NO_x in Turbulent Systems

<u>Species continuity</u>: (steady-state)

$$\rho u \frac{\partial y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\Gamma_{y_k} \frac{\partial y_k}{\partial x_i} \right) = \dot{W}_k$$

If y_k is small, $y_k', \rho', and\ \overline{y_k' y_k'}$ are small, so

$$\bar{\rho}\tilde{u} \frac{\partial \tilde{y}_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\Gamma_{y_k} \frac{\partial \tilde{y}_k}{\partial x_i} \right) = \tilde{\dot{W}}_k$$

How do you get W_k that is meaningful?

$$\tilde{\dot{W}}_k \neq \dot{W}_k\left(\tilde{T}, \tilde{y}_k\right)$$

NO_x Measurements (background)

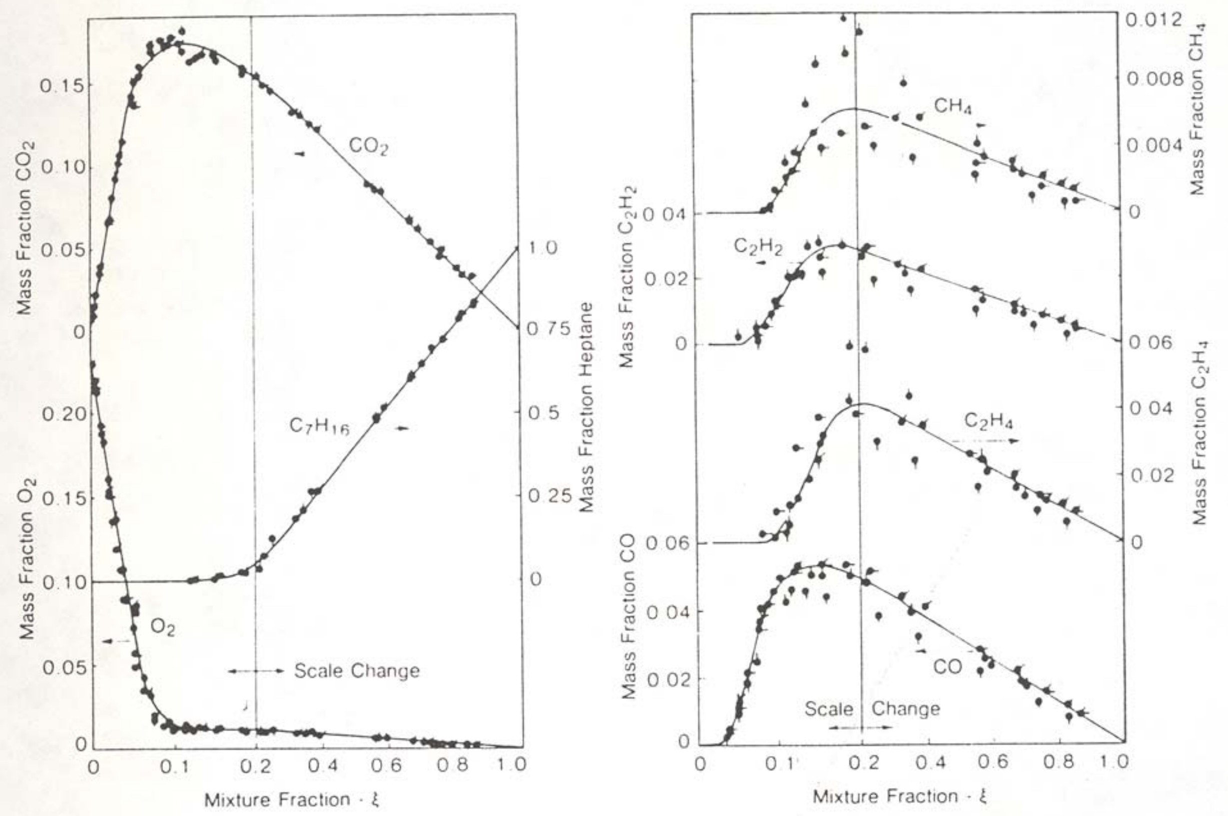
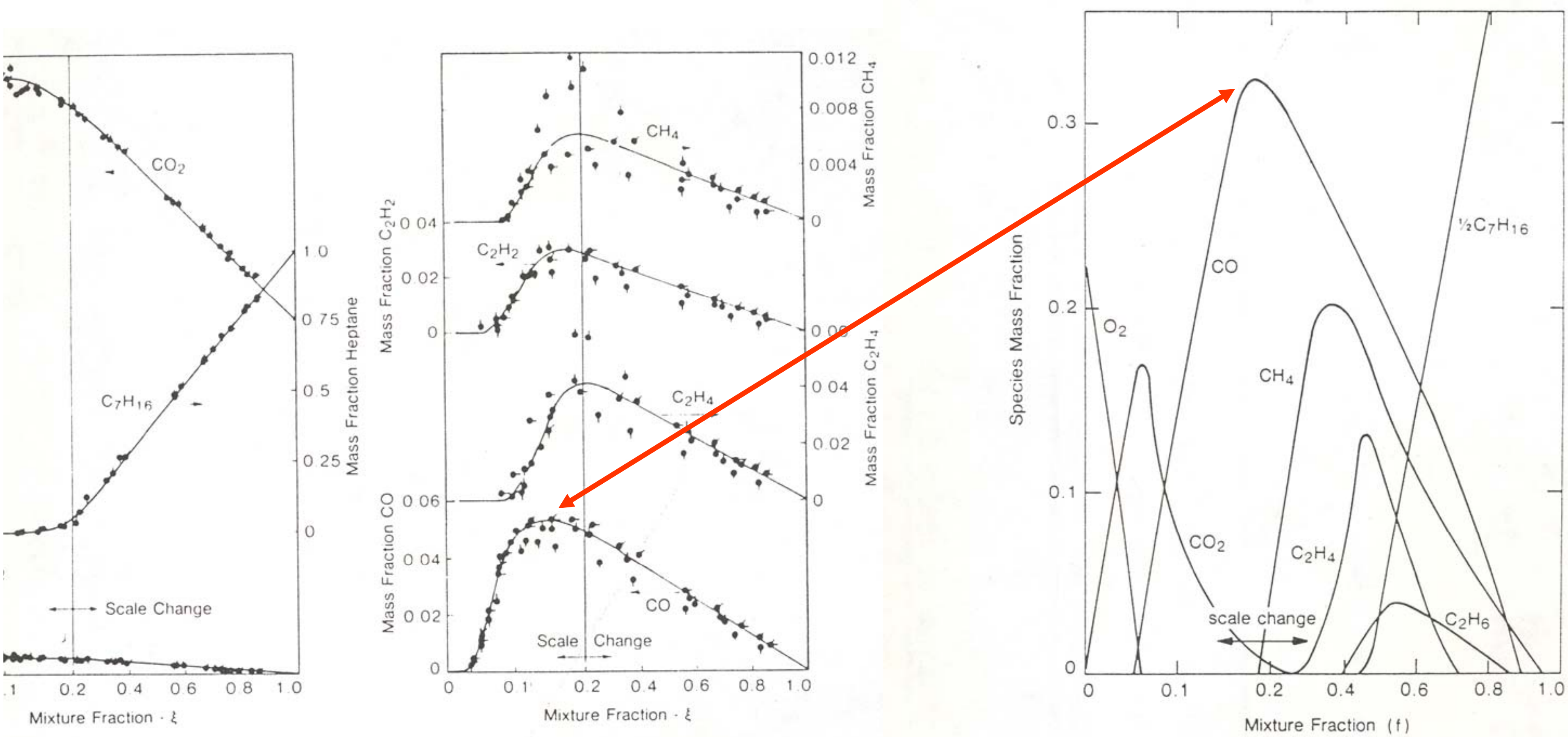


Figure 15.2. Composition correlation between (a) major and (b) minor species composition and mixture fraction in heptane diffusion flames. (Figure used with permission from Bilger, 1978.)

Comparison with Equilibrium (CO)

NO$_x$ POLLUTANT FORMATION



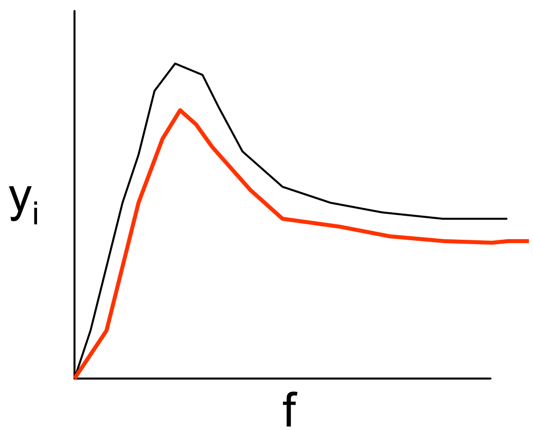
.2. Composition correlation between (a) major and (b) minor species composition and raction in heptane diffusion flames. (Figure used with permission from Bilger, 1978.)

Figure 15.3. Equilibrium composition for the heptane/air flame data shown in Figure 15.2. The equilibrium predictions were performed without solid carbon as an allowed species. (Figure us with permission from Bilger, 1978.)

Idea

Partial Equilibrium

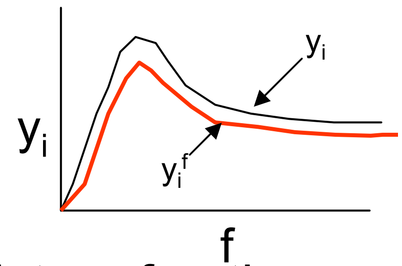
- Some reactions are too slow to achieve equilibrium (i.e., NO, CO)
- Perhaps some characteristic curve is more typical (called partial equilibrium)



Assume that the ratio of actual to equilibrium is constant!

NO_x Approach Used in PCGC-3

Define a variable (π_k) for the extent of reaction:



$$\pi_i = \frac{y_i}{y_i^f}$$

Where y_k^f is computed at equilibrium from the mixture fraction.
Assume that π_k does not fluctuate!

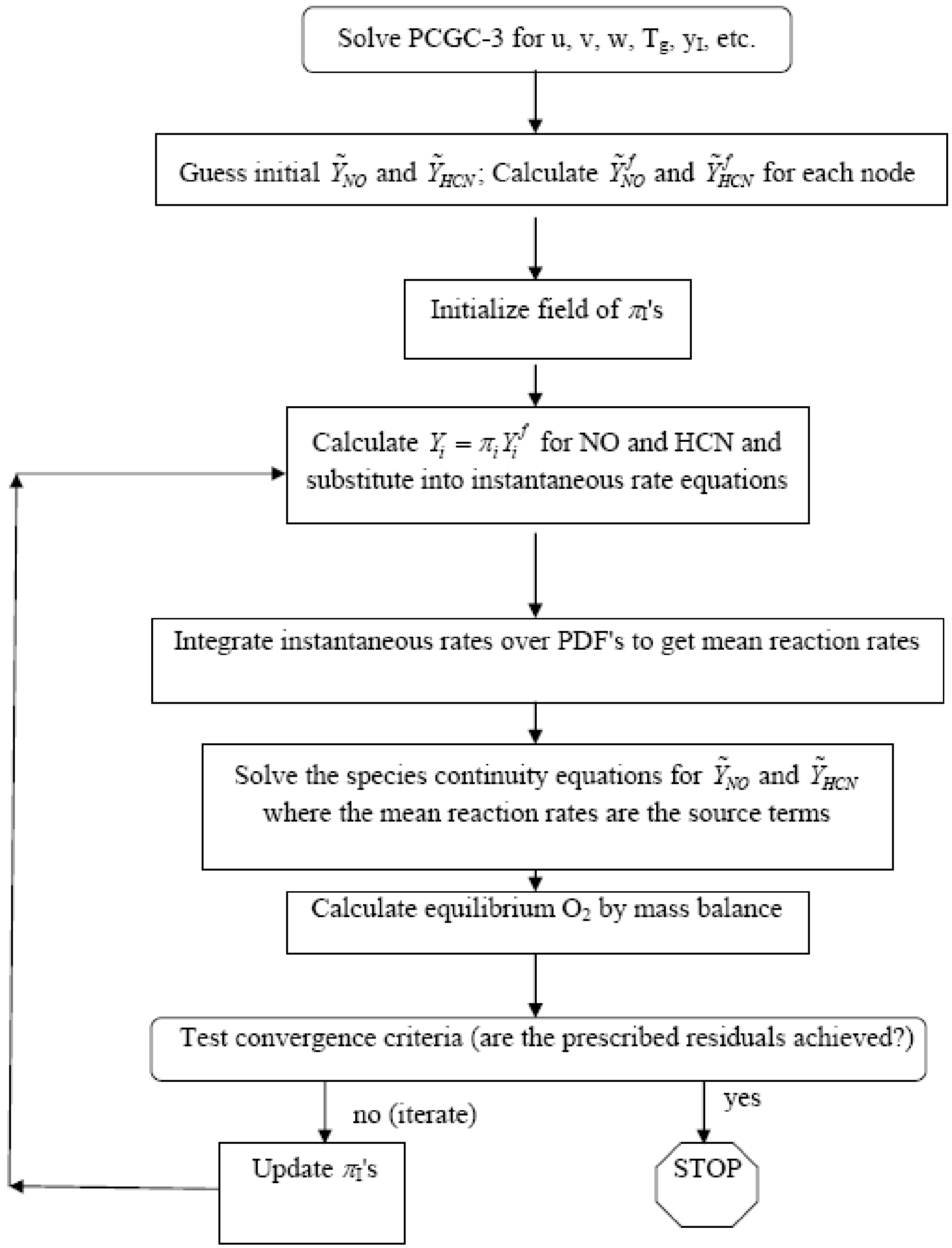
$$\pi_i = \frac{y_i}{y_i^f} = \frac{\tilde{y}_i}{\tilde{y}_i^f}$$

And π_i ≠ function of f, but is constant for each cell

$$\tilde{\dot{W}}_i = \rho \int_\eta \int_f \frac{w_i(\eta, f)}{\rho(\eta, f)} P(\eta) P(f)\, d\eta\, df$$

Where $w_i(\eta,f)$ = rate calculated at y_i (= $\pi_i\, y_i^f$) and T.

NO_x Calculations in PCGC-3



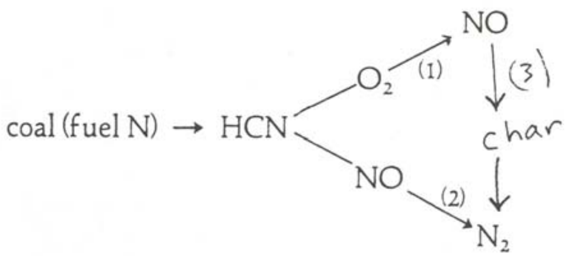


TABLE 15.1. Equation Set for NO Formation and Reduction Model in Turbulent, Coal-Laden, Reacting Flow Processes[a]

Description		Equation
1. Mass balance for O_2	(A)	$\tilde{Y}_{O_2} = \tilde{Y}^0_{O_2} - \tilde{Y}_{NO} M_{O_2}/M_{NO}$
2. Species continuity for $i =$ NO and HCN	(B)	$\bar{\rho}\tilde{u}(\partial \tilde{Y}_i/\partial x) + \bar{\rho}\tilde{v}(\partial \tilde{Y}_i/\partial r) - (\partial/\partial x)(\tilde{D}_Y \partial \tilde{Y}_i/\partial x) - (1/r)(\partial/\partial r)(r\tilde{D}_Y \partial \tilde{Y}_i/\partial r) = \bar{W}_i$
3. Overall mean reaction rates for each species	(C)	$\bar{W}_{NO} = (\bar{w}_1 - \bar{w}_2 - \bar{w}_3) M_{NO}$
	(D)	$\bar{W}_{HCN} = (\bar{w}_0 - \bar{w}_1 - \bar{w}_2) M_{HCN}$
4. Rate of nitrogen release from the coal	(E)	$\bar{w}_0 = \omega_N \bar{S}_p / M_N$
5. Instantaneous reaction rate terms	(F)	$w_1 = \rho(1 \times 10^{11}) X_{HCN} X^b_{O_2} \exp(-67.0\ \text{kcal}/RT)/M_m$
	(G)	$w_2 = \rho(3 \times 10^{12}) X_{HCN} X_{NO} \exp(-60.0\ \text{kcal}/RT)/M_m$
6. Mean reaction rate term by convolution over probability density functions	(H)	$\bar{w}_i = \bar{\rho} \int_f \int_\eta [w_i(f,n)/\rho(f,n)] \tilde{P}(f) \tilde{P}(n)\, df\, dn$
7. NO–Char reduction reaction	(I)	$\bar{w}_3 = \alpha_p n_p (4.18 \times 10^7) A_E \tilde{p}_{NO} \exp(-34.7\ \text{kcal}/R\tilde{T})$
8. Instantaneous mole fractions	(J)	$X_i = Y_i M_m / M_i$
9. Instantaneous mass fractions	(K)	$Y_i = \pi_i Y_i^f$
10. Deviation from fully reacted mass fractions	(L)	$\pi_i = \tilde{Y}_i / \tilde{Y}_i^f$

[a]From Smith *et al.* (1983).

(not referenced)

X_i = mole fraction
Y_i = mass fraction