1. Business

   a. Teams
   b. Schedule
   c. Don't be afraid to explore → gridding

2. Review (where are we?)

   - Equilibrium
   - Detailed Chemistry
   - Turbulent Reacting Gaseous Flow (Fluent)

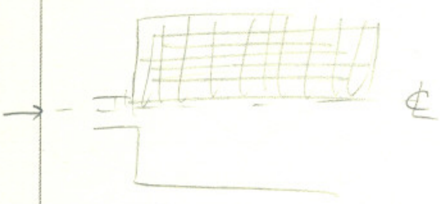
3. Now add a condensed phase!

   - droplet combustion ⇒ engines for transportation
   - particle combustion
     - → pulverized coal ⇒ electricity
     - → biomass
     - → propellants

4. Class Outline (typed sheet)

Lecture 30 — Approaches to Particle Flow

Eulerian



- solve on a grid
- transport properties between cells based on ν, ρ, T
- finite volume approach
- Use void fraction

$$\theta = \frac{V_{gas}}{V_{gas} + V_{solid}}$$

dispersed when $\theta \cong 1$

Advantages

→ Easy

Disadvantages

→ Hard to get Eulerian transport properties for particles (no equ. of state for particles)

→ particle history effects not modeled

→ Turbulence affects particles differently than gas

Lagrangian

- solve along particle trajectories
  - continuity, momentum, energy

get x_p from $u_p = \frac{dx_p}{dt}$

y_p from $v_p = \frac{dy_p}{dt}$

z_p from $w_p = \frac{dz_p}{dt}$

(i.e., solve time-dependent particle equs.)

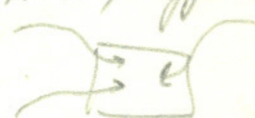
- Save source terms for gas phase equs.
- use gas properties from Eulerian approach

solve gas phase → solve particle phase → converged? — no →; yes → Be happy!

Advantages

→ Easier to get physical parameters to solve conservation equations

→ History effect modeled



(particle properties dependent on path to the cell)

→ Can use small time steps when needed

Disadvantage

→ Need lots of particles to represent system

→ Interface with gas phase is sometimes hard

Table 1. Summary of Conservation Equations for Gas–Particle Mixtures

Continuity equation

Gas phase:	$\partial\rho'_g/\partial t + \nabla\cdot(\rho'_g \mathbf{v}_g) = r_p$
Particle phase:	$\partial\rho'_p/\partial t + \nabla\cdot(\rho'_p \mathbf{v}_p) = -r_p$
Mixture:	$(\partial/\partial t)(\rho'_p + \rho'_g) + \nabla\cdot(\rho'_g \mathbf{v}_g + \rho'_p \mathbf{v}_p) = 0$

Eulerian Approach

(for particles)

$\rho'_g = \theta\rho_g$

θ = void fraction

ρ'_p = bulk particle density

Momentum equation

Gas phase: $(\partial/\partial t)(\rho'_g \mathbf{v}_g) + \nabla\cdot(\rho'_g \mathbf{v}_g \mathbf{v}_g) = -\nabla p + \nabla\cdot[\theta\boldsymbol{\tau} + (1-\theta)\boldsymbol{\tau}_a] - \mathbf{f}_p + \rho'_g \mathbf{g} + \mathbf{v}_p r_p$

Particle phase: $(\partial/\partial t)(\rho'_p \mathbf{v}_p) + \nabla\cdot(\rho'_p \mathbf{v}_p \mathbf{v}_p) = \mathbf{f}_p + \rho'_p \mathbf{g} - \mathbf{v}_p r_p$

Mixture:
$$(\partial/\partial t)(\rho'_g \mathbf{v}_g + \rho'_p \mathbf{v}_p) + \nabla\cdot(\rho'_g \mathbf{v}_g \mathbf{v}_g + \rho'_p \mathbf{v}_p \mathbf{v}_p)$$
$$= -\nabla p + \nabla\cdot[\theta\boldsymbol{\tau} + (1-\theta)\boldsymbol{\tau}_a] + (\rho'_g + \rho'_p)\mathbf{g}$$

Energy equation (total)

Gas phase:
$$(\partial/\partial t)[\rho'_g(i_g + v_g^2/2)] + \nabla\cdot[\rho'_g \mathbf{v}_g(h_g + v_g^2/2)]$$
$$= -\nabla\cdot[\theta\mathbf{q} + (1-\theta)\mathbf{q}_s] - q_{cp} + q_{rg} + r_p(\overline{h}_s + v_p^2/2 + w'^2/2) - \nabla\cdot[(1-\theta)p\mathbf{v}_p]$$
$$+ \nabla\cdot[\theta\boldsymbol{\tau}\cdot\mathbf{v}_g + (1-\theta)\boldsymbol{\tau}_a\cdot\mathbf{v}_p] - \mathbf{v}_p\cdot\mathbf{f}_p + \rho'_g\mathbf{g}\cdot\mathbf{v}_g + \bar{p}_s s_v$$

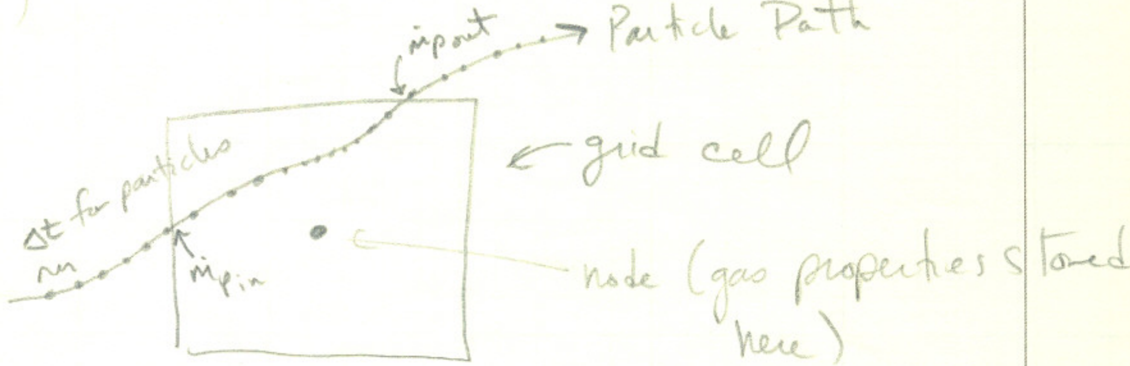
Particle phase:
$$(\partial/\partial t)[\rho'_p(i_p + v_p^2/2)] + \nabla\cdot[\rho'_p \mathbf{v}_p(i_p + v_p^2/2)]$$
$$= -r_p(\overline{h}_s + v_p^2/2 + w'^2/2) + \mathbf{v}_p\cdot\mathbf{f}_p + \rho'_p\mathbf{g}\cdot\mathbf{v}_p + q_{cp} + q_{rp} - \bar{p}_s s_v$$

Mixture:
$$(\partial/\partial t)[\rho'_g(i_g + v_g^2/2) + \rho'_p(i_p + v_p^2/2)] + \nabla\cdot[\rho'_g \mathbf{v}_g(h_g + v_g^2/2) + \rho'_p \mathbf{v}_p(i_p + p/\rho_p + v_p^2/2)]$$
$$= -\nabla\cdot[\theta\mathbf{q} + (1-\theta)\mathbf{q}_s] + \theta q_{rg} + q_{rp} + \nabla\cdot[\theta\boldsymbol{\tau}\cdot\mathbf{v}_g + (1-\theta)\boldsymbol{\tau}_a\cdot\mathbf{v}_p]$$
$$+ \mathbf{g}\cdot(\rho'_p \mathbf{v}_p + \rho'_g \mathbf{v}_g)$$

from Smoot and Pratt, Pulverized-Coal Combustion and Gasification, Plenum, New York, p. 39 (1979). (See Table 9.1, p. 239 of Smoot and Smith, 1985)

PSI-Cell Technique

(Clayton Crowe)



Idea: what is the source term to gas phase from particles

A. Mass

$$\vec{\nabla}\cdot\rho\vec{v} = S_p^m$$

$$S_{p\,cell}^m = \frac{\Delta\dot{m}_p}{V_{cell}}$$

mass/particle

$$\Delta\dot{m}_p = \dot{n}_p\left[\alpha_{p\,in} - \alpha_{p\,out}\right]$$

$\frac{\#\text{ of particles}}{\text{time}}$ represented by this trajectory

Procedure: - compute $\Delta\dot{m}_p$ whenever particle crosses cell boundaries
- interpolate to get gas properties based on neighboring cells

B. Momentum

Axial $$S_p^u = \frac{1}{V}\dot{n}_p\left[(u_p\alpha_p)_{in} - (u_p\alpha_p)_{out}\right]$$

same for v, w velocities $\Rightarrow S_p^v, S_p^w$

c. Energy (neglecting radiation for now)

$$S_p^h = \frac{1}{V} \dot{n}_p \left[(h_p \alpha_p)_{in} - (h_p \alpha_p)_{out} \right]$$

⇒ more complicated when radiation is involved

⇒ includes chemical reaction and convective heat transfer effects

In Practice, many different particles are used

i = index for particle size

j = index for starting location, etc.

$$S^m_{Pcell} = \frac{1}{V} \left(\sum_i \sum_j \Delta \dot{m}_{P_{ij}} \right)$$

(sum contributions from all particles)

If we wanted to do species continuity

$S^m_{P,k}$ ← species or element contribution

D. To start trajectories, need

- size distribution
- starting location
- composition

Turbulence Effects on Particle Motion

A. Ignore Turbulence $\frac{d[\ ]_p}{dt} = f$ (mean gas properties)

B. $u_p = u_{p_m}(f[\ ]_g) + u_{p_t}$

$$\frac{d\vec{V}_p}{dt} = \underbrace{f_p(\vec{V}_g - \vec{V}_p)}_{\text{drag}} + \underbrace{\vec{g}}_{\text{gravity (sign change)}}$$

$f_p = \frac{C_d Re_p}{24\tau_p}$, $\tau_p = \frac{\alpha_p}{3\pi\mu_g d_p}$

1. Empirical ways to get u_{p_t} based on gradient analogies (Smith & Smoot, 1985)

$$u_{p_t} = -\Gamma_p^t \frac{\vec{\nabla}\bar{n}_p}{\bar{n}_p}$$

n_p = particle number density $\left(\frac{\#}{\text{volume}}\right)$

$\Gamma_p^t = \frac{\nu_g^t}{\sigma_p^t}$ ← turbulent eddy viscosity / ← turbulent schmidt number (empirical)

problems: ① Have to use Eulerian eqn. to get $\bar{n}_p$

② Physics not right (not gradient-dependent, since it is not a continuum)

2. Stochastic methods (Shuen, et al., AIAA J, 23:3, 396-404, 1985)

$u_p = u_p(f[\ ]_g) + u_{pt}$

u_{p_t} = random element based on k & ε

v_{pt}

w_{pt} randomly select from

⇒ Gaussian PDF with isotropic Standard deviations $\sqrt{\frac{2}{3}k}$ ← turbulent kinetic energy

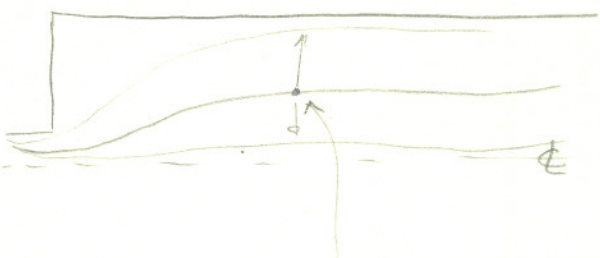
and $\bar{u} = \bar{v} = \bar{w} = 0$

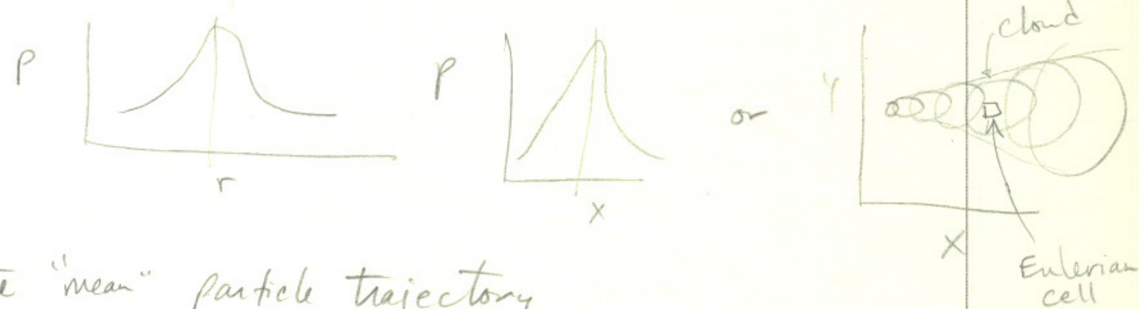
keep this "extra" velocity for eddy lifetime or distance

$t_e = \frac{L_e}{\sqrt{\frac{2}{3}k}}$, $L_e = C_\mu^{3/4} k^{3/2}/\varepsilon$

* LOTS OF PARTICLES (~ 5000)

3. Cloud method





→ compute "mean" particle trajectory

→ compute distribution as a function of time assuming a distribution function

Markovian ⇒ $R = -\int_0^t \tau_g(t')\,dt'$

$$\tau_g = \frac{C_\mu^{2/3} k^{3/2}}{\varepsilon \left(\frac{2k}{3}\right)^{1/2}}$$

- get contribution to cell from different clouds, weight appropriately

* distribution function sacrifices physics
* "easy" to use (not so many particles)
* gas properties computed only at mean position
* wall boundaries are complicated

Reference: Baxter & Smith, Energy & Fuels, 7, 852-859 (1993)

Bottom Line: No perfect method

Fluent ⇒ Stochastic

PCGC-3 ⇒ Empirical $\overline{n}_p$ (want to change) - gradient method
; stochastic option

Jasper ⇒ Cloud
U of U

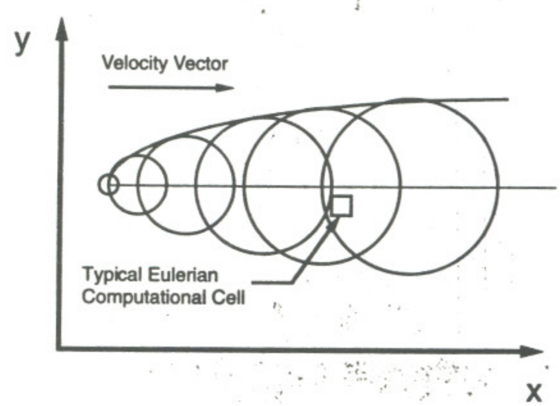


Figure 4. Lagrangian view of dispersion in a one-dimensional flow. Each circle is a measure of the spatial extent of a pdf for particle position at successive times during the flow. The position of a typical Eulerian computational cell is also illustrated. Particles of many different residence times contribute to the overall population of particles in the cell.