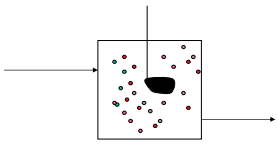
Partially-Stirred Reactor



PASR Flow Diagram

(initialization)

1. Read in Input Parameters
   - Mixing frequency
   - Residence time
   - Number of particles
   - Mixture fraction
   - Number of iterations
   - Output interval
   - Fraction of time for splitting
   - Flags for restart, combustion, mixing, and throughflow

2. Initialize Chemkin calling routines

3. Set up thermochemical properties (concentration and enthalpy)
   - Incoming oxidizer & fuel particles
   - Initial reactor particles

4. Calculate time step size

   $\Delta t_{mix} = t_{timesplit} / \omega_{mix}$

   $\Delta t_{res} = t_{timesplit} * \tau_{res}$

   $\Delta t = \min(\Delta t_{mix}, \Delta t_{res})$

PASR Flow Diagram

(iteration loop)

5. Throughflow of replacement particles
   - # of replaced particles = $N_p * \Delta t/\tau_{res}$
   - Manage influx of fuel and oxidizer
   - Replace randomly chosen (without repetition) particles with fresh fuel and oxidizer particles

time stepping

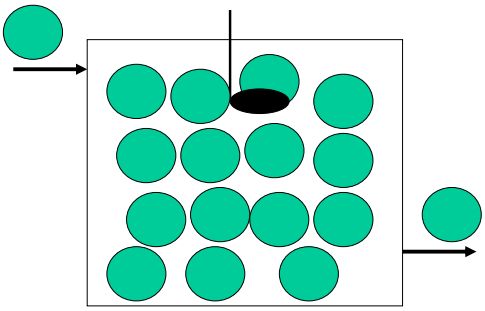
6. Simulate Molecular mixing process in turbulent flow (choose a method)
   - Modified Curl's method
   - Interaction-by-exchange-with-the-mean (IEM) method

7. Integrate chemical kinetic equations
   - Update thermochemical properties for each Monte Carlo particle

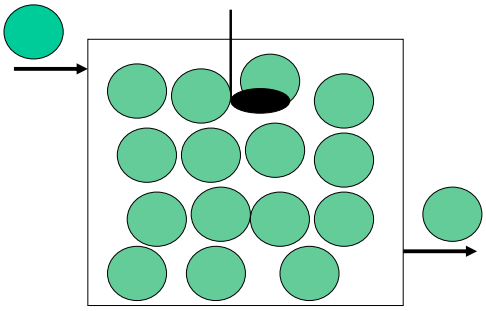
8. Post-process the data
   - Calculate mean T and ρ
   - Calculate the first two moments of scalars (mean and variance)
   - Calculate first six moments of mixture fraction
   - Write to output files

time stepping

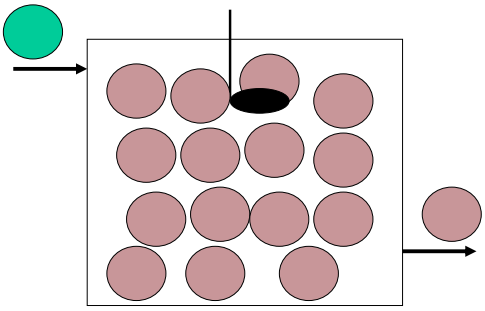
Start reactor

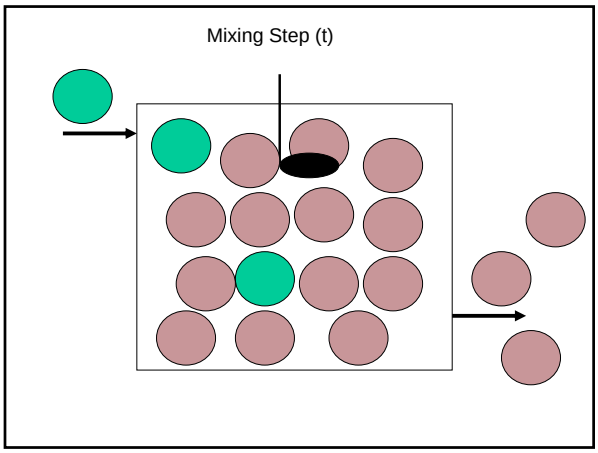


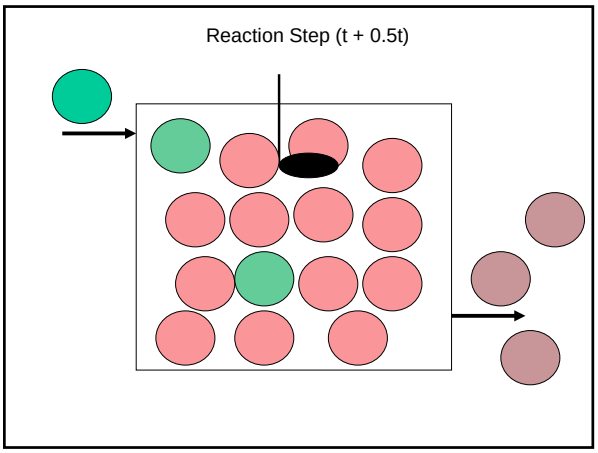
Reaction Step (0.5t)

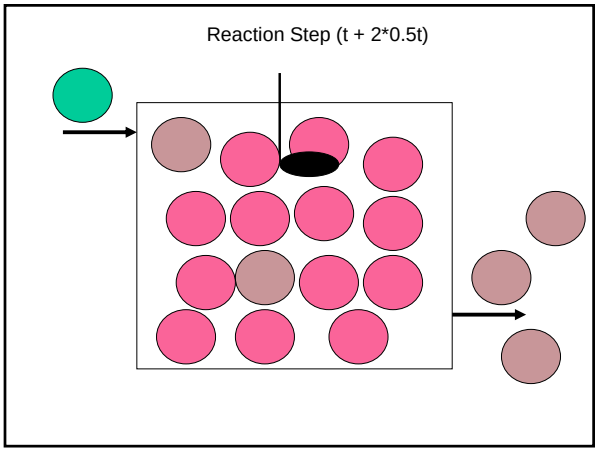


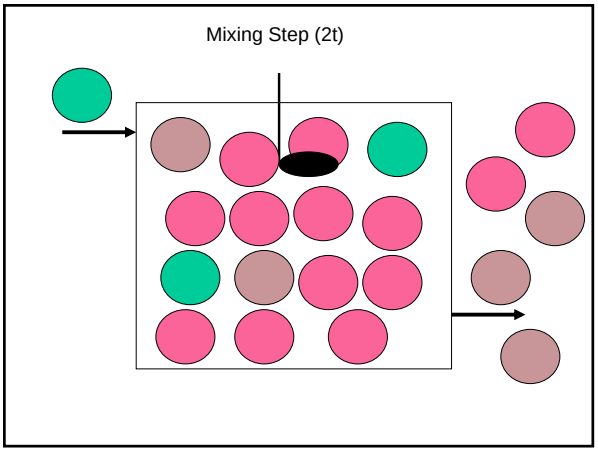
Reaction Step (additional 0.5t)

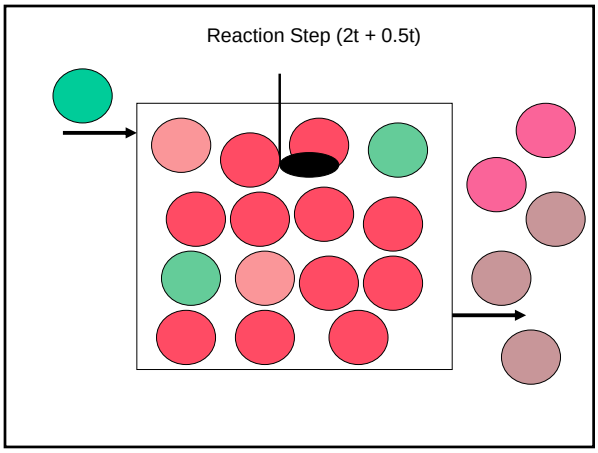


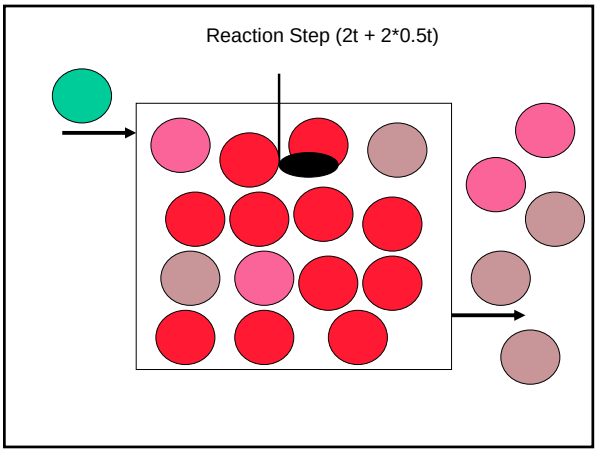

Mixing Step (t)


Reaction Step (t + 0.5t)

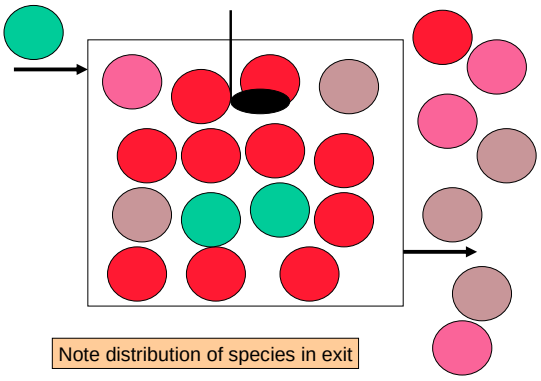

Reaction Step (t + 2*0.5t)


Mixing Step (2t)


Reaction Step (2t + 0.5t)


Reaction Step (2t + 2*0.5t)

Mixing Step (3t)



Note distribution of species in exit

PaSR Predictions, Premixed CO-Air

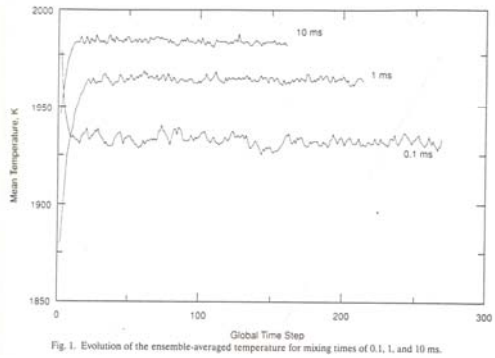


Fig. 1. Evolution of the ensemble-averaged temperature for mixing times of 0.1, 1, and 10 ms.

from Correa, Combustion & Flame, 93, 41-60 (1993)

PaSR Predictions, Premixed CO-Air

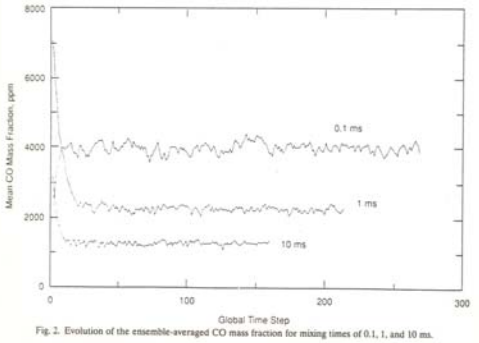


Fig. 2. Evolution of the ensemble-averaged CO mass fraction for mixing times of 0.1, 1, and 10 ms.

from Correa, Combustion & Flame, 93, 41-60 (1993)

PaSR Predictions, Premixed CO-Air

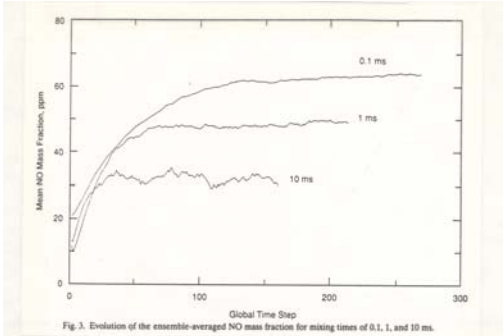


Fig. 3. Evolution of the ensemble-averaged NO mass fraction for mixing times of 0.1, 1, and 10 ms.

from Correa, Combustion & Flame, 93, 41-60 (1993)

PaSR vs PSR and PFR

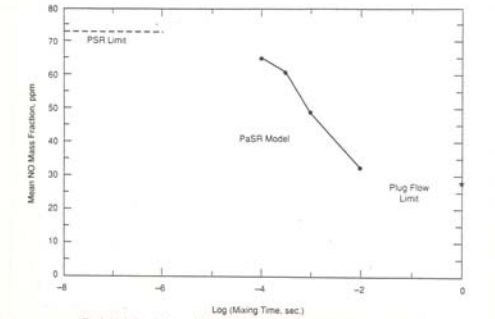


Fig. 6. Variation of the ensemble-averaged NO mass fraction with mixing time scale.

from Correa, Combustion & Flame, 93, 41-60 (1993)

PaSR vs PSR and PFR

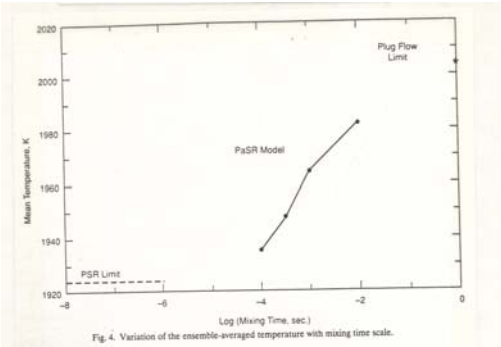


Fig. 4. Variation of the ensemble-averaged temperature with mixing time scale.

from Correa, Combustion & Flame, 93, 41-60 (1993)

Age Plot

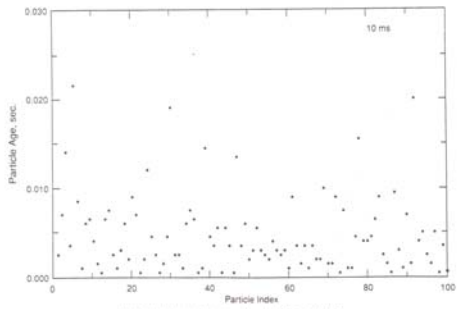


Fig. 9. Particle age in the ensemble, mixing time = 10 ms.

from Correa, Combustion & Flame, 93, 41-60 (1993)

NO "Age" Plot

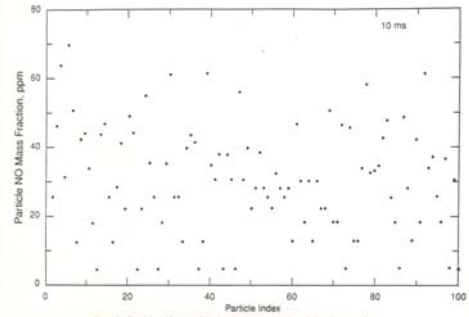
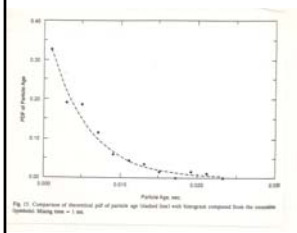


Fig. 10. Particle NO mass fraction in the ensemble, mixing time = 10 ms.

from Correa, Combustion & Flame, 93, 41-60 (1993)

Steady-State Age Distribution



- At steady-state, age distribution should approach a theoretical limit

$$P(\Psi) = \frac{e^{-\Psi/\tau}}{\tau}$$

- where τ is the reactor residence time
- This arises from the random selection of particles exiting the PaSR

from Correa, Combustion & Flame, 93, 41-60 (1993)