Turbulence-Chemistry w/ Solid Reactions

1. Review of mixture fraction approach
   - definition of f
   - definition of g_f
   - what are conserved scalars?
   - what is a PDF & how is it used?
   - what assumptions are involved?
   - why can't this approach be used for premixed systems?
   - why can't we just use mean values of T; C_i in reaction rate expressions?
   - how do you get mean values of T; C_i?
2. The Coal Gas Mixture Fraction

   Useful to define additional progress variable:

   η = the coal gas mixture fraction

   $= \dfrac{m_c}{m_c + m_p + m_s}$) m_c = mass of gas originating in the coal

   (13.1 Smoot & Smith)

   Examples: Devolatilization coal → volatiles $\xrightarrow{+O_2}$ $CO_2 + H_2O$

   m_c = mass of volatiles only

   Char Oxidation $C_{(s)} + O_2 \rightarrow CO_2$

   m_c = mass of Carbon released only) i.e., the "C" part of the CO_2

3. Calculating the Coal Gas Mixture Fraction

Conservation Equation → convection ; diffusion plus source term

$$\vec{\nabla}\cdot\left(\bar{\rho}\tilde{\vec{v}}\tilde{\eta} - \Gamma_\eta^t \vec{\nabla}\tilde{\eta}\right) = S_p^m$$

S_{pm} = net rate of mass addition to the gas phase from the condensed phase (due to evaporation, devolatilization, or heterogeneous oxidation).

Also, since $\rho = \frac{\text{total mass of gas}}{\text{volume}} = \frac{m_c + m_y + m_s}{\text{volume}}$)

the equation for f has to be changed!

Let $f_p = \frac{m_p}{m_p + m_s + m_c} = \underbrace{\left(\frac{m_p}{m_p + m_s}\right)}_{f}\underbrace{\left(\frac{m_p + m_s}{m_p + m_s + m_c}\right)}_{(1-\eta)}$

so $f_p = f(1-\eta)$

So equation for f_p becomes

$$\vec{\nabla}\cdot\left(\bar{\rho}\tilde{\vec{v}}\tilde{f}_p - \Gamma_{f_p}^t \nabla\tilde{f}_p\right) = 0$$

→ refer to Figure 13.1 in Smoot ; Smith

Idea is (a) get split between pri ; sec using f (elemental composition)

(b) get coal off-gas using η (elemental composition)

Assumptions 1. η ; f are independent ⇒ $\tilde{f}_p = \tilde{f}(1-\tilde{\eta})$

2. All coal off-gas has the same elemental composition throughout combustion

(see Figs. 13.2, 13.3, ; 13.4 in Smoot ; Smith)

4. How do you use η?

To get elemental composition,

$$b_k = b_{kc}\,\eta + (1-\eta)\left[f\,b_{kp} + (1-f)\,b_{ks}\right]$$

13.7 Smoot & Smith

where b_k = elemental mass fraction of element k, { c = coal gas, p = primary, s = secondary }

Then, if we assume local equilibrium, we only need the enthalpy (h) and pressure

$$Y_i = f(b_k, h) = f(f, \eta, h)$$

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

etc.

locally adiabatic cases: $h = f(f, \eta)$!! (very rare) ↳ we'll fix this later

let β = some gas property { Y_i, T, ρ, etc. }

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

↑ Joint PDF

13.13 Smoot & Smith

Assume $\tilde{P}(\eta) = \tilde{P}(\eta)\,\tilde{P}(f)$

- Convenience mainly, although they come from different sources

$$\therefore \quad \tilde{\beta} = \int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} \beta(\eta, f)\, \tilde{P}(f)\, df\right] \tilde{P}(\eta)\, d\eta$$

↑ ↑ limits are out of bounds ⇒ introduce intermittency

integral with respect to f

13.17 Smoot & Smith

$$\tilde{\beta} = \int_{-\infty}^{\infty}\left[\alpha_p\,\beta(\eta, 1) + \alpha_s\,\beta(\eta, 0) + \int_0^1 \beta(\eta, f)\, df\right] \tilde{P}(\eta)\, d\eta$$

↑ pure primary ($f=1$) ⇒ really, no secondary

↑ pure secondary ($f=0$) really, no primary

Consider intermittency of η:

α_c = when $\eta = 1$; pure coal off-gas

α_I = when $\eta = 0$, pure inlet gases (mixture of m_p; m_s only)

$$\tilde{\beta} = \alpha_c \beta_c + \alpha_I \left[\alpha_p \beta_p + \alpha_s \beta_s + \int_0^1 \beta(0,f)\, \tilde{P}(f)\, df \right]$$

$$+ \alpha_p \int_0^1 \tilde{P}(\eta)\, \beta(\eta,1)\, d\eta + \alpha_s \int_0^1 \tilde{P}(\eta)\, \beta(\eta,0)\, d\eta$$

$$+ \int_0^1 \int_0^1 \beta(\eta,f)\, \tilde{P}(f)\, \tilde{P}(\eta)\, df\, d\eta$$

13.14 Smoot; Smith

to get $\tilde{P}(\eta)$, we need to specify a shape and a variance (g_η)

→ Equation for g_η is derived in a manner similar to g_f

$$\nabla \cdot \left(\bar{\rho} \tilde{\vec{v}}\, g_\eta - D_\eta^t \vec{\nabla} g_\eta \right) = S_{g_\eta} = \begin{cases} C_{g_1} D_\eta^t \left[\left(\frac{\partial \tilde{\eta}}{\partial x} \right)^2 + \left(\frac{\partial \tilde{\eta}}{\partial r} \right)^2 + \left(\frac{\partial \tilde{\eta}}{\partial \theta} \right)^2 \right] \\ - C_{g_2} \bar{\rho} \left(\frac{\varepsilon}{k} \right) g_\eta \end{cases}$$

$$D_\eta^t = \frac{\nu_g^t}{\sigma_\eta}$$

Idea: ① get $\begin{Bmatrix} \tilde{\eta}, g_\eta \\ \tilde{f}, g_f \end{Bmatrix}$ from transport equations

② use PDF to get $\tilde{Y}_i$, $\tilde{T}$, $\tilde{\rho}$, etc.

What about h? (we left it out earlier)

Possible approaches:

(1) assume adiabatic locally, then $h = f(f, \eta)$

NOT GOOD!

(2) assume no fluctuations in h

NOT GOOD, also hard to separate from fluctuations in f; η

(3) PDF in h $P(f, \eta, h) \stackrel{?}{=} P(f)\, P(\eta)\, P(h)$, need η, etc.

$P(h)$ too costly, somewhat coupled to η : f

(4) Divide up h into mixing part and residual

$$\tilde{h} = \tilde{h}_m + \tilde{h}_r$$

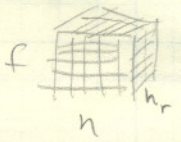
$$h_m = h_c \tilde{\eta} + (1-\tilde{\eta})\left[\tilde{f} h_f + (1-f) h_s\right]$$

h_r = residual $(\tilde{h} - h_m)$, where $\tilde{h}$ is from conservation equation for $\tilde{h}$.

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

- Don't allow fluctuations in h_r
- Equilibrium table for β

(given η, f, h_r, find β from pre-stored array)

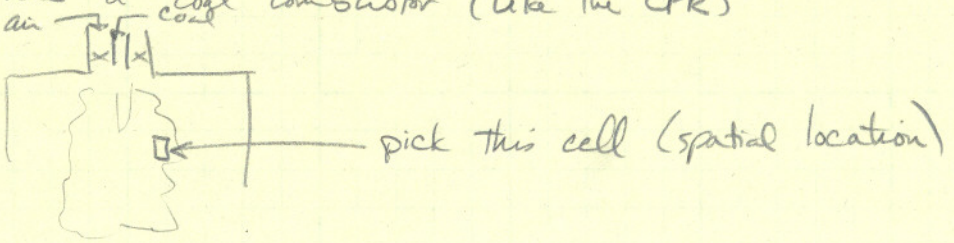


Advantage: you are able to set limits on the values of h_r, and don't have to call the equilibrium program so many times.

(i.e., $h_r = h_m \pm 20\%$ or so)

Different Look at η

Suppose we had a coal combustor (like the CPR)



1. How do we tell what the equilibrium species are at this point?
   - → energy level (suppose we know this)
   - → pressure (known)
   - → composition unknown

2. What do we do to get composition? (~~i.e., elemental composition~~)
   a. Need to know how much of coal has reacted
   b. Ratio of air to coal off-gas
   c. compute the elemental composition

   Say 10 g air (23 wt% O_2, 77% N_2)
   1 g coal off-gas (80% C, 5% H, 15% O)

   net: .8 g C
   .05 g H → get mass fractions → NASA-Lewis
   2.45 g O
   7.7 g N

3. Mixture fraction approach
   η tells how much coal off gas ($= \frac{1}{11}$)

   $$X_C = X_{C,coal}\,\eta + (1-\eta)X_{C,air} = (.8)\left(\tfrac{1}{11}\right) + \left(1-\tfrac{1}{11}\right)(0.0) = .07273$$

   $X_H = -$
   $X_O = -$
   $X_N = -$

Alternatively $\frac{.8\text{ g C}}{11\text{ g tot}} = .07273$

Now suppose that we account for turbulence

for 10% of time, 1 g coal, 10 g air
40% of time 2 g coal, 9.5 g air
etc.

⇒ get average by weighting by time

$$\frac{\Sigma(f_{time})(comp.)}{\Sigma f_{time}}$$

This is what is done by

$$\bar{\beta} = \int \beta(f)\, df \quad \text{or} \quad \iint \beta(\eta, f)\, P(\eta)\, P(f)\, d\eta\, df$$

How do we do this?

⇒ Set up table of equilibrium properties vs. every combination of f; η, then interpolate

for $\eta = 0$

f	Y_{CO_2}	Y_{O_2}	Y_{N_2}	...	T	ρ	ER	...
0								
.01								
.02								
⋮								
f_{st}								
⋮								
.2								
.3								
.5								
1								

for $\eta = .05$

f	Y_i	...	T	ρ	...
0					
.01					
.02					
⋮					

2-η Model

Idea: Treat elemental composition of volatiles separately from char off-gas

$$\text{Coal} \xrightarrow{\text{heat}} \underbrace{\text{Char}}_{\text{mainly C}} + \underbrace{\text{Volatiles}}_{\text{enriched in H, O}}$$

$$\underbrace{O_2}_{\text{from inlet gases (f)}} + \text{char} \Rightarrow \underbrace{CO_2}_{\text{only the C is from char}} + \text{heat}$$

Let $\eta_1 = \dfrac{m_v}{m_v + m_p + m_s}$

$$\eta_2 = \frac{m_{ch}}{m_{ch} + m_v + m_p + m_s}$$

(conserved scalar) b_k = mass fraction of element k

$$= b_{k,ch}\,\eta_2 + (1-\eta_2)\left\{ b_{kv}\,\eta_1 + (1-\eta_1)\left[b_{kp} f + b_{ks}(1-f) \right] \right\}$$

(Average gas property)

$$\tilde{\beta}(f, \eta_1, \eta_2, h) = \iiint \beta(f, \eta_1, \eta_2, h)\, \tilde{P}(f, \eta_1, \eta_2, h)\, df\, d\eta_1\, d\eta_2\, dh$$

Assumptions

$g_{\eta_2} = 0$ (O_2 + char have to be mixed to burn anyway)

$\alpha_{ch} = 0$ (cannot vaporize C in char)

fluctuations in h treated by $h = h_a + \tilde{h}_r$ ← does not fluctuate

$= f(\eta_1, f, \tilde{\eta}_2)$

$$\tilde{\beta}(f, \eta_1, \tilde{\eta}_2, \tilde{h}_r) = \alpha_v \beta_v(\tilde{\eta}_2, \tilde{h}_r) + \alpha_I \left[\alpha_p \beta_p(\tilde{\eta}_2, \tilde{h}_r) + \alpha_s \beta_s(\tilde{\eta}_2, \tilde{h}_r) + \int_0^1 \beta(f, 0, \tilde{\eta}_2, \tilde{h}_r)\, \tilde{P}(f)\, df \right]$$

$$+ \alpha_p \int_0^1 \beta(1, \eta_1, \tilde{\eta}_2, \tilde{h}_r) P(\eta_1) d\eta_1 + \alpha_s \int_0^1 \beta(0, \eta_1, \tilde{\eta}_2, \tilde{h}_r) P(\eta_1) d\eta_1$$

$$+ \int_0^1 \int_0^1 \beta(f, \eta_1, \tilde{\eta}_2, \tilde{h}_r)\, \tilde{P}(f)\, P(\eta_1)\, df\, d\eta_1$$

⇒ 4-D table (f, η_1, η_2, h_a)