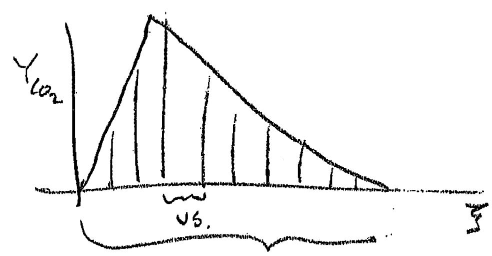
CMC - Conditional Moment Closure,

- SLFM: map everything to ξ in a lookup table, and transport ξ.
- CMC
  - $\overline{\omega}(x) \neq \omega(\overline{x})$, because of nonlinear Dependence and fluctuations.
  - BUT, for a Given ξ, $\overline{\omega}(x) \approx \omega(\overline{x})$
  - 

  - Bin up the ξ Domain and Solve not $\langle Y_i \rangle \equiv \overline{Y}_i$ but $\langle Y_i | \xi \rangle$ (That is, the avg Y_i in a given ξ bin)

    $\rightarrow \langle Y_i \rangle = \int \langle Y_i | \xi \rangle \, P(\xi) \, d\xi$

→ (*) See slide

CMC Equation

Normal: $\bar{\rho}\frac{\partial \tilde{Y}_i}{\partial t} + \bar{\rho}\tilde{v}\,\nabla \tilde{Y}_i + \nabla\cdot(\bar{\rho}\,\widetilde{v''Y_i''}) = \overline{\rho R_i}$

CMC: $\rho_\xi P_\xi \frac{\partial\langle Y_i|\xi\rangle}{\partial t} + \rho_\xi P_\xi \langle v|\xi\rangle \nabla\langle Y_i|\xi\rangle + \nabla\cdot(\langle v''Y_i''|\xi\rangle \rho_\xi P_\xi) = \langle R_i|\xi\rangle P_\xi + \rho_\xi P_\xi \frac{\chi_\xi}{2}\frac{\partial^2\langle Y|\xi\rangle}{\partial \xi^2}$

- $Y_i \longrightarrow \langle Y_i|\xi\rangle$
- $\bar{\rho} \longrightarrow \bar{\rho} P_\xi$
- $\tilde{v} \longrightarrow \langle v|\xi\rangle$
- $R \to \langle R|\xi\rangle$
- $\widetilde{v''Y_i''} \longrightarrow \langle v''Y_i|\xi\rangle$

- Models for $\langle v|\xi\rangle$, χ_ξ, $\langle v''Y_i''|\xi\rangle$
- Also solve a Transport P_ξ

- 4-D $\longrightarrow$ 5-D $\longrightarrow$ more expensive
  t, x, y, z $\quad$ t, x, y, z, ξ
- Rxn term is "closed"
- S.S., Homogeneous $\longrightarrow$ looks like Flamelets
- retain Unsteady & spatial Terms $\longrightarrow$ obtain history effects
- $(\bar{\rho} P_\xi)$ is Density in x, y, z, ξ Space like
  $\bar{\rho}$ is Density in x, y, z Space.

Transported PDF (From Cont)

η is sample space variable for random var ϕ

$$\frac{\partial}{\partial t}\left[\rho P(\eta)\right] = -\frac{\partial}{\partial x_k}\left[\langle u_k|\eta\rangle \rho P(\eta)\right] - \frac{\partial}{\partial \eta}\left[\omega(\eta) P(\eta)\right] - \frac{\partial^2}{\partial \eta^2}\left[\rho P(\eta)\langle N_\phi|\eta\rangle\right]$$

$N_\phi = D\left(\frac{\partial \phi}{\partial x_k}\right)^2$ is the Dissipation rate.

$$\langle u_k|\eta\rangle P(\eta) = \bar{u}_k P(\eta) - D_t \frac{\partial P(\eta)}{\partial x_k}$$

Mixing model for the last term,

Monte Carlo approach,

- fluid = virtual particles
  - evolution by a random walk = turb. Dispersion (macromixing)
  - micromixing: $\frac{d\phi^n}{dt} = -\frac{(\phi^n - \bar{\phi})}{\tau_{turb}} + \omega^n$

IEM.

others: · Curl
· Mod. Curl.
· EMST
· SPL.

~~Langevin model~~ Random walk: Langevin model.

$$dx_i = u_i dt.$$

$$du_i = -\left(\frac{1}{2} + \frac{3}{4}C_0\right)\frac{u_i - \bar{u}_i}{\tau_t}dt + (C_0\epsilon)^{1/2}\zeta(dt)^{1/2}$$

$$\tau_t = k/\epsilon$$

ζ is random w/ normal Dist w/ 0 mean and unity variance.

$$\epsilon \sim \frac{1}{\sqrt{N_p}}.$$

· Part rep the PDF.

Chemical Engineering 641

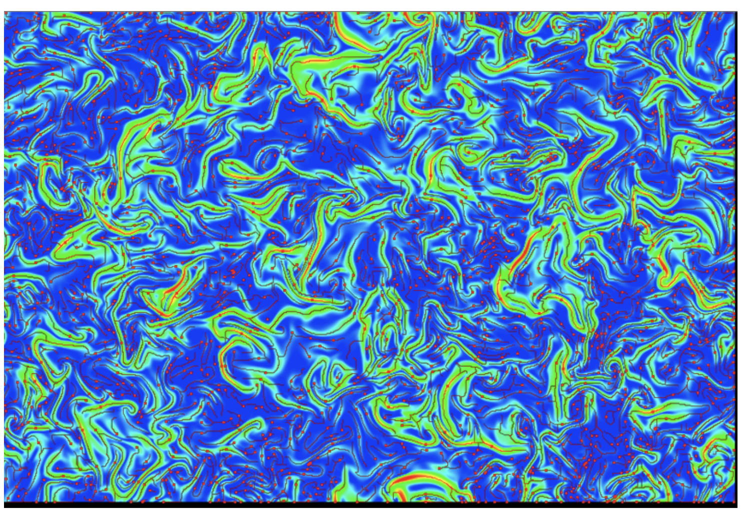
Combustion Modeling

Turbulent Nonpremixed
Combustion Models

1

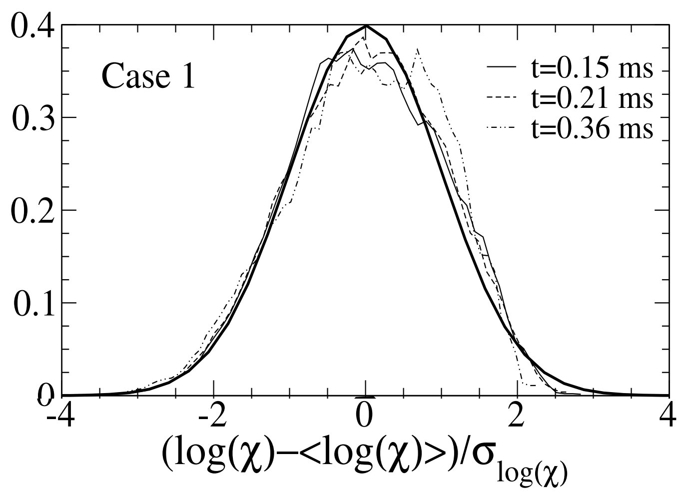
2

Mixing Field: Thin Structures



http://www.vacet.org/gallery/combustion.html

Lognormal PDF



CMC Equations—Derivation

$$\psi = \prod_i \delta(Z_i - Y_i(x,t))$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial Z_i}\left(\psi \frac{\partial Y_i}{\partial t}\right)$$

$$\frac{\partial Y_i}{\partial t} = -\boldsymbol{v}\cdot\nabla Y_i + \frac{1}{\rho}\nabla\cdot(\rho D_i \nabla Y_i) + \frac{1}{\rho}\nabla\cdot(\rho^{-1}D_{T,i}Y_i\nabla\ln T) + \frac{\omega_i}{\rho}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial Z_i}\left(\psi \boldsymbol{v}\cdot\nabla Y_i - \frac{\psi}{\rho}\nabla\cdot(\rho D_i\nabla Y_i) - \frac{\psi}{\rho}\nabla\cdot(\rho^{-1}D_{T,i}Y_i\nabla\ln T) - \psi\frac{\omega_i}{\rho}\right)$$

$$\begin{aligned}\frac{\partial \rho\psi}{\partial t} + \nabla\cdot(\rho\boldsymbol{v}\psi) = &-\frac{\partial}{\partial Z_i}(\psi\omega_i)\\ &-\frac{\partial}{\partial Z_i}\left(\psi\nabla\cdot(\rho^{-1}D_{T,i}Y_i\nabla\ln T)\right)\\ &-\frac{\partial}{\partial Z_i}\left(\psi\nabla\cdot(\rho(D_i - D)\nabla Y_i)\right)\\ &-\frac{\partial}{\partial Z_i}\frac{\partial}{\partial Z_j}(\psi\rho D\nabla Y_i\cdot\nabla Y_j)\\ &+\nabla\cdot(\nabla(\rho D\psi)) - \nabla\cdot(\psi\nabla(\rho D)).\end{aligned}$$

$$\begin{aligned}\frac{\partial\langle\rho|\boldsymbol{Z}\rangle P}{\partial t} + \nabla\cdot(\langle\rho\boldsymbol{v}|\boldsymbol{Z}\rangle P) = &-\frac{\partial}{\partial Z_i}(\langle\omega_i|\boldsymbol{Z}\rangle P)\\ &-\frac{\partial}{\partial Z_i}\left(\langle\nabla\cdot(\rho^{-1}D_{T,i}Y_i\nabla\ln T)|\boldsymbol{Z}\rangle P\right)\\ &-\frac{\partial}{\partial Z_i}\left(\langle\nabla\cdot(\rho(D_i - D)\nabla Y_i)|\boldsymbol{Z}\rangle P\right)\\ &-\frac{\partial}{\partial Z_i}\frac{\partial}{\partial Z_j}\left(\langle\rho D\nabla Y_i\cdot\nabla Y_j|\boldsymbol{Z}\rangle P\right)\\ &+\nabla^2(\langle\rho D|\boldsymbol{Z}\rangle P) - \nabla\cdot(\langle\nabla(\rho D)|\boldsymbol{Z}\rangle P)\end{aligned}$$

(skipping lots of steps)

$$\begin{aligned}\frac{\partial\langle\rho Y_s|\eta\rangle P(\eta)}{\partial t} + \nabla\cdot(\langle\rho Y_s\boldsymbol{v}|\eta\rangle P(\eta)) = &\langle\omega_{Y_s}|\eta\rangle P(\eta)\\ &+\langle\nabla\cdot(\rho Y_s D_{T,i}\nabla\ln T)|\eta\rangle P(\eta)\\ &-\frac{\partial}{\partial\eta}\left(\langle\nabla\cdot[\rho(D_\xi - D_s)\nabla\xi]Y_s|\eta\rangle P(\eta)\right)\\ &-\frac{\partial^2}{\partial\eta^2}\left(\langle\rho D_s(\nabla\xi)^2 Y_s|\eta\rangle P(\eta)\right)\\ &+\frac{\partial}{\partial\eta}\left(\langle 2\rho D_s(\nabla Y_s\nabla\xi)|\eta\rangle P(\eta)\right)\\ &+\nabla^2(\langle\rho D_s Y_s|\eta\rangle P(\eta)) - \nabla\cdot(\langle\nabla(\rho D_s Y_s)|\eta\rangle P(\eta)),\end{aligned} \qquad \text{(D.27)}$$

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$$\frac{\partial Y_i}{\partial t} = -v\cdot\nabla Y_i + \frac{1}{\rho}\nabla\cdot(\rho D_i \nabla Y_i) + \frac{1}{\rho}\nabla\cdot(\rho^{-1} D_{T,i} Y_i \nabla \ln T) + \frac{\omega_i}{\rho}$$

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial Z_i}\left(\psi v\cdot\nabla Y_i - \frac{\psi}{\rho}\nabla\cdot(\rho D_i\nabla Y_i) - \frac{\psi}{\rho}\nabla\cdot(\rho^{-1} D_{T,i} Y_i \nabla \ln T) - \psi\frac{\omega_i}{\rho}\right)$$

(skipping lots of steps)

$$\frac{\partial \rho\psi}{\partial t} + \nabla\cdot(\rho v \psi) = -$$

$$- \frac{\partial}{\partial Z_i}\frac{\partial}{\partial Z_j}(\psi\rho D\nabla Y_i\cdot\nabla Y_j)$$
$$+ \nabla\cdot(\nabla(\rho D\psi)) - \nabla\cdot(\psi\nabla(\rho D)).$$

$$\frac{\partial\langle\rho|Z\rangle P}{\partial t} + \nabla\cdot(\langle\rho v|Z\rangle P) = -\frac{\partial}{\partial Z_i}(\langle\omega_i|Z\rangle P)$$
$$- \frac{\partial}{\partial Z_i}\left(\langle\nabla\cdot(\rho^{-1}D_{T,i}Y_i\nabla\ln T)|Z\rangle P\right)$$
$$- \frac{\partial}{\partial Z_i}\left(\langle\nabla\cdot(\rho(D_i - D)\nabla Y_i)|Z\rangle P\right)$$
$$- \frac{\partial}{\partial Z_i}\frac{\partial}{\partial Z_j}\left(\langle\rho D\nabla Y_i\cdot\nabla Y_j|Z\rangle P\right)$$
$$+ \nabla^2(\langle\rho D|Z\rangle P) - \nabla\cdot(\langle\nabla(\rho D)|Z\rangle P)$$

$$\frac{\partial}{\partial t} + \nabla\cdot(\langle\rho Y_s v|\eta\rangle P(\eta)) = \langle\omega_{Y_s}|\eta\rangle P(\eta) \quad \text{(D.27)}$$
$$+ \langle\nabla\cdot(\rho Y_s D_{T,i}\nabla\ln T)|\eta\rangle P(\eta)$$
$$- \frac{\partial}{\partial\eta}(\langle\nabla\cdot[\rho(D_\xi - D_s)\nabla\xi]Y_s|\eta\rangle P(\eta))$$
$$- \frac{\partial^2}{\partial\eta^2}(\langle\rho D_s(\nabla\xi)^2 Y_s|\eta\rangle P(\eta))$$
$$+ \frac{\partial}{\partial\eta}(\langle 2\rho D_s(\nabla Y_s\nabla\xi)|\eta\rangle P(\eta))$$
$$+ \nabla^2(\langle\rho D_s Y_s|\eta\rangle P(\eta)) - \nabla\cdot(\langle\nabla(\rho D_s Y_s)|\eta\rangle P(\eta)),$$

Derivation of Conditional Transport Equations

- Two approaches to deriving CMC equations
  - Decomposition method
  - Joint PDF method: Follow Klimenko and Bilger (1999)
- Procedure

$$\psi = \prod_i \delta(Z_i - Y_i) \qquad P(Z_i) = \langle\psi\rangle = \int \psi(Z - Y)P(Y)dY$$

  - Joint PDF is the mean of the fine grain PDF
  - Insert the transport equations for scalars into the derivative of fine grain PDF

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial Z_i}\left(\psi \frac{\partial Y_i}{\partial t}\right)$$

  - Average the result to obtain the joint PDF transport equation
  - Multiply by Z_k and integrate over all Z_i except η to obtain the conditional transport equation
- Differential diffusion is treated with each individual component diffusivity written in terms of a reference diffusitvity.
  - Reference diffusivity taken as soot rather than mixture fraction.

$$D_i = D_{ref} + (D_i - D_{ref})$$

CMC Summary

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$$\frac{\partial \langle \rho Y_i | \xi \rangle}{\partial t} + \nabla \cdot \langle \rho v Y_i | \xi \rangle + \frac{1}{P_\xi} \nabla \cdot [\langle u' Y_i' \rangle \rho P_\xi] = \frac{\bar{\rho}\tilde{\chi}}{2} \frac{\partial^2 \langle Y_i | \xi \rangle}{\partial \xi^2} + \langle R_i | \xi \rangle$$

Unsteady | Transport | Turbulent Transport | Transport in the Mixture Fraction Coordinate | Source

$Y_i = Y_i(x,y,z,t,\xi)$