The NO_x Model

The Problem: NO_x is very far from mixing-limited

→ show equilibrium vs measured NO_x

air / utah coal, 1atm Pressure, 2000 K, $\phi = 1.0$

Equilibrium: mole fraction = .0008 = 800 ppm

Practice: 100 to 800 ppm, depending on flame (co-flow, swirl, opposed jet, etc.)

⇒ NO_x formation is generally reaction rate limited to a large degree

Types of NO_x

A. Thermal NO_x — N_2 in air, O_2 in air ⇒ NO — high temperature (Zeldovich)

B. Fuel NO_x — N in fuel, O_2 in air ⇒ HCN, NH_3 ⇒ NO, ↘ N_2

C. Prompt NO_x — CH_x radicals, N_2 in air ⇒ HCN ⇒ NO, ↘ N_2 — fuel rich only

D. Reburning — CH_x radicals, NO ⇒ HCN ⇒ N_2, ↘ NO — temperature window

WANTED: Method to incorporate kinetics into turbulent system

<u>Idea</u>: (1) From laminar diffusion flame data, species are a function of ϕ (although not necessarily at equilibrium)

(2) The reaction rates are even a stronger function of ϕ

(3) $\phi = f(f, \eta)$ the mixing variables

<u>Hence</u>: let the reaction rates be a function of f and η !!!

(Show Figs. 15.2 & 15.3 from Smoot & Smith)

→ NO_x is like CO in these figures (falls in a line, but non-equilibrium)

<u>Also note</u>: NO_x is low, & does not seriously affect major variables such as T, Y_{O_2}, etc.

⇒ do NO_x as post-process

i.e., solve entire field, <u>then</u> do NO_x.

Another look

$\overline{W}_{NO}$ = net mass production of NO (source term for species continuity)

$$= \left(\bar{\omega}_1 - \bar{\omega}_2 - \bar{\omega}_3\right) M_{NO}$$

$\uparrow$ molar rates $\qquad$ $\uparrow$ MW_{NO}

$$\bar{\omega}_i = \bar{\rho} \iint_{f\,\eta} \frac{\omega_i}{\rho} P(f)\, P(\eta)\, df\, d\eta$$

mole fractions

$$\bar{\omega}_1 = \bar{\rho} \int_f \int_\eta \frac{1}{\rho} \frac{\rho A e^{-E/RT} X_{HCN} X_{O_2}^{b}}{M_{mix}} \, d\eta \, df$$

$$X_i = Y_i \frac{M_{mix}}{M_i}$$

$$\left[= \frac{mass_i}{mass_t} \frac{\frac{mass_t}{mole_t}}{\frac{mass_i}{mole_i}} = \frac{mole_i}{mole_t} \right]$$

$$Y_i = \pi_i Y_i^f$$

$\uparrow$ computed at equilibrium as a function of f !!!

Note: ω_3 not allowed to fluctuate

How do we get π_i ??

1. use current guess at each cell to get $\overline{W}_i$
2. use $\overline{W}_i$ to solve species continuity eqns. to get $\tilde{Y}_i$
3. compute new $\pi_i = \dfrac{\tilde{Y}_i}{\tilde{Y}_i^f}$

$\nwarrow$ Computed from $\tilde{f}$ and g_f

$$\tilde{Y}_i^f = \iint Y_i^f \, P(f)\, P(\eta)\, df\, d\eta$$

$\uparrow$ equil

4. Does new π_i = old π_i ?

Why Does this Work?

① NO_x is small ($< 0.1\%$)

- doesn't affect other variables < $\overline{Y'_{NO} Y'_k} \cong 0$; change in O_2 is small

② Decoupled from T calculation
(NO_x doesn't affect T, hence ρ and then u, v, etc.)

③ Global rates have been determined

④ Reaction rates seem to be strong functions of the local equivalence ratios

⑤ Coal is inherently a diffusion flame, and therefore mixing is usually important.

Other applications

⇒ CO (assumptions may be flawed)

1. Electromagnetic spectrum

2. Planck's law

$$\rightarrow \int_0^\infty e_{b,\lambda}(\lambda)\, d\lambda = \underset{\substack{\uparrow \\ \text{Stefan-Boltzman constant}}}{\sigma} T^4$$

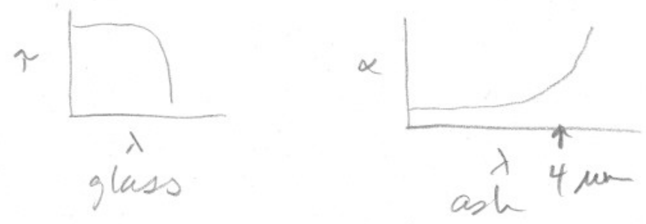
3. Glossary

4. Spectral : directional radiation

5. Radiative transfer equation
   - solved using a "discrete ordinates" method (break up into discrete directions, not along grid, and solve for I_λ field with spatial variations in properties)

6. Put in radiation term for particles in Lagrangian system (Q_{rad}) that includes radiation absorbed and emitted.

7. Emphasize path length dependence
   - like how far can you see in the fog
   - gases are spectral
   - glasses (ash) are a continuum with spectral variation



   - show plot from Terry Wall

The Radiative Transfer Equation (RTE)

$$\underbrace{\frac{1}{c}\frac{\partial I_\lambda}{\partial t}}_{\text{transient}} + \overbrace{\vec{\nabla}\bullet\hat{\Omega}}^{\text{Change in intensity in direction }\Omega}\, I_\lambda + (\underset{\substack{\uparrow \\ \text{absorption}}}{\kappa_\lambda} + \underset{\substack{\nwarrow \\ \text{outscattering}}}{\sigma_\lambda})\, I_\lambda = \overbrace{\kappa_\lambda\, I_{\lambda b}(T)}^{\text{emission}} + \underbrace{\frac{\sigma_\lambda}{4\pi}\int_{\Omega'=4\pi} \Phi_\lambda(\Omega',\Omega)\, I_\lambda(\Omega')\, d\Omega'}_{\text{inscattering}}$$

c = speed of light

Ω = direction

I_λ = intensity

$I_{\lambda b}$ = blackbody emission

κ_λ = absorption coefficient

σ_λ = scattering coefficient

$\Phi_\lambda(\Omega',\Omega)$ = Phase function for light scattered into Ω direction from Ω' direction

I_λ' = intensity of light from Ω' direction

So what does PCGC-3 do?

(1) Discrete Ordinates method for treating RTE

(2) Calculates net emissivity (non-spectral) of gases in each cell (CO_2 and H_2O)

(3) Calculates particle number density

(4) Needs absorption and scattering coefficients for each particle size

(5) Alex → soot model

(6) Solves for I_λ at each cell

(7) Calculates wall heat fluxes