chemical equilibrium for the *j*-th reaction step, i.e. forward and backward reaction rates are equal and then:

$$\frac{k_{\mathrm{f}j}}{k_{\mathrm{b}j}} = K_j(T)$$

Rate constants are often expressed as:

$$k_{\mathrm{f}j} = B_{\mathrm{f}j} T^{\alpha_{\mathrm{f}j}} \exp\left(-\frac{T_{\mathrm{af}j}}{T}\right)$$

where the pre-exponential factor $B_{\mathrm{f}j}$, the temperature exponent $\alpha_{\mathrm{f}j}$ and the activation temperature $T_{\mathrm{af}j}$ are constants which characterize the rate of the *j*-th reaction in forward direction.

in general Arrhenius form:

$$k_n = A_n T^{n_{\mathrm{n}}} \exp\left(-\frac{E_{\mathrm{n}}}{RT}\right)$$

with the frequency factor A_{n}, the temperature exponent n_n and the activation energy E_n.

Modelling Combustion

Temperature Dependency of Reaction Rate (1)

Let's consider a simple bimolecular reaction with negligible backward reaction. $M_1 + M_2 = M_3$ Eqn (5)

The contribution of this reaction step to the chemical source term in the conservation equation for M_1 can be found from Eqn 4 to be (with α =0):

$$-\rho^2 Y_1 Y_2 B \exp\left[-\frac{T_a}{T}\right]$$

Now $B \exp\left[-\frac{T_a}{T}\right]$ is usually in the order of $10^{10}/\rho_0\tau_0$ times $exp\,(-20 \cdot 10^3/2 \cdot 10^3)$ or larger with

ρ_0 is a representative density and τ_0 a representative chemical time.

Let's now consider a temperature T_c such that $\rho_c \tau_c\, B = exp(T_a/T_c)$ and then we get

$$-\frac{\rho^2}{\rho_0 \tau_c} Y_1 Y_2 B \exp\left[\frac{T_a}{T_c}\left(1-\frac{T_c}{T}\right)\right] \qquad \text{Eqn (6)}$$

Modelling Combustion

Temperature Dependency of Reaction Rate (2)

and with

$$ln(\rho_c \tau_c B) = T_a/T_c \gg 1$$

we may conclude that the consumption of M_1 due to this reaction step is limited to regions in the flow where $T \approx T_c$;

for $T < T_c$ T the reaction rate is very slow while for

$T > T_c$ either Y_1 or Y_2 must be so small that again little M_1 is consumed.

The small magnitude of either Y_1 or Y_2 is reminiscent of the Burke-Schuman model of non-premixed combustion where a flame sheet separates fuel and oxidizer and creating product.

If B and ρ_0 are known, we can determine the representative chemical time scale τ_c of reaction Eqn (5).

Modelling Combustion

Temperature Dependency of Reaction Rate (3)

Many chemical reactions in applications of interest behave in a fashion that can be represented by Eqn (6), i.e. they have rates extremely sensitive to temperature which implies the chemical reaction is very localized, a fact of great importance for laminar and turbulent flows.

In laminar flows, this means that very thin reaction zones are embedded in viscous layers devoid of significant chemical activity but possibly with large temperature gradients.
(There are many models which aim at the description of stability and/or heat loss on flame extinction which treat the flame as indefinitely thin, i.e. as discontinuity.)

In many (not all) turbulent flows, a high sensitivity of chemical reactions to temperature results in reactions being confined to laminar flamelets (will be discussed later), molecularly dominated surfaces which are moved around and strained by the turbulent flow field (reaction sheet regime).

Modelling Combustion

Modeling Premixed Turbulent Flames

Most models employ assumptions which aren't satisfied by real flames, e.g.

• Adiabatic	may sometimes be ok
• Homogeneous, isotropic turbulence over many length scales	never holds
• Low Karlowitz or high Damköhler numbers which results in thin flame fronts	may be sometimes ok
• Lewis number Le = 1	may sometimes be ok, e.g. for CH4-air combustion
• Constant transport properties	never holds, up to a factor of 25 increase of viscosity and thermal diffusivity across flame front
• u' doesn't change across flame front	never holds due to thermal expansion across flame which generates turbulence, however, increase in viscosity across flame front will decrease turbulence and this counterworking effects may cancel themselves out sometimes
• Constant density	never holds

Combustion Models

Eddy Dissipation Model (EDM)

Extension (Magnussen & Hjertager) of old Eddy Break-Up Model (Spalding)

- Assumes extremely fast chemistry → mixing time is the dominant time scale and thus controls the process
- Can be applied to both turbulent premixed and non-premixed combustion since it couples turbulent mixing with chemical reaction

Source term (1-step reaction)

$$\widetilde{S}_i = A\,\nu_i' M_i \frac{\widetilde{\varepsilon}}{\widetilde{k}} \min\left(\frac{\widetilde{Y}_R}{\nu_R' M_R}, B \frac{\sum \widetilde{Y}_P}{\sum \upsilon_P'' M_P} \right)$$

Y_R, Y_P: mass fraction of reactant/product
A, B: model parameters (experimentally)

- has to be adjusted to lean/rich mixtures

- Approach is simple and numerically robust,
- However
  - No finite rate chemistry and no extinction
  - Often overestimates fuel consumption and yields too high temperatures

Combustion Models

Finite Rate Chemistry Model (FRCM)

Combustion model for cases where chemistry is controlling the combustion process

- Assumes $t_{chemistry} > t_{mixing}$ (laminar and or turbulent) and is applicable for both laminar and turbulent non-premixed situations when non-equilibrium effects become important

Source term (species *i* in reaction *j*)

$$\widetilde{S}_{i,j} = A\widetilde{\Gamma}M_i\left(\nu''_{i,j} - \nu'_{i,j}\right)\left(k_{f,j}\prod_i\left(\frac{\overline{\rho}\widetilde{Y}_i}{M_i}\right)^{\upsilon'_{i,j}} - k_{b,j}\prod_i\left(\frac{\overline{\rho}\widetilde{Y}_i}{M_i}\right)^{\upsilon''_{i,j}}\right)$$

$k_{f,j}$, $k_{b,j}$: rates of reaction j (forward/backward) determined by Arrhenius expressions $f(\widetilde{T})$

$\widetilde{\Gamma}$: models influence of third body reactions $\widetilde{\Gamma} = \sum \gamma_{i,j}\frac{\overline{\rho}\widetilde{Y}_i}{M_i}M_i$

- Source term linearization centered on operating point which allows for integration into species equations and realization of larger time steps

However

- Takes only mean values for temperature in the Arrhenius expression and thus ignores effect of turbulent fluctuations which yields an under-prediction of temperatures

Combustion Models

Combination of EDM and FRCM

Model computes for each cell two reaction rates, one based on EDM and the other on FRCM assumptions and the smaller rate is then used to determine the local reaction rate.

$$r_i = \min\left(r_i^{EDM}, r_i^{FRCM}\right)$$

Hence, the model automatically decides if the process is controlled by mixing or by chemistry.

Although this combined approach enlarges the range of applicability, it still does not account for turbulence / chemistry interaction.

Combustion Models

Eddy Dissipation Concept (EDC)

EDC is an extension of EDM insofar as it considers detailed chemical kinetics and it assumes that reactions take place at small scales`*´

$$\xi^* = C_\xi \left(\frac{\upsilon \bar{\varepsilon}}{\tilde{k}^2} \right)^{1/4} \quad \text{with a volume:} \quad \xi^{*3}$$

Reaction rates are derived from Arrhenius expression (FRCM) with time scale of reactions:

$$\tau^* = C_\tau \left(\frac{\upsilon}{\tilde{\varepsilon}} \right)^{1/2}$$

Boundary/Initial conditions for reactions:

- Assumption: *p = const.*
- Initial condition: temperature and species concentration in a cell
- Reactions at time scale τ^*
- Numerical integration (e.g. ISAT-Algorithm) → $\tilde{Y}_{i^*}$

Combustion Models

Eddy Dissipation Concept (EDC)

Source term model

$$\widetilde{S}_i = \frac{\xi^{*2}}{\tau^*\left(1-\xi^{*3}\right)}\left(\widetilde{Y}_{i^*} - \widetilde{Y}_i\right)$$

Mass fraction of species i on small scales after reaction time τ^*

Requires processing power
System of differential equations very stiff

Combustion Models

Transport PDF Equation Model

Model bases on transport equation for velocity and reactive scalars for a one-point statistics (joint pdf, Pope)

$$P = f\left(\mathbf{v}, \boldsymbol{\psi}, \mathbf{x}, t\right)$$

Reactive scalar: mass fraction of all components and temperature

$$\psi_i = \left(Y_1, Y_2, Y_3, , , Y_N, T\right)^T$$

Balance for all ψ_i:

$$\rho \frac{\partial \psi_i}{\partial t} + \rho u_j \frac{\partial \psi_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_i \frac{\partial \psi_i}{\partial x_j}\right) + \rho S_i$$

- D_i, mass diffusivity, thermal diffusivity
- S_i, mass/temperature source term

in conservative form:

$$\frac{\partial \rho P}{\partial t} + \nabla\left(\rho \mathbf{v} P\right) + \left(\rho g - \overline{p}\right) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^{N} \frac{\partial \psi_i}{\partial x_j}\left(\omega_i P\right) = \nabla_{\mathbf{v}} \cdot \left[\left\langle -\nabla \cdot \tau + \nabla\left\langle p' \middle| \mathbf{v}, \psi \right\rangle P \right\rangle\right] - \sum_{i=1}^{N} \frac{\partial}{\partial \psi_i}\left[\left\langle \nabla \cdot \left(\rho D \nabla \psi_i\right) \middle| \mathbf{v}, \psi \right\rangle P\right]$$

$\nabla_{\mathbf{v}}$ is the gradient with respect to velocity components,
$\langle\ \rangle$ angular brackets are conditional means,
same symbol used for random and sample space variables

Combustion Models

PDF Closure Problem

Analysis of individual terms (l.h.s.)

- the first two are local change and convection of the pdf in physical space
- the third is the transport in velocity space by gravity and mean pressure gradient
- the fourth represents the chemical sources

$$\frac{\partial \rho P}{\partial t} + \nabla(\rho \mathbf{v} P) + (\rho g - \bar{p}) \cdot \nabla_{\mathbf{v}} P + \sum_{i=1}^{N} \frac{\partial \psi_i}{\partial x_j} (\omega_i P) =$$

all the l.h.s. terms are closed since they are local in physical space.

Analysis of individual terms (r.h.s.)

- the first describes the transport of the pdf in velocity space as a result of viscous stresses and fluctuating pressure gradient
- the second represents transport in reactive scalar space by molecular fluxes (molecular mixing).

$$\nabla_{\mathbf{v}} \cdot \left[\left\langle -\nabla \cdot \tau + \nabla \left\langle p' \middle| \mathbf{v}, \psi \right\rangle P \right\rangle \right] - \sum_{i=1}^{N} \frac{\partial}{\partial \psi_i} \left[\left\langle \nabla \cdot (\rho D \nabla \psi_i) \middle| \mathbf{v}, \psi \right\rangle P \right]$$

all r.h.s. terms, which contain gradients of conditioned quantities (velocity and composition) are unclosed and have to be modelled.

Monte-Carlo Methods are applied (linear dependency memory requirement on problem dimensionality)

Combustion Models

PDF Closure Problem

In case of fast chemical reactions, mixing and reaction happen in thin layers where chemical source terms and molecular transport are balanced

→ Both the closed chemical term and the unclosed molecular mixing term are important and closely linked which results in steep local gradients of the reactive scalars and makes closure assumptions of the molecular mixing term.

One solution for this problem is the presumed pdf approach

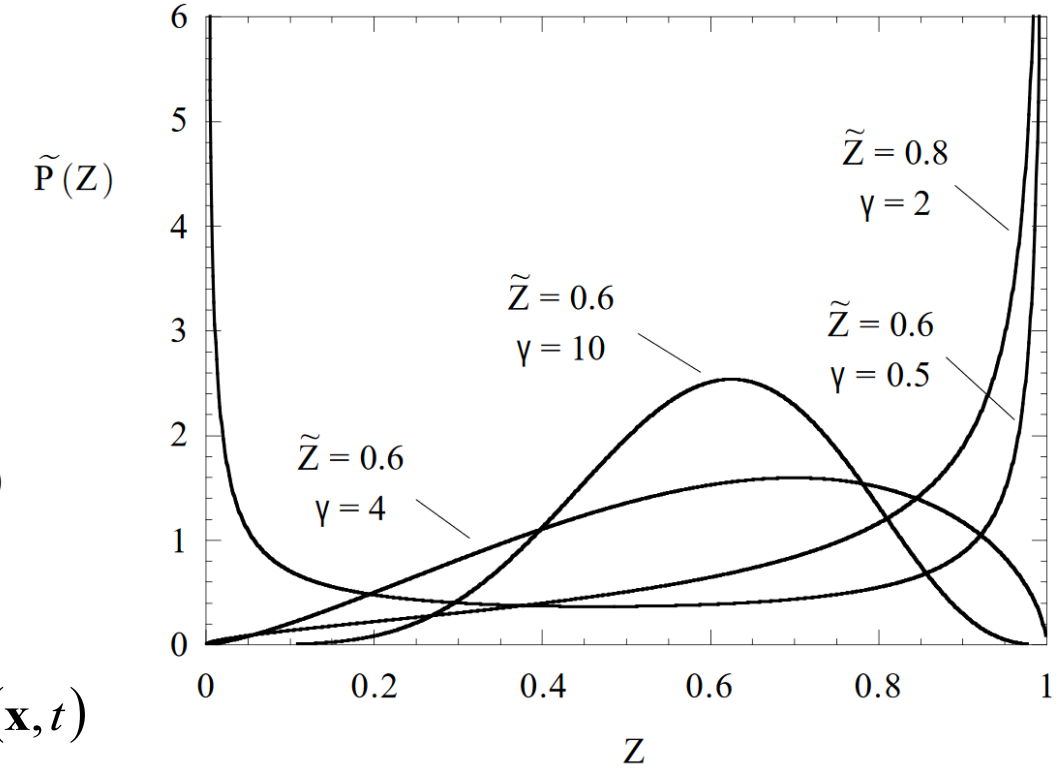
Basic assumptions: within this thin layers and in their vicinity, temperature and reactive species concentrations profiles can be described as functions of the mixture fraction which doesn't contain chemical source terms thus bypassing the problem.

For non-premixed combustion a beta function pdf

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

is applied with $\gamma=\frac{\widetilde{Z}(1-\widetilde{Z})}{\widetilde{Z}''^2}-1\geq 0$ and $\alpha=\widetilde{Z}\gamma;\quad \beta=\left(1-\widetilde{Z}\right)\gamma$

α and β are related to the Favre mean and variance: $\widetilde{Z}(\mathbf{x},t);\ \widetilde{Z}''^2(\mathbf{x},t)$



Combustion Models

Bray-Moss-Libby Model (BML)

Pre-mixed Turbulent Combustion

Lewis number Le = 1

Definition of a progress variable: $c = \frac{T - T_u}{T_b - T};\ or\ \ c = \frac{Y_P}{Y_{P,b}}$

Favre-averaged transport (molecular transport neglected):

$$\bar{\rho}\frac{\partial \tilde{c}}{\partial t} + \bar{\rho}\tilde{u}_i \frac{\partial \tilde{c}}{\partial x_i} = -\frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i'' c''}\right) + \bar{\omega}_c$$

Closure required for turbulent transport and chemical source term (very fast chemistry →

flame thickness $l_F << \eta << l_t$ length scale of turbulence (eddies).

Fuel consumption happens only within the thin flame front, hence there is either a flow of burnt gases (c = 1) or the unburnt mixture (c = 0) and intermediate states (finite rate chemistry) are highly unlikely.

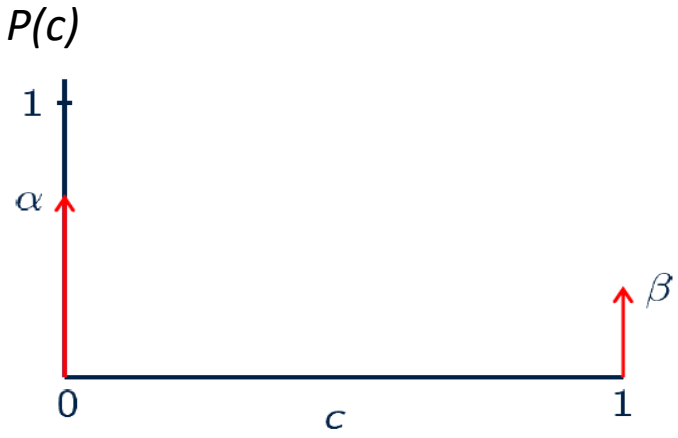
Combustion Models

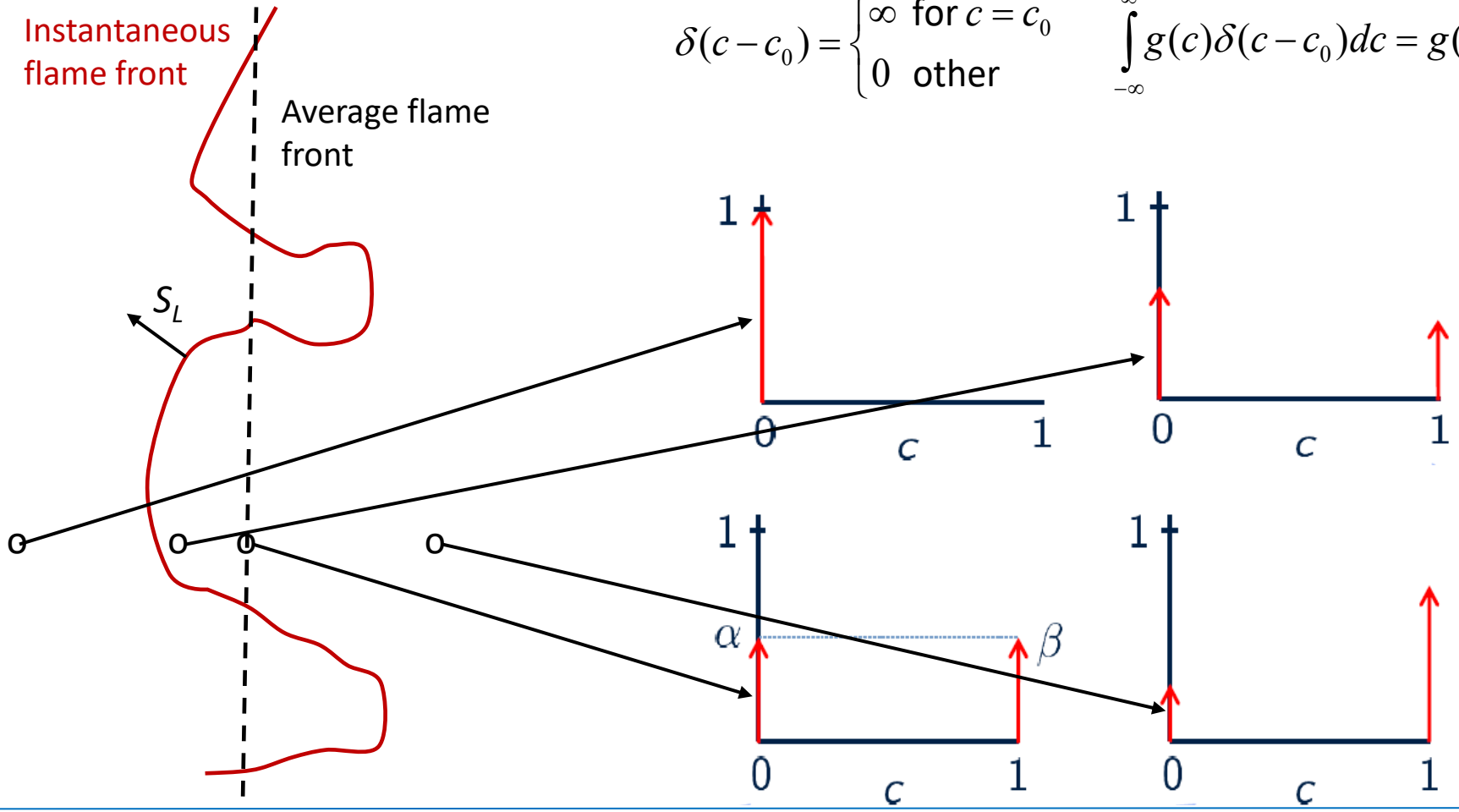
BML Model

Probability density function

$P(c) = \alpha\delta(c) + \beta\delta(1-c); \quad \alpha + \beta = 1; \quad \delta$ delta function

$$\delta(c-c_0) = \begin{cases} \infty & \text{for } c = c_0 \\ 0 & \text{other} \end{cases} \qquad \int_{-\infty}^{\infty} g(c)\delta(c-c_0)dc = g(c_0)$$





Probability density function at different positions relative to the instantaneous flame front.

Combustion Models

BML Turbulent Transport Closure

Favre average $\tilde{Q} = \frac{1}{\bar{\rho}} \int_{c_{min}}^{c_{max}} \int_{u_{min}}^{u_{max}} \rho Q(u,c) P_{u,c}(u,c) du dc;$

The unclosed correlation $\widetilde{u_i'' c''}$ can be derived from a joint pdf for u and c

$P_{u,c}(u,c) = P(c) P_{u|c}(u|c)$ Bayes-Theorem

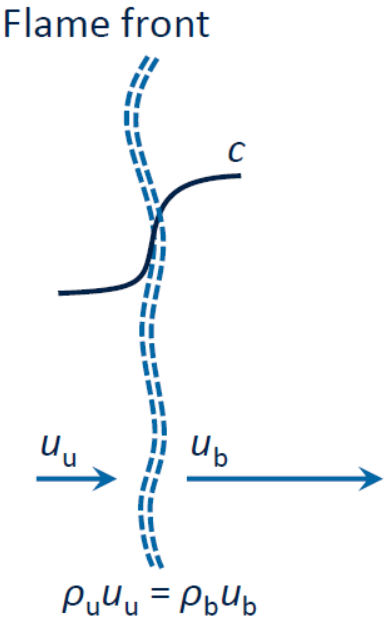
$P_{u,c}(u,c) = \alpha \delta(c) P_{u|c}(u|c=0) + \beta \delta(1-c) P_{u|c}(u|c=1)$

conditional pdf delta function

with the BML approach of P(c) we get:

and with follows: $\widetilde{u_i'' c''} = \frac{\overline{\rho u_i'' c''}}{\bar{\rho}} = \frac{\overline{\rho (u-\tilde{u})(c-\tilde{c})}}{\bar{\rho}} = \frac{1}{\bar{\rho}} \int_0^1 \int_{-\infty}^{\infty} \rho (u-\tilde{u})(c-\tilde{c}) P_{u,c}(u,c) du dc$

$\widetilde{u_i'' c''} = \tilde{c}(1-\tilde{c})(\bar{u}_b - \bar{u}_u)$



However, through the flame front, the velocity increases while the density decreases and thus:

$(\bar{u}_b - \bar{u}_u) > 0$ and because $c \geq 0$ → $\widetilde{u_i'' c''} = \tilde{c}(1-\tilde{c})(\bar{u}_b - \bar{u}_u) \geq 0$

Combustion Models

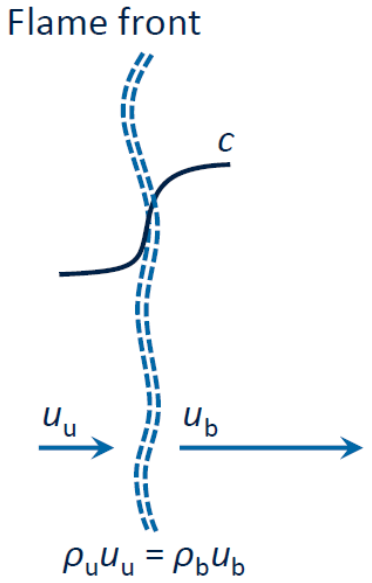
BML Turbulent Transport Closure Problem

Within the flame: $\frac{\partial \tilde{c}}{\partial x} \geq 0$

Gradient transport would yield $\widetilde{u_i'' c''} = -D_t \frac{\partial \tilde{c}}{\partial x_i} \leq 0$

which contradicts the previous result $\widetilde{u_i'' c''} = \tilde{c}(1-\tilde{c})(\bar{u}_b - \bar{u}_u) \geq 0$

Hence, this means we have a counter-gradient diffusion



Two limiting cases:

1. Low turbulence levels: fluid dynamics is imposed by thermal expansion (chemistry generated/enhanced turbulence)

→ counter-gradient transport

2. High turbulence levels: fluid dynamics is imposed by turbulence

→ Gradient transport

Bray Criterion: $N_B = \frac{\tau S_L}{\alpha u'}$

Combustion Models

BML Chemical Source Term Closure

Flame surface density model

- $\overline{\omega}$: chemical source term
- I_0: strain factor (describes the change of burn rate by strain)
- S_L^0: laminar flame velocity
- $\sum$: Flame surface density (flames per volume)
- $u_c(s)$: consumption speed of flame with stretch s
- c: reaction progress variable or dimensionless temperature

number of flames per volume

$$\overline{\omega}_c = \rho_u S_L^0 I_0 \sum$$

local conversion of mass per area

$$I_0 = \frac{1}{S_L^0} \int_{-\infty}^{\infty} u_c(\dot{s}) P(\dot{s}, \mathbf{x}) d\dot{s}$$

$$u_c = \frac{1}{\rho_u} \int_{-\infty}^{\infty} \omega(z, \dot{s}) P dz$$

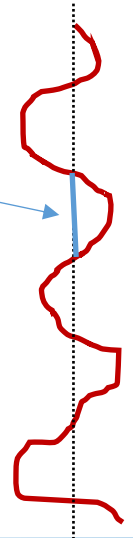
Chemical source term is product of density in the unburnt mixture times the laminar flame velocity times the change of burning velocity by local strain times the number of flames per volume.

Closure of flame surface density by

a) algebraic equation:

$$\sum \sim \frac{\bar{c}(1-\bar{c})}{L_y}$$

L_y: average length between flame crossings



b) transport equation:

$$\bar{\rho} \frac{\partial \sum}{\partial t} + \bar{\rho} \tilde{u}_i \frac{\partial \sum}{\partial x_i} = -\frac{\partial}{\partial x_i} D_t \frac{\partial \sum}{\partial x_i} + C_1 \frac{\varepsilon}{k} \sum - C_2 S_L \frac{\sum^2}{1-\bar{c}}$$

Local change	Convective transport	Turbulent transport	Production due to strain	Flame quenching

Combustion Models

Turbulent Non-Premixed Models

Conserved Scalar Based Models (Mixture Fraction Z)

$$\upsilon Y_F - Y_O = \upsilon Y_{F,u} - Y_{O,u} = \upsilon Y_1 Y_{F,1} - Y_2 Y_{O,2} = \upsilon Y_1 Y_{F,1} - (1 - Y_1) Y_{O,2}$$

$$Z = \frac{\upsilon Y_F - Y_O + Y_{O,2}}{\upsilon Y_{F,1} + Y_{O,2}} = \frac{m_1}{m_1 + m_2} = \frac{1}{1 + \frac{m_2}{m_1}}$$

For stoichiometric conditions:

$$Z_{st} = \left. \frac{\upsilon Y_F - Y_O + Y_{O,2}}{\upsilon Y_{F,1} + Y_{O,2}} \right|_{st} = \frac{1}{1 + \upsilon \frac{Y_{F,1}}{Y_{O,2}}}$$

Transport Equation

Boundary conditions: *Z=1* in fuel, *Z=0* in oxidizer

$$\overline{\rho} \frac{\partial Z}{\partial t} + \overline{\rho} \widetilde{u}_i \frac{\partial Z}{\partial xj} = \frac{\partial}{\partial xj} \left(\rho D \frac{\partial Z}{\partial x_j} \right)$$

If species and temperature are function of mixture ratio

$$\widetilde{Y}_i = \int_{-\infty}^{\infty} Y_i(Z) \widetilde{f}(Z) dZ; \text{ and } \widetilde{T} = \int_{-\infty}^{\infty} T(Z) \widetilde{f}(Z) dZ$$

Closure

- local statistics of Z (as pdf)
- Species/temperature functions $Y_i(Z)$, $T(Z)$

Combustion Models

Turbulent Non-Premixed Models

Conserved Scalar Based Models (Mixture Fraction Z)

Equation for the mean

$$\rho\frac{\partial\tilde{Z}}{\partial t}+\rho\tilde{u}_i\frac{\partial\tilde{Z}}{\partial x_i}=\frac{\partial}{\partial x_i}\left(\bar{\rho}D_t\frac{\partial\tilde{Z}}{\partial x_j}\right)$$

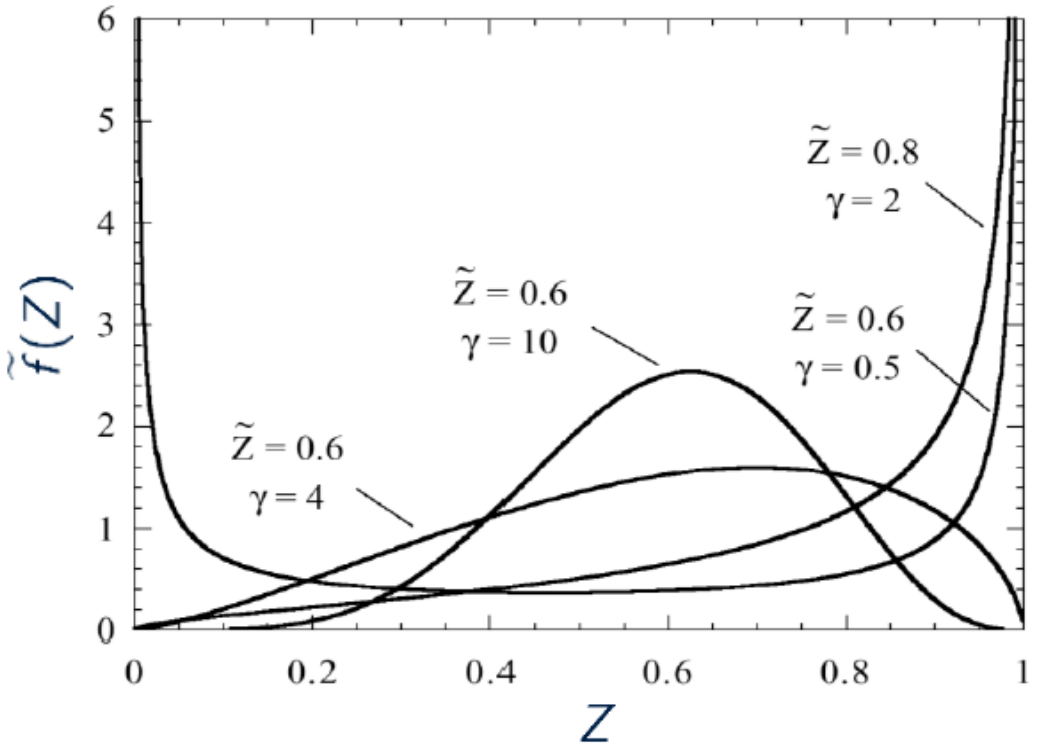
Variance

$$\bar{\rho}\frac{\partial\tilde{Z}''^2}{\partial t}+\bar{\rho}\tilde{u}_i\frac{\partial\tilde{Z}''^2}{\partial x_i}=-\frac{\partial}{\partial x_i}\left(\bar{\rho}D_t\frac{\partial\tilde{Z}''^2}{\partial x_i}\right)+2\bar{\rho}\left(D_t\frac{\partial\tilde{Z}''}{\partial x_i}\right)\frac{\partial\tilde{Z}}{\partial x_i}-\bar{\rho}c_\chi\frac{\tilde{\varepsilon}}{\tilde{k}}\tilde{Z}''^2$$

β-function pdf for Z

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

Recall $\alpha=\tilde{Z}\gamma;\quad \beta=(1-\tilde{Z})\gamma$ and $\gamma=\frac{\tilde{Z}(1-\tilde{Z})}{\tilde{Z}''^2}-1\geq 0$



Combustion Models

Turbulent Non-Premixed Models

Conserved Scalar Based Models (Mixture Fraction Z)

1. Infinitely fast irreversible chemistry (see lecture on combustion theory)
   - Burke-Schuman
   - Solution = *f(Z)*
2. Infinitely fast reversible chemistry
   - Chemical equilibrium
   - Solution = *f(Z)*
3. Flamelet for non-premixed combustion
   - Chemistry fast, but not infinitely fast
   - Solution = *f(Z,χ)*
4. Conditional Moment Closure (CMC)
   - Similar to flamelet approach
   - Solution = *f(Z,<χ IZ>)*

Combustion Models

Turbulent Non-Premixed Models

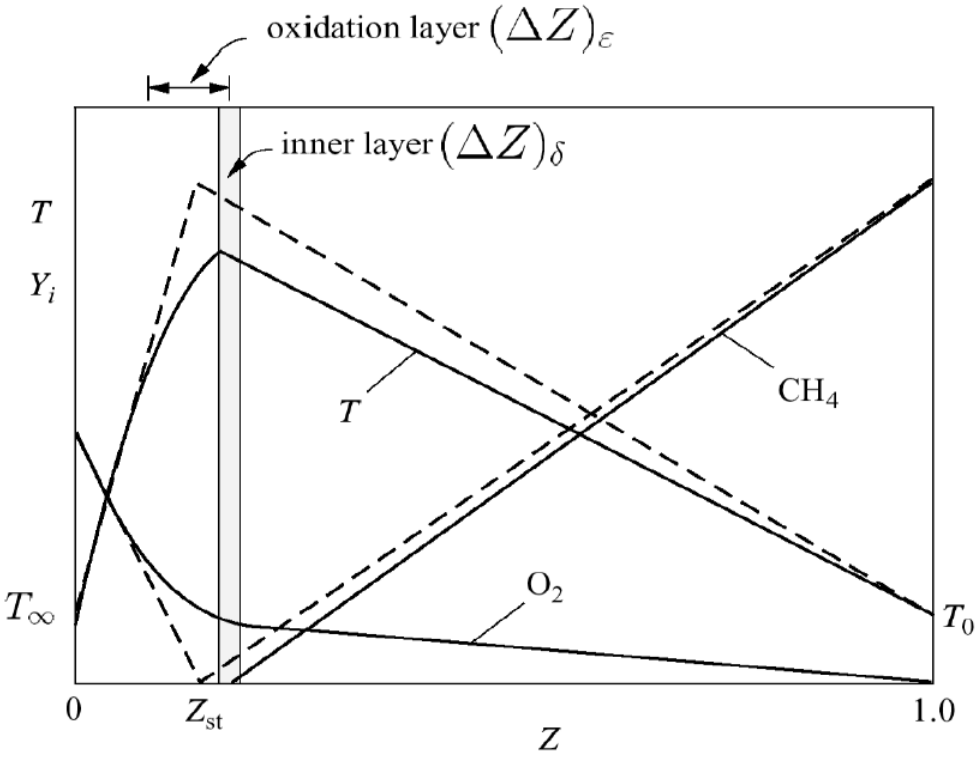
Flamelet

- Bases on the idea of scale separation
- Assumes fast, but not infinitely fast chemistry (1 << Da << 1
- reaction zone thin compared to small turbulence scales (laminar)
- Transformation and asymptotic approximation leads to flamelet equations

$$\rho\frac{\partial T}{\partial t}+\rho u_i\frac{\partial T}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial T}{\partial x_i}\right)=-\sum_{\alpha=1}^{n}\frac{h_\alpha}{c_p}\dot{m}_\alpha'''+\frac{\dot{q}_R'''}{c_p}+\frac{1}{c_p}\frac{\partial p}{\partial t}$$

$$\rho\frac{\partial Y_\alpha}{\partial t}+\rho u_i\frac{\partial Y_\alpha}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial T}{\partial x_i}\right)=-\dot{m}_\alpha'''$$

$$\rho\frac{\partial Z}{\partial t}+\rho u_i\frac{\partial Z}{\partial x_i}-\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial Z}{\partial x_i}\right)=0$$



Example of an oxygen/methane flame in temperature / mixture fraction space

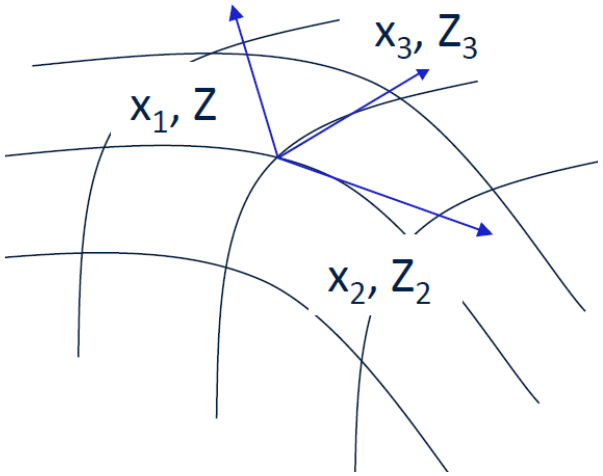
Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

with $L \equiv \rho \frac{\partial}{\partial t} + \rho u_i \frac{\partial}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D \frac{\partial}{\partial x_i}\right)$ follows $L(T) = -\sum_{\alpha=1}^{n} \frac{h_\alpha}{c_p} \dot{m}_\alpha''' + \frac{\dot{q}_R'''}{c_p} + \frac{1}{c_p}\frac{\partial p}{\partial t}$, $L(Y_a) = -\dot{m}_\alpha'''$ and $L(Z) = 0$

Transformation



- Surface of stoichiometric mixture
- Reaction zone confined to thin layer around this surface
- Transformation to surface attached coordinate system
- $x_1, x_2, x_3, t \rightarrow Z(x_1, x_2, x_3, t), Z_2=x_2, Z=x_3, \tau$
- $\Psi(x_1, x_2, x_3, t) \rightarrow \Psi[Z(x_1, x_2, x_3, t), Z_2, Z_3, \tau]$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t}\rho D \frac{\partial}{\partial Z}$$

$$\frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1}\frac{\partial}{\partial Z}$$

$$\frac{\partial}{\partial x_j} = \frac{\partial}{\partial Z_j} + \frac{\partial Z}{\partial x_j}\frac{\partial}{\partial Z}, j = 2,3$$

Combustion Models

Turbulent Non-Premixed Models

Transformation example for temperature:

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \tau} + \frac{\partial Z}{\partial t}\rho D \frac{\partial}{\partial Z}$$

$$\frac{\partial}{\partial x_1} = \frac{\partial Z}{\partial x_1}\frac{\partial}{\partial Z}$$

$$\frac{\partial}{\partial x_j} = \frac{\partial}{\partial Z_j} + \frac{\partial Z}{\partial x_j}\frac{\partial}{\partial Z}, j = 2,3$$

$$\mathrm{L}(T) = -\sum_{\alpha=1}^{n}\frac{h_\alpha}{c_p}\dot{m}_\alpha''' + \frac{\dot{q}_R'''}{c_p} + \frac{1}{c_p}\frac{\partial p}{\partial t} = \dot{\omega}_T$$

yields transformed temperature equation

$$\rho\frac{\partial T}{\partial \tau} + \rho u_j \frac{\partial T}{\partial Z_j} - \rho D\left[2\frac{\partial Z}{\partial x_j}\frac{\partial^2 T}{\partial Z \partial Z_j} + \frac{\partial^2 T}{\partial Z_j^2}\right] - \frac{\partial}{\partial x_j}\left(\rho D\frac{\partial T}{\partial Z_j}\right) - \rho D\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_T; j = 2,3$$

Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

$$\rho\frac{\partial T}{\partial \tau}+\rho u_j\frac{\partial T}{\partial Z_j}-\rho D\left(2\frac{\partial Z}{\partial x_j}\frac{\partial^2 T}{\partial Z\partial Z_j}+\frac{\partial^2 T}{\partial Z_j^2}\right)-\frac{\partial}{\partial x_j}\left(\rho D\frac{\partial T}{\partial Z_j}\right)-\rho D\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2}=\dot{\omega}_\tau,\quad j=2,3$$

Local change

small, not dominating

mixing

Chemical source term

For flamelets thin in Z direction, a similarity analysis shows that $\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2}$ is the dominating term of the spatial variables;

→ $$-\rho D\left(\frac{\partial Z}{\partial x_i}\right)^2\frac{\partial^2 T}{\partial Z^2}=\dot{\omega}_\tau$$

$\rho\frac{\partial T}{\partial \tau}$

This is equivalent to the assumption that temperature derivatives normal to the flame surface are much larger than those in tangential direction.

The local change term is important for very rapid changes which may yield extinction.

Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

- Similar procedure for mass fraction
- Flamelet structure is to leading order described by one-dimensional time dependent equations

$$\rho \frac{\partial T}{\partial \tau} + \rho \frac{\chi_{st}}{2} \frac{\partial^2 T}{\partial Z^2} = \dot{\omega}_T$$

$$\rho \frac{\partial Y\alpha}{\partial \tau} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 Y_\alpha}{\partial Z^2} = \dot{m}'''_\alpha$$

$$\rho \frac{\partial \psi_i}{\partial \tau} - \rho \frac{\chi_{st}}{2} \frac{\partial^2 \psi_i}{\partial Z^2} = \dot{\omega}_{\psi_i}$$

- Instantaneous scalar dissipation rate χ_{st} at stoichiometric conditions,

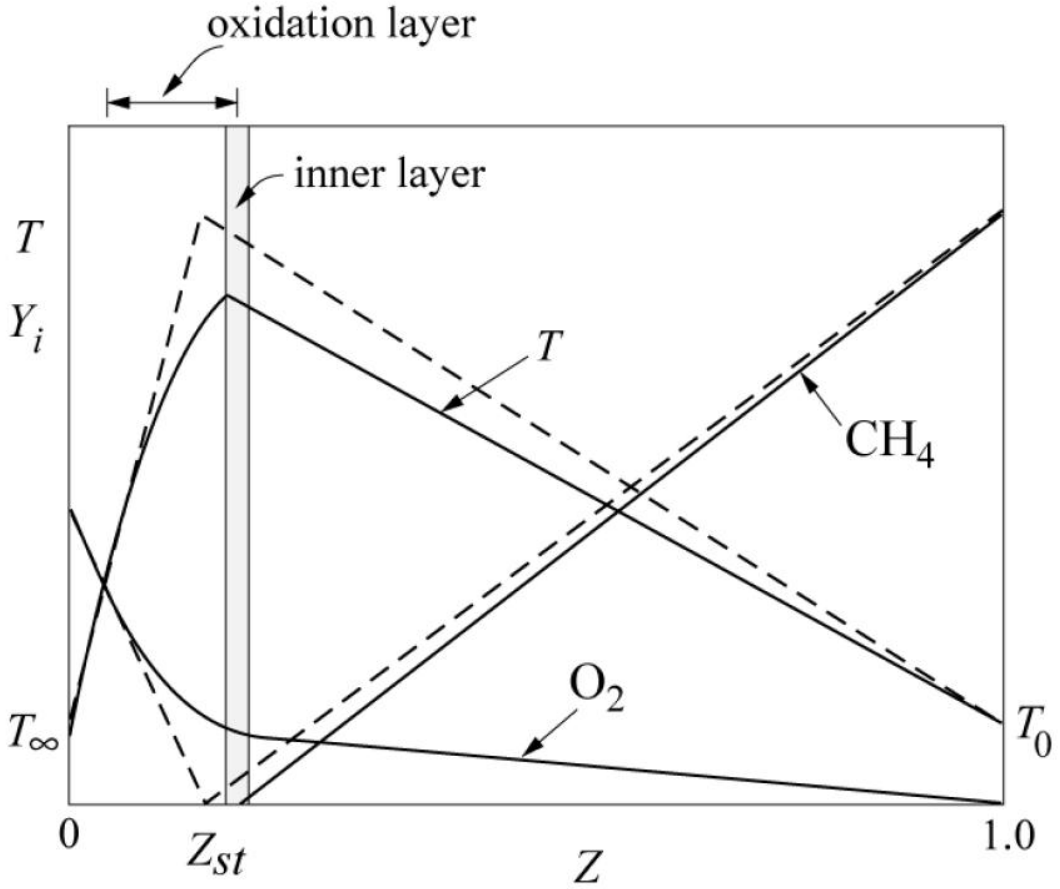
$$\chi_{st} = 2D\left(\frac{\partial Z}{\partial x_i}\right)^2\Big|_{st}$$

may be interpreted as inverse of a characteristic time for diffusion

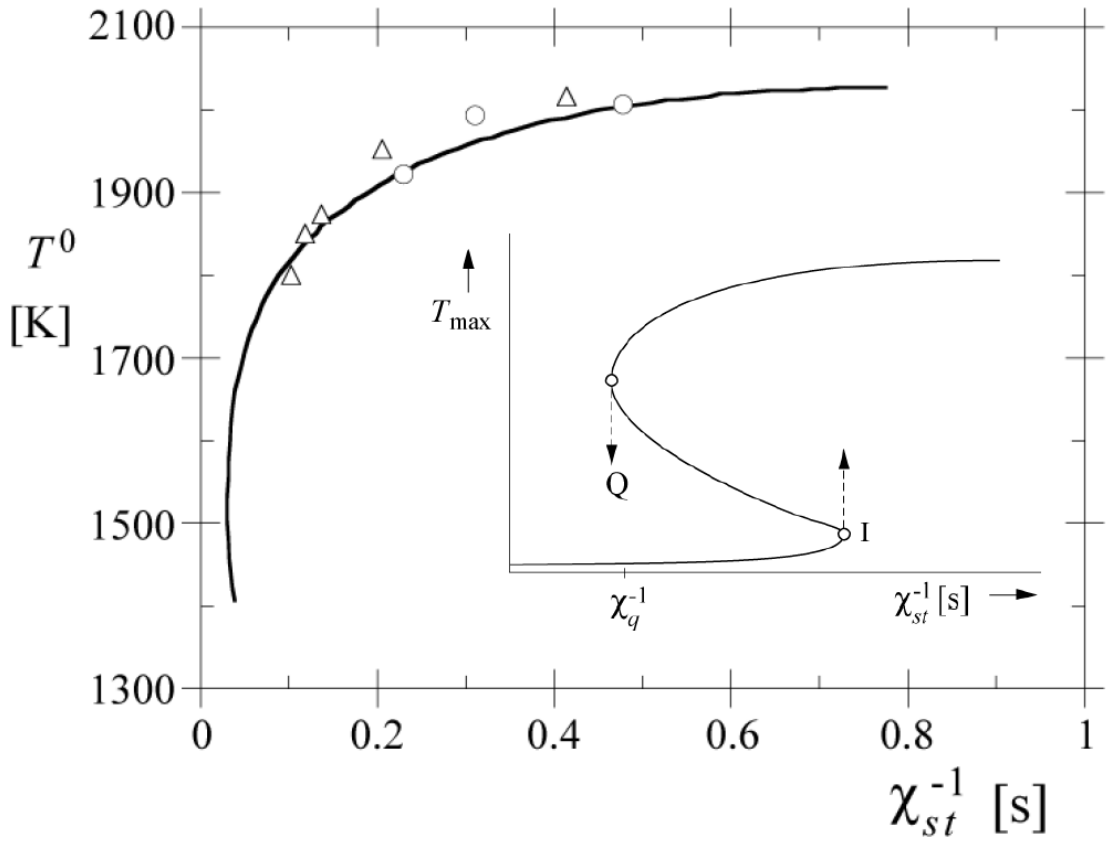
Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation



Asymptotic analysis (Seshadri)



Calculations agree pretty well with numerical (DNS) data and experiments and reveal the vertical slop which corresponds to extinction.

Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

Steady flamelet equation provides $\psi_i = f(Z, \chi_{st})$

if a joint pdf $\widetilde{P}(Z, \chi_{st})$ is known, then the Favre mean of ψ_i is:

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

If the unsteadiness has to be retained, joint statistics of Z and χ_{st} become impractical and a different approach has to be taken.

→ Reduction of dimensionality through introduction of multiple flamelets which each represent different ranges of χ – distributions, i.e. Eulerian Particle Flamelet Model.

Then, the scalar dissipation rate may be formulated as a function of the mixture fraction.

Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

Modeling the conditional Favre mean scalar dissipation rate

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

Flamelet equation

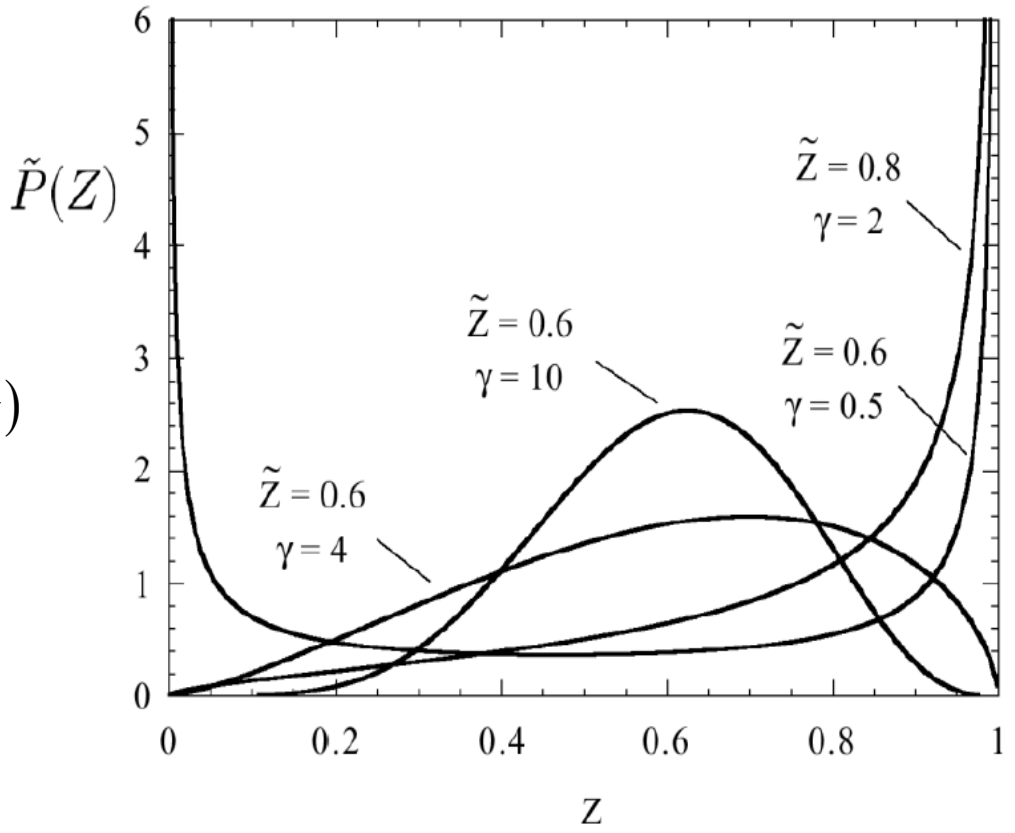
$$\rho \frac{\partial \psi_i}{\partial t} - \frac{\rho}{Le_i} \frac{\chi_Z}{2} \frac{\partial^2 \psi_i}{\partial Z^2} = \dot{\omega}_{\psi_i} \quad \Longrightarrow \quad \psi_i(Z, \tilde{\chi}_Z, t)$$

Favre mean

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

with

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



Combustion Models

Turbulent Non-Premixed Models

Flamelet Equation

Requires a model for the conditional scalar dissipation rate $\tilde{\chi}_Z$

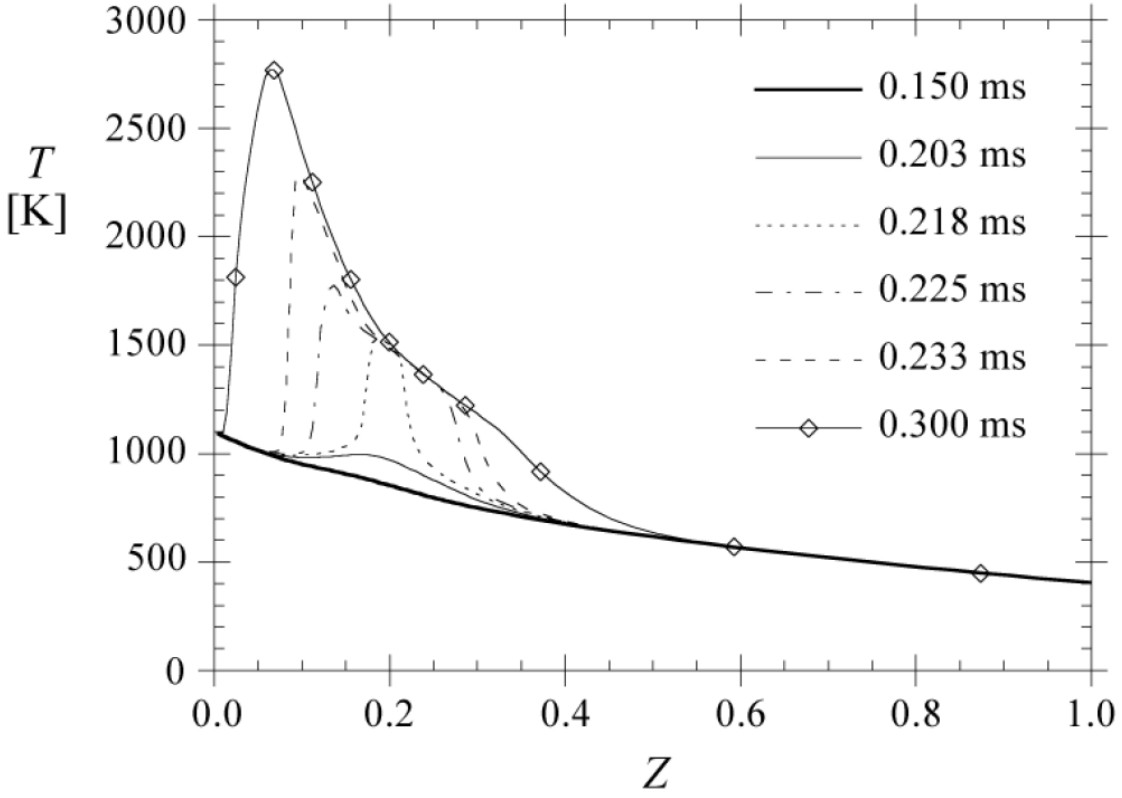
Relate the conditional scalar dissipation rate to the one at a fixed value of Z_{st}.

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

and with

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

$$\tilde{\chi}_{st} = \frac{\tilde{\chi} f(Z_{st})}{\int_0^1 f(Z)\tilde{P}(Z)dZ} = \frac{c_\chi \frac{\tilde{\varepsilon}}{\tilde{k}} \tilde{Z}''^2}{\int_0^1 f(Z)\tilde{P}(Z)dZ}$$



Example of the impact of time for n-heptane/air ignition with an initial air temperature of 1100 K and initial fuel temperature of 400 K.

Combustion Modelling

What you should not forget

- Key assumption in all combustion models (diffusion coefficients, Schmidt = Prandtl number)
- What can we conclude from the temperature dependency of chemical reactions ?
- Assumptions and short-comings of EDM and FRCM , and EDC approaches
- BML assumptions and closure models
- Flamelet assumptions and closures

Annex

Available Models for Premixed Combustion (may be used for Non-Premixed too but be cautious)

*Nota: Slide from Suresh Menon (GeorgiaTech)

Model family/concept	Some assumptions	What the model typically needs?	Benefits	Some Drawbacks
G-equation (Markstein 1964, Williams 1985)	- physical flame thickness $\delta << \Delta x$ - flame at G = const. i.e. level-set approach - separation to **burnt** and **unburnt** regions	- Correlation S_L - an algorithm to find the flame position	- single equation to describe premixed combustion	- G=G(x,y,z,t) has no physical meaning elsewhere than at flame - level set approach so the flame really needs to be tracked → compications for implementation
Flame surface density (c-equation)	- Thin flame $\delta << \Delta x$ - c is defined everywhere in contrast to level-set -	- Correlation S_L - Correlation for flame surface density (effect of unresolved flame deviation from planar)	- single equation to describe premixed combustion - rather simple to implement	-assumption of single step chemistry -a particular link between emissions and c needed - possibly even extra eqn for surface density needed
Flamelet method	- flame=ensemble of 1d flames	- pre-calculated chemistry look-up tables	- fast in runtime with accurate description of species from tables	- pre-tabulation can be a tedious task
Direct chemistry	- full Navier-Stokes + species eqs solved - flame is resolved DNS	- low Reynolds number - accurate diffusion model	- computational 'experiment' with all possible data available	- very heavy and limited to small mechanisms
Thickened flame	- flame artificially thickened to numerically resolve the flame - reaction rate scaled by L and thermal diffusivity by 1/L while S_L is const.	- reduced or accurate chemical mechanism which gives correct flame speed and IDT	- flame front is really resolved with important species	- is the physics still the same ?

Combustion Models for LES

A large variety of models applicable for LES exist can be split in two combustion fields

- Models suited for pre-mixed cases
  - **FSD** Flame surface-density models with or without tabulated chemistry
  - **FPV** Flamelet progress variable models
  - **TFM** Thickened flame model (flamelet-based)
  - **CMC** Conditional moment closure (flamelet-based)
  - **G-eqn** G equation
  - **LEM** Linear eddy model
- Models suited for Non-Premixed Combustion
  - **SSLF** Steady strained laminar flamelet
    Z eqn with scalar dissipation rate
  - **FPV** flamelet progress variable
    Z and c equations
  - **CMC** conditional moment closure (flamelet-based)
  - **PDF** PDF transport methods (parcels)