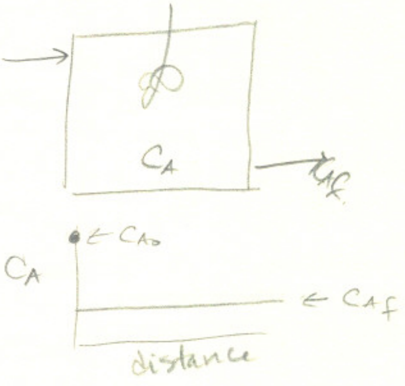
Partially - Stirred Reactors

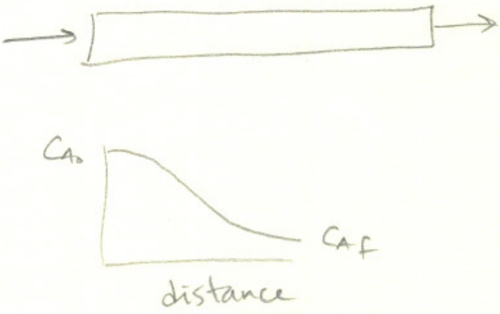
So far, we have looked at 2 ideal reactors that are useful in examining reactions:

A. PSR



very fast mixing (infinite turbulence)
$(C_A = C_{Af})$

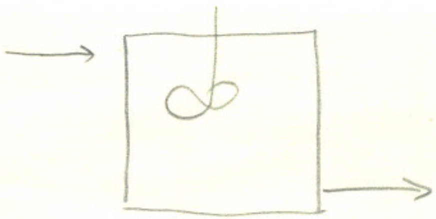
B. Premixed / Plug



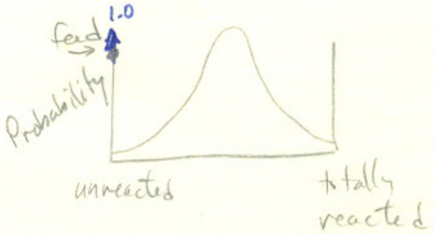
no axial mixing (laminar)
(some diffusion)
$C_A = f(\text{distance})$

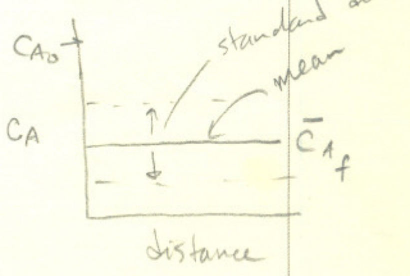
C. Partially - Stirred Reactor

- intermediate to the two extremes
- mixing introduced as a possible controlling step
- chemistry also calculated



at steady-state,

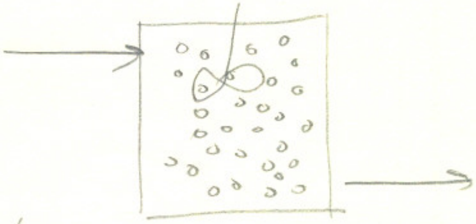




Partially - Stirred Reactor

Idea: Represent the fluid as a series of "particles" of fluid. Start with $N_p = 500$ in the system.

Consider premixed, $T_{initial}$



Principles

① Perform kinetic calculations on each individual "particle" as a function of time (microscale)

② Remove "particles" randomly from the system after a global (macro) time step

③ Introduce new "particles" of feed into the system at Y_k^0, T^0 to replace particles that were removed (i.e., this is a steady-state flow system)

④ Perform some mixing between the particles in the system according to some mixing rule (i.e., new "particles" just fed into the system mix with older "particles" according to some arbitrary mixing frequency "ω")

⑤ Increment time until some steady-state is achieved

Good reference: Correa, S.M., Combustion & Flame, 93, 41-60 (1993)

PaSR

For each individual particle, continuity:

← nth particle

$$\frac{dY_k^{(n)}}{dt} = \underbrace{-C_\phi\,\omega\left(Y_k^{(n)} - \bar{Y}_k\right)}_{\text{mixing model}} + \underbrace{\dot{w}_k^{(n)}\, M_k / \rho^{(n)}}_{\text{net reaction rate}}$$

$Y_k^{(n)}$ = mass fraction of species k in nth particle

$\bar{Y}_k$ = ensemble-averaged mass fraction (updated every Δt_{global})

ω = mixing frequency (user-specified)

→ IEM (Interactive-exchange-with-mean) vs other methods (CURL)

Energy:

$$\boxed{\bar{C}_p \frac{dT^{(n)}}{dt} = \frac{dH^{(n)}}{dt} - \Sigma h_k \frac{dy_k^{(n)}}{dt}}$$

Where did this come from?

for premixed, adiabatic PaSR, $h^{(n)}$ = constant!

$$H = \Sigma y_k h_k \qquad (1)$$

$$\bar{c}_p = \Sigma y_k c_{pk} \qquad (2)$$

$$dh_k = c_{pk}\, dT \qquad (3)$$

From (1),

$$\frac{dH}{dt} = \Sigma\left(y_k \frac{dh_k}{dt}\right) + \Sigma\left(h_k \frac{dy_k}{dt}\right) \qquad (4)$$

from (3), multiplying by y_k,

$$y_k \frac{dh_k}{dt} = y_k c_{pk} \frac{dT}{dt} \qquad (5)$$

or

$$\Sigma y_k \frac{dh_k}{dt} = \Sigma y_k c_{pk} \frac{dT}{dt} = \bar{c}_p \frac{dT}{dt} \qquad (6)$$

Substituting into (4) from definition of $\Sigma y_k \frac{dh_k}{dt}$ from (6),

$$\frac{dH}{dt} = \bar{c}_p \frac{dT}{dt} + \Sigma h_k \frac{dy_k}{dt}$$

, which leads to the final eqn.

$$H = \Sigma y_k h_k$$

$$\frac{dH}{dt} = \Sigma y_k \frac{dh_k}{dt} + \Sigma h_k \frac{dy_k}{dt}$$

$$y_k \frac{dh_k}{dt} = y_k c_{pk} \frac{dT}{dt}$$

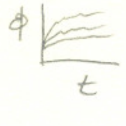
$$\frac{dH}{dt} = \left(\Sigma y_k c_{pk} \right) \frac{dT}{dt} + \Sigma h_k \frac{dy_k}{dt}$$

$$\frac{dH}{dt} = c_{p_{mix}} \frac{dT}{dt} + \Sigma h_k \frac{dy_k}{dt}$$

OR

$$c_{p_{mix}} \frac{dT}{dt} = \frac{dH}{dt} - \Sigma h_k \frac{dy_k}{dt}$$

— Examples of predictions

A. 

(achieving steady-state)
(sensitivity to mixing time)

B. Relationship to PSR ; Plug Flow predictions

C. Scatter plots (a few)

D. PDF of particle age

— Why <u>use</u> the PaSR at all?

→ Provides <u>another</u> tool to evaluate kinetic schemes in a system where turbulence may be important.

→ provides basis for application to large-scale CFD (although large scale computations probably limited to global mechanisms of ~4-8 steps).

Partially - Stirred Reactor

- The selected # of particles and the volume of the reactor determines the mass per particle

$$\rho V = N_p m_p$$

(each "particle" has equal mass)

- The # of particles removed or injected after a certain time step must match the specified mass flow rate.

$$\dot{m} = \frac{N_{in} m_p}{\Delta t} = \frac{N_{out} m_p}{\Delta t}$$

$$(N_{in} = N_{out})$$

- Since the removal of particles is a random process, each particle will have a different residence time. The <u>average</u> residence time is

$$\tau = \frac{\bar{\rho} V}{\dot{m}}$$, where $\bar{\rho}$ is the #-averaged ρ

- Two time scales are used:

  (a) time step for integrating chemical reaction rate

  (b) "global" time step for
    - removing particles
    - injecting replacement feed particles
    - mixing of particles