Class 17

Turbulence-Chemistry with Solid Reactions

Review of Mixture Fraction Approach

- 1. Definition of f
- **2**. Definition of g_f
- 3. What are conserved scalars?
- 4. What is a PDF & how is it used?
- 5. What assumptions are involved?
- 6. Why can't this system be used for premixed systems?
- 7. Why can't we just used the mean values of T and C_i in the reaction rate expressions?
- 8. How do you get mean values of T and C_i ?

The Coal Gas Mixture Fraction

It is useful to define another progress variable η = the coal gas mixture fraction

$$\eta = \frac{m_c}{m_c + m_p + m_s}$$

Devolatilization

Char Oxidation

where $m_c = mass$ of gas originating in the coal **Examples**:

 $\begin{array}{l} \text{volatiles} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \\ m_c = \text{mass of volatiles only} \\ \text{C(s)} + \text{O}_2 \rightarrow \text{CO}_2 \\ m_c = \text{mass of carbon released only} \\ (\text{i.....e., the "C" part of the CO}_2) \end{array}$

Calculating The Coal Gas Mixture Fraction

Conservation Equation (convection, diffusion, source term)

$$\vec{\nabla} \cdot \left(\overline{\rho} \widetilde{\vec{v}} \, \widetilde{\eta} - D_{\eta}^{t} \overline{\nabla} \, \widetilde{\eta} \right) = S_{p}^{m}$$

 S_p^m = net mass addition to the gas phase from the condensed phase (due to evaporation, devolatilization, and heterogeneous oxidation)

Also calculate variation in η

$$\vec{\nabla} \cdot \left(\overline{\rho} \widetilde{\vec{v}} g_{\eta} - D_{\eta}^{t} \overline{\nabla} g_{\eta} \right) = S_{g_{\eta}}$$

$$S_{g_{\eta}} = C_{g_{1}} D_{\eta}^{t} \left[\left(\frac{\partial \widetilde{\eta}}{\partial x} \right)^{2} + \left(\frac{\partial \widetilde{\eta}}{\partial r} \right)^{2} + \left(\frac{\partial \widetilde{\eta}}{\partial \theta} \right)^{2} \right] - C_{g_{2}} \overline{\rho} \left(\frac{\varepsilon}{k} \right) g_{\eta}$$

Equation	¢	Γ_{ϕ}	Sé
Continuity	1	0	S_p^m
X Momentum	\tilde{u}	μ_{e}	$-\frac{\partial \tilde{p}}{\partial x} + \frac{\partial}{\partial x} \left(\mu_e \frac{\partial \tilde{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu_e \frac{\partial \tilde{v}}{\partial x} \right) + \frac{\partial}{\partial z} \left(\mu_e \frac{\partial \tilde{w}}{\partial x} \right) + \tilde{\rho} g_x - \frac{2}{3} \tilde{\rho} \tilde{k} + S_p^u + \tilde{u} S_y^u + \tilde{v} S_y^u + \tilde{v}$
Y Momentum	\tilde{v}	μ_e	$-\frac{\partial \rho}{\partial y} + \frac{\partial}{\partial x} \left(\mu_{e} \frac{\partial \tilde{u}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\mu_{e} \frac{\partial \tilde{v}}{\partial y} \right) + \frac{\partial}{\partial z} \left(\mu_{e} \frac{\partial \tilde{w}}{\partial y} \right) + \tilde{\rho} g_{y} - \frac{2}{3} \tilde{\rho} \tilde{k} + S_{p}^{y} + \tilde{v} S_{p}^{m}$
Z Momentum	ŵ	μ	$\cdot \frac{\partial p}{\partial z} + \frac{\partial}{\partial x} \left(\mu_{e} \frac{\partial \widetilde{u}}{\partial z} \right) + \frac{\partial}{\partial y} \left(\mu_{e} \frac{\partial \widetilde{v}}{\partial z} \right) + \frac{\partial}{\partial \overline{z}} \left(\mu_{e} \frac{\partial \widetilde{w}}{\partial \overline{z}} \right) + \widetilde{\rho}_{g_{z}} - \frac{2}{3} \widetilde{\rho} \widetilde{k} + S_{p}^{W} + \widetilde{w} S_{p}^{M}$
Turbulent Energy	k	$\frac{\mu_s}{\overline{\sigma}_k}$	$G = \widetilde{p}\widetilde{c}$
Dissipation Rate	ŝ	14 17	$\binom{\hat{i}}{\hat{j}}(e_1G - e_2\tilde{p}\tilde{i})$
Mixture Fraction	\overline{f}	$\frac{\mu_{\theta}}{\overline{\sigma}_{f}}$	S_p^f
Mixture Fraction Variance	ŝ	$\frac{\mu_{e}}{\sigma_{g}}$	$\frac{c_{g1}}{c_{g}}^{\mu_{g}} \left[\left(\frac{\delta j}{\delta_{g}} \right)^{2} + \left(\frac{\delta j}{\delta_{y}} \right)^{2} + \left(\frac{\delta j}{\delta_{g}} \right)^{2} \right] - c_{g2} \tilde{\rho}_{g2}^{\mu\nu} / \tilde{\lambda}$
Coal Gas Mixture Fraction	ñ	$\frac{\mu_{a}}{\alpha_{\eta}}$	S_p^{η}
Coal Gas Mixture Praction Variance	ε̃ _n	$\frac{\alpha}{\frac{\alpha}{g\eta}}$	$c_{g^{1}}\frac{\mu_{g}}{\sigma_{g^{q}}}\left[\left(\frac{\partial \tilde{\eta}}{\partial s}\right)^{2} + \left(\frac{\partial \tilde{\eta}}{\partial y}\right)^{2} + \left(\frac{\partial \tilde{\eta}}{\partial s}\right)^{2}\right] - c_{g^{2}}\tilde{p}\tilde{q}_{\eta}\frac{\tilde{q}}{\tilde{s}}$
Enthalpy	\vec{h}	$\frac{\mu_d}{\sigma_h}$	$q'_{rg} + \left(\tilde{u}\frac{\partial p}{\partial x} + \tilde{v}\frac{\partial p}{\partial y} + \tilde{w}\frac{\partial p}{\partial z}\right) + S^h_p + \tilde{h}S^m_p$
where:	-		

Need new mixture fraction

Since $\rho = \frac{total \ mass}{volume} = \frac{m_c + m_p + m_s}{volume}$

the equation for f must be changed. Define f_p

$$f_{p} = \frac{m_{p}}{m_{c} + m_{p} + m_{s}} = \left\{ \frac{m_{p}}{(m_{p} + m_{s})} \right\} \left\{ \frac{(m_{p} + m_{s})}{m_{c} + m_{p} + m_{s}} \right\} = f \cdot (1 - \eta)$$

The equation for f_p becomes:

 $\vec{\nabla} \cdot \left(\overline{\rho} \widetilde{\vec{v}} \widetilde{f}_p - D_{f_p}^t \overline{\nabla} \widetilde{f}_p \right) = 0$

refer to Smoot & Smith, Figure 13.1



f = mass fraction of primary carrier gas
 in inlet gas (dmi)

 $= dm_p/dm_i = dm_p/(dm_p + dm_s)$

- fp= mass fraction of primary carrier gas in total gas mass (dm)
 - $= dm_p/dm = dm_p/(dm_i + dm_c)$
 - $= dm_p/(dm_p + dm_s + dm_c)$

 $\begin{aligned} \eta &= \text{ mass fraction of coal off-gas} \\ &\text{ in total gas mass (dm)} \\ &= dm_c/dm = dm_c/(dm_i + dm_c) \\ &= dm_c/(dm_p + dm_s + dm_c) \end{aligned}$

Figure 13.1. Components of an element of gas mass dm.

Main Idea

- (a) Get split between pri & sec using f (elemental composition)
- (b) Get coal off-gas using η (elemental composition)

Assumptions:

- 1. η and f are independent $\Rightarrow \tilde{f}_p = \tilde{f} \cdot (1 \tilde{\eta})$
- All coal off-gas has the same elemental composition throughout combustion (see Figs. 13.2, 13.3, & 13.4 in Smoot & Smith)





Figure 13.2. Fraction of carbon released to the gas phase from the coal particles for two different coal types (used with permission from Asay, 1982). Points are experimental data; solid line has slope of 1.0. Primary velocity \sim 15 m/s, primary temperature 300 K, and secondary temperature 590 K.

Figure 13.4. Fraction of hydrogen released to the gas phase from the coal for two different coal types. Solid line has a slope of 1.0. (Figure used with permission from Asay, 1982.)



Figure 13.3. Fraction of nitrogen released to the gas phase from the coal from two different coal types. Solid line has a slope of 1.0. (Figure used with permission from Asay, 1982.)

Nitrogen

How do you use η ?

To get elemental composition,

$$b_{k} = b_{kc}\eta + (1 - \eta) [fb_{kp} + (1 - f)b_{ks}] \quad (Eqn.13.7)$$

Where b_k = elemental mass fraction of element "k". If we assume local equilibrium, we only need the enthalpy and the pressure to get properties:

$$y_i = f(b_k, h) = f(f, \eta, h)$$
$$T = f(b_k, h) = f(f, \eta, h)$$

etc.

Locally adiabatic means $h = f(f,\eta)$!! (very rare) (We'll discuss this later)

Putting it all together

Assume $P(\eta, f) = P(\eta) P(f)$ (for convenience mainly)

Mean value, convoluted over joint PDF is:

$$\widetilde{\beta} = \int_{-\infty-\infty}^{\infty} \int_{-\infty}^{\infty} \beta(\eta, f) P(f) P(\eta) df d\eta$$

• 2-D table needed for T, y_i , etc., vs. η and f

Consider Intermittency of f

- α_p = when f = 1 (i.e., pure primary)
- α_s = when f = 0 (i.e., pure secondary)
- Use intermittency to limit integrals to be from 0 to 1

$$\widetilde{\beta} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{\infty} \beta(\eta, f) P(f) df \right] P(\eta) d\eta$$
$$\widetilde{\beta} = \int_{-\infty}^{\infty} \left[\int_{-\infty}^{0} \beta(\eta, f) P(f) df + \int_{0}^{1} \beta(\eta, f) P(f) df + \int_{1}^{\infty} \beta(\eta, f) P(f) df \right] P(\eta) d\eta$$

Intermittency (cont.)

Changing inside integrals to intermittency:



Consider Intermittency of η

 α_c = when η = 1 (i.e., pure coal off-gas) α_i = when η = 0 (i.e., pure inlet gas; pri & sec only)

$$\widetilde{\beta} = \alpha_c \beta_c + \alpha_s \beta_s + \int_0^1 \beta(0, f) P(f) df + \alpha_s \beta_s + \int_0^1 \beta(\eta, f) P(f) df + \alpha_s \int_0^1 \beta(\eta, f) P(\eta) d\eta + \alpha_s \int_0^1 \beta(\eta, f) P(\eta) d\eta + \alpha_s \int_0^1 \beta(\eta, f) P(f) df P(\eta) d\eta$$

What about h???

Possible approaches:

Assume adiabatic locally so $h = f(f,\eta)$ Assume no fluctuations in h PDF in h so $P(f,\eta,h) = P(f)P(\eta)P(h)$ Divide up h into mixing part and residual $\tilde{h} = \tilde{h}_m + \tilde{h}_r$ $h_m = h_c \eta + (1-\eta) [fh_p + (1-f)h_s]$ $\tilde{h}_m = \int_{-\infty-\infty}^{\infty} \tilde{h}_m P(f)P(\eta) df d\eta$ $h_r = residual (\tilde{h} - h_m)$, where \tilde{h} is from conservation equation

How does this help?

 $\beta(\eta, f, h) = \beta(\eta, f, h_r)$

- Don't allow fluctuations in h_r
- Equilibrium table for β (i.e., given η,f,h_r, find β from pre-stored array)
- Advantage: you can set limits on h_r, and hence limit table size



2-η Approach