Turbulent Combustion Modelling - Chemistry.

- Previously Discussed wide Range of Scales in turbulent flows.
- Rans, LES Don't resolve these Scales $\longrightarrow$ Models
- Key issues.
    - wide Range of Scales
    - Nonlinear interactions : $RR \sim e^{-E/RT}$
    - Many Species
    - Differential Diffusion
- Turbulence is "Random" $\longrightarrow$ Deal with Statistics.
    - Mean $\vec{V}$
    - Mean T
    - Mean ω, etc.
    - Mean, RMS fluctuations.

$\longrightarrow$ Closure Problem

- Decompose : $u \rightarrow \bar{u} + u'$
- Average $\longrightarrow$ eqn for $\bar{u}$, with new terms $\overline{u_i' u_j'}$

Species eqn:

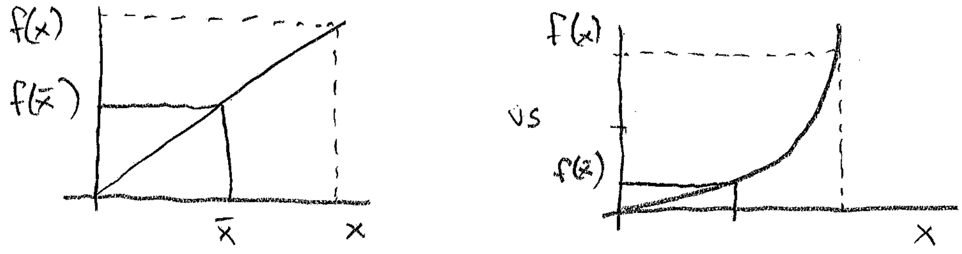
$$\frac{\partial \bar{\rho} \tilde{Y}_i}{\partial t} + \nabla \cdot (\bar{\rho} \tilde{V} \tilde{Y}_i) + \nabla \cdot (\bar{\rho} \widetilde{V'' Y_i''}) + \nabla \cdot \bar{j}_i = \bar{R}_i$$

How to evaluate $\bar{R}_i$?

$$A + B \longrightarrow C \quad ; \quad R_A = [A][B] k e^{-E/RT}$$

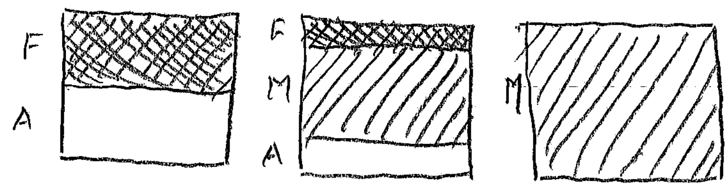
$$R_A = R_A(Y_A, Y_B, T)$$

$$\bar{R}_A \neq R_A(\bar{Y}_A, \bar{Y}_B, \bar{T})$$ Because R is nonlinear



$\bar{f} = f(\bar{x})$ $\qquad\qquad$ $\bar{f} \neq f(\bar{x})$

- With fluctuations, we can have a given average, with a wide variety of states
  - Stoic Fuel, Air



$R=0$ $\qquad$ $R=$ intermediate $\qquad$ $R=\max$

Segregated ⟶ Mixed

$$* \quad \bar{R} = \iiint R(Y_A, Y_B, T)\, P(Y_A, Y_B, T)\, dY_A, dY_B, dT$$

- Need Joint PDF : Multi-D
  Unknown

Approaches

F = Fluent has a basic implementation.

- F • Transported PDF
- • Conditional Moment Closure
- F • Presumed PDF
  - Equilibrium
  - Flamelets
  - ...
- F • EDC
- • LEM / ODT
- • Multi-Environment PDF

Presumed PDF Approach – Mixture-fraction based

- Observation
  - Typical Combustion Scalars (T, Y_α, ρ) are Strong functions of mixture fraction: ξ
  - See Examples
- Result: Eval means as $\bar{\phi}(\xi) = \int_0^1 \phi(\xi) P(\xi) \, d\xi$

  where ϕ is some Scalar, like T, Y_α, ρ, radiation absorption coeff., etc.

  → Don't explicitly Transport Species / Reactions

  → Instead
  - Specify $\phi(\xi)$ (somehow) = Reaction Model
  - Specify $P(\xi)$ (somehow) = Mixing Model

Equilibrium Model

Take $\phi(\xi)$ from equilibrium.

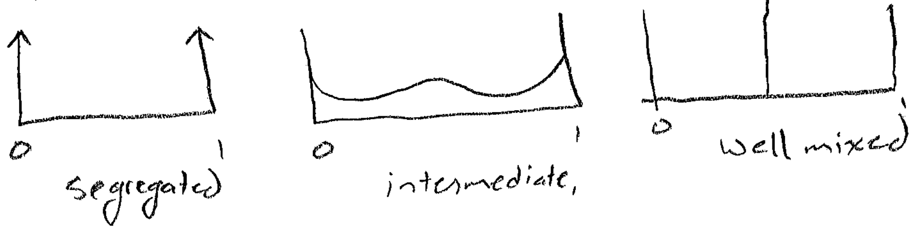
- Discretize ξ into Bins (say 100)
- Eval all Desired properties as equilibrium in each ξ_i
- Tabulate $\phi_i(\xi_i)$

→ Given ξ_i, lookup ϕ_i from Table (interpolate)

$$\bar{T} = \int_0^1 T(\xi) \, P(\xi) \, d\xi$$

Need $P(\xi)$

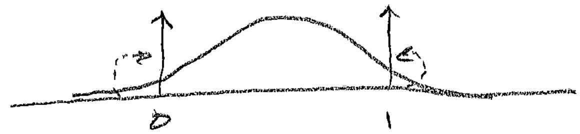
- For given $\bar{\xi}$, limitis of $P(\xi)$:



- PDF is specied by ① Form
  ② $\bar{\xi}$
  ③ σ_{ξ}^2

$$\left.\begin{array}{l} \bar{\xi} \\ \sigma_{\xi}^2 \end{array}\right\} \longrightarrow \bar{\xi}', \ \sigma_{\xi}'^2$$

Clipped Gaussian



- Clip tails $\pm\infty$, add δ functions at 0, 1
- $$P(\xi) = \begin{cases} \alpha_0 = \frac{1}{2}\left(1-\mathrm{erf}\left(\bar{\xi}/\sqrt{2\sigma_{\xi}'^2}\right)\right) & : \xi = 0 \\ \frac{1}{\sqrt{2\pi\sigma_{\xi}^2}} \cdot \exp\left[-\frac{(\xi-\bar{\xi})^2}{2\sigma_{\xi}'^2}\right] & : 0 < \xi < 1 \\ \alpha_1 = \frac{1}{2}\left(1-\mathrm{erf}\left((\bar{\xi}-1)/\sqrt{2\sigma_{\xi}'^2}\right)\right) & : \xi = 1 \end{cases}$$

β-PDF

- Similar, but more natural

$$P(\xi) = \xi^{a-1}(1-\xi)^{b-1} \cdot \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}$$

$$a = \bar{\xi}\left[\frac{\bar{\xi}(1-\bar{\xi})}{\sigma_{\xi}^2} - 1\right] = \bar{\xi}\left(\sigma_{\xi,max}^2/\sigma_{\xi}^2 - 1\right)$$

$$b = a(1-\bar{\xi})/\bar{\xi}$$

Γ is the gamma function.

See Examples.

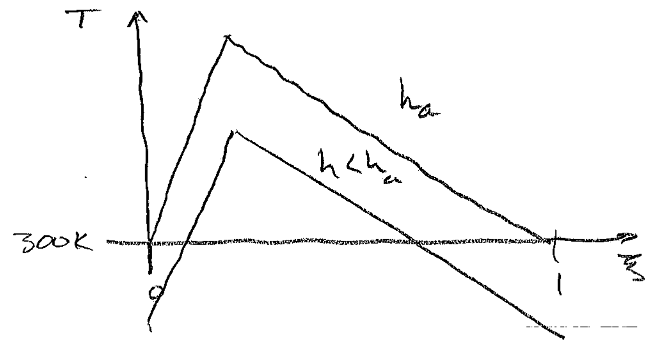
For Equilibrium Model

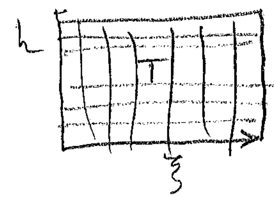
- Build a 2-D Table $\bar{\phi} = \bar{\phi}(\bar{\xi}, \sigma_{\xi}^2)$
  - computed as $\bar{\phi} = \int_0^1 \phi(\xi)\, P(\bar{\xi}, \sigma_{\xi}^2)\, d\xi$
- CFD Solves Transport equations for $\bar{\xi}$, σ_{ξ}^2
  $\longrightarrow$ Lookup $\bar{\phi}$ as needed

* Note, The Table is needed for Closing terms in the resulting Transport eqns (like $\bar{\rho}$), not e.g. Y_i

Heat loss.

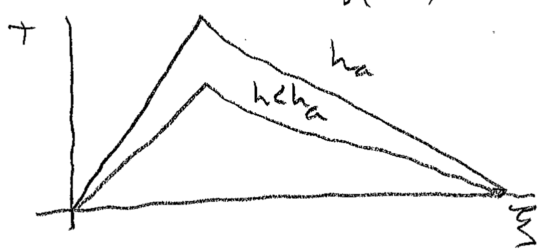
- Via Radiation, Wall transfer
- Code Solves Enthalpy, but it is inconvenient to tabulate Chemistry in terms of h:



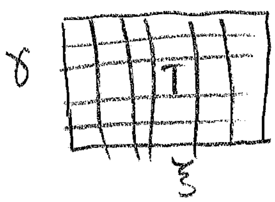


} not realistic

- instead, use $\gamma = \dfrac{h_a(\xi) - h}{h_s(\xi)}$



· Pure fuel, air have $h_s \to 0$
$\Rightarrow h \to h_a$



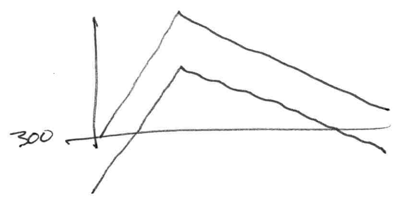
- $\bar{\phi} = \bar{\phi}(\bar{\xi}, \sigma^2_\xi, \gamma)$ Table.
- Transport $\bar{\xi}$, σ^2_ξ, $\bar{h}$
- Lookup $\bar{\phi}(\bar{\xi}, \sigma^2_\xi, \gamma)$ as needed

* Compute $\bar{\phi}$ as

$$\begin{aligned}\bar{\phi} &= \iint \phi(\xi,\gamma')\, P(\xi,\gamma')\, d\xi\, d\gamma' \\ &\simeq \iint \phi(\xi,\gamma')\, P(\xi)\, P(\gamma')\, d\xi\, d\gamma' \\ &\approx \iint \phi(\xi,\gamma')\, P(\xi)\, \delta(\gamma'-\gamma)\, d\xi\, d\gamma' \\ &= \int \phi(\xi,\gamma)\, P(\xi)\, d\xi\end{aligned}$$

Heat loss Note

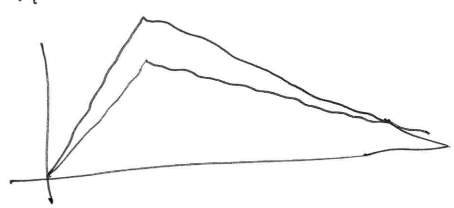
- When using an equilibrium model, the various ξ are independent, unlike a 1-D laminar flamelet.
- Then, to integrate over the β-PDF, we need some appropriate measure of h that applies across the ξ space.
- Cannot use a uniform value of h (or $\underline{\underline{\Delta h}}$) since we would go "negative" on the boundaries.



e.g. uniform Δh

- γ scales Δh by h_s which vanishes on the edges.

$h = h_a - h_s \cdot \gamma$ $\rightsquigarrow$ as $h_s \to 0$ $h \to h_a$



e.g. uniform γ.

- Other possibilities could work:
  - Radiate to $\underbrace{\text{"cold" surroundings}}_{T_{mix}(\xi)}$ for some Δt.

  Do this for all ξ for <u>same</u> Δt.

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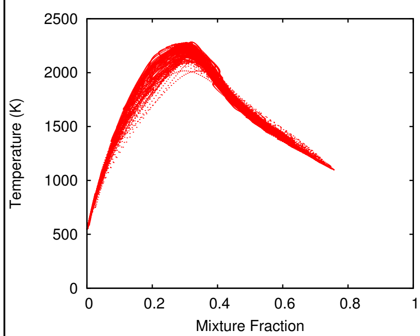
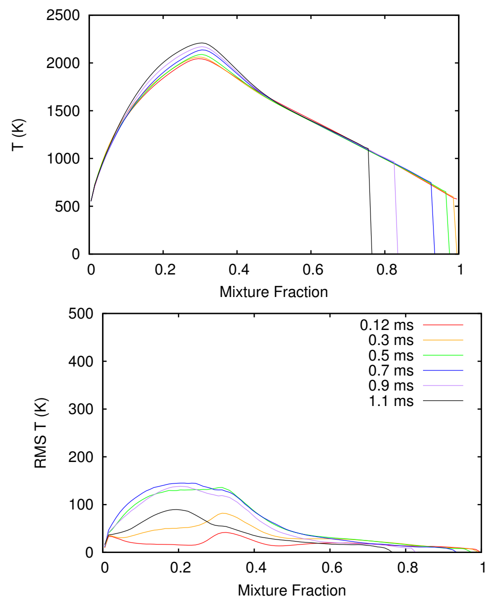
Jet Temperature Profiles





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Experimental Profiles

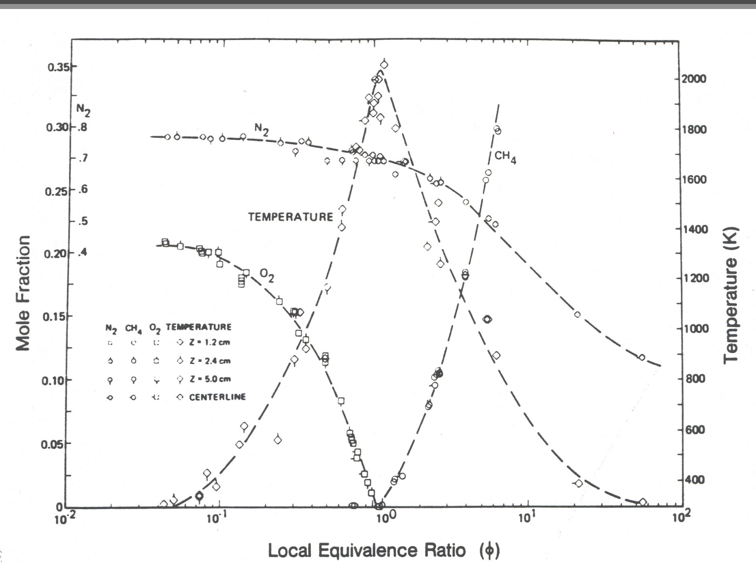
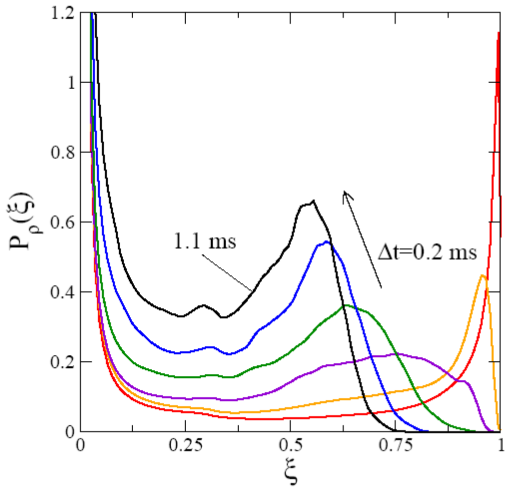


Figure 11.4. Measured temperature and reactant concentration as a function of the local equivalence ratio in a laminar methane diffusion flame. (Figure used with permission from Mitchell *et al.*, 1980.)

Mixture Fraction PDFs



Sample Equilibrium Table