PDF Methods:

The use of PDF methods historically saw their rise with respect to their convenience in solving for reacting flows.

Modeling reacting flows is not a significant aspect of this coarse. But it does serve to motivate some general discussions we will have on PDF methods.

Look at a convection-diffusion, reaction equation:

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} = D\frac{\partial^2 c}{\partial x^2} + \dot{\omega}_c$$

$\dot{\omega}_c$ = rate of conversion (generation or consumption) of C

$\dot{\omega}_c$ is usually a nonlinear function of other scalar values

Consider a case where C is produced in a simple reaction

$$A + B \rightarrow C$$

And assume $\dot{\omega}_c = K A B$.

For K = constant, we have

$$\overline{\dot{\omega}_c} = K\,\bar{A}\,\bar{B} + \overline{a'b'}$$

$\overline{a'b'}$ must be modeled.

How to do it?

More realistic:

$$\dot{\omega}_c = KAB \quad \text{where } k = K_0\, e^{(-T_a/T)}$$

Then $\overline{\dot{\omega}_c} = (\bar{A}+a')(\bar{B}+b')\, e^{-(T_a/(\bar{T}+T'))}$

When T dependences are important, the above approach is not practical!

And More realistic: $\overline{\dot{\omega}_c} = K A^n B^m$

$$K = K_o(T,p)\, e^{-(T_a/T)}$$

There are many ways to simplify
e.g. assume local equilibrium

But for finite rate chemistry need something else:

Go back to properties of PDF

recall $P_\phi(\psi; x,t)\, d\psi$ = probability that
$\psi < \phi < \psi + d\psi$ at x,t

& for some scalar ϕ

$$\int_{-\infty}^{\infty} P_\phi(\psi; x,t)\, d\psi = 1$$

(We'll drop x, t, ϕ in notation from now)

Also $\bar{\phi} = \int_{-\infty}^{\infty} \psi\, P(\psi)\, d\psi$

$$\overline{\phi'^2} = \int_{-\infty}^{\infty} (\psi - \bar{\phi})\, P(\psi)\, d\psi$$

All single point statistics available from properties of pdf

Consider next the joint pdf of n scalars:

$$P(\psi_1, \psi_2, \psi_3, \ldots \psi_n ; x, t) = P(\psi_n)$$

then,

$P(\psi_n)$ = probability that

$$\psi_1 < \phi_1 < \psi_1 + d\psi_1 \;\&\; \psi_2 < \phi_2 < \psi_2 + d\psi_2 \;\ldots\; \& \;\psi_n < \phi_n < \psi_n + d\psi_n$$

Then, from the properties of the pdf:

$$\overline{\dot{\omega}_\alpha} = \int \cdots \int \dot{\omega}_\alpha P(\psi) \, d\psi_1 \, d\psi_2 \ldots d\psi_n$$

where $\dot{\omega}_\alpha = f(\phi_1, \phi_2, \ldots \phi_n)$

So if you know the pdf, you can get the mean of any single point, non-linear property!

The problem now shifts to finding the PDF

Two approaches commonly taken:

a) Assume functional form for PDF
b) Solve a transport equation for PDF

a) Assumed PDF

Commonly use approach to model mixing.

We assume a general form for the pdf

e.g. Guassian, Beta,

Both the Guassian & Beta are characterized by their first two moments

$$\overline{\Phi}\ ,\ \overline{\phi'^2}$$

This illustrates one reason understanding shape & evolution of pdf is important

A typical use for this is in reaction modeling

B) <u>Evolution equation for pdf</u>

It is possible to derive an evolution or transport equation for the pdf of a scalar (or vector) quantity

Let's review and introduce some properties & definitions related to PDF's

<u>Joint Pdf</u> $P_{\phi v}(\phi', v'; x\, t)$ we defined already

<u>Conditional Pdf</u>

$$P_{\phi|v}(\phi', v') = \frac{P_{\phi v}(\phi', v')}{P_v(v')}$$ (dropped x, t dependence

" The probability that $\phi' < \phi < \phi' + d\phi'$ given that $v' < v < v' + dv'$

Short hand $P_{\phi v}$

$P_{\phi|v}$

Conditional Mean

Consider a function, g that is a function of ϕ & V, $g(\phi, V)$

The conditional mean

$$\langle g(\phi, V) \,|\, \phi = \phi' \rangle = \int_{-\infty}^{\infty} g(\phi', V') \, P_{\phi|V} \, dV'$$

mean value of g given that $\phi = \phi'$

Independence:

Assume the random variables ϕ & V are independent.

then $P_{\phi|V} = P_\phi$

& $P_{\phi V} = P_\phi P_V$

Derivation of PDF transport equation (See Pope Appendix H)

To derive the PDF transport equation we start with the "fine grained" PDF

$$P'_{V_i}(V'_i; x, t) \equiv \delta(V_i(x,t) - V'_i)$$

Note that $\boxed{\langle P'_{V_i} \rangle = P_{V_i}}$

Proof (Pope, 702)

$$\langle P'_{V_i} \rangle = \langle \delta(V_i(x,t) - V'_i) \rangle$$

definition of mean in terms of Pdf

$$= \int \delta(V''_i - V'_i) \, P_V(V''; x, t) \, dV''$$

property of integrating with δ functions

$$= P_{V_i}(V'_i; x, t)$$

A final Equality use

$$V_i(x,t)\frac{\partial}{\partial x_i}P_V'(V';x,t) = \frac{\partial}{\partial x_i}\left(V_i(x,t)\,P_{V_i}'(V';x,t)\right)$$ incompressib

$$= \frac{\partial}{\partial x_i}\left[V_i' P_V'(V';x,t)\right]$$ from $g(x)\,\delta(x-a) = g(a)\,\delta(x-a)$

$$= V_i'\frac{\partial}{\partial x_i}P_V'(V';x,t)$$ V_i' independent of x_i ☆☆☆

Using ☆, ☆☆, ☆☆☆ we can write

$$\to \frac{\partial P'}{\partial t} + V_i'\frac{\partial P'}{\partial x_i} = -\frac{\partial}{\partial V_i'}\left(P'\,\frac{DV_i}{Dt}\right)$$

Next take mean of this equation

$$\frac{\partial P}{\partial t} + V_i'\frac{\partial P}{\partial x_i} = -\frac{\partial}{\partial V_i'}\left(P\left\langle \frac{DV_i}{Dt}\middle| V'\right\rangle\right)$$ ☆☆☆☆

look at proof a couple of pages back for;

$$\langle \phi(x,t)\,P_{V_i}'\rangle = \langle \phi(x,t)\,|\,V_i(x,t)\,P_{V_i}\rangle$$

☆☆☆☆ still doesn't give us information on the velocity evolution as there is no physics.

Next use Navier Stokes Equation

$$\frac{DV_i}{Dt} = \nu\nabla^2 V_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i}$$

Plug this into ☆☆☆☆

$$\frac{\partial P}{\partial t} + V_i'\frac{\partial P}{\partial x_i} = -\frac{\partial}{\partial V_i'}\left(P\left\langle \nu\nabla^2 V_i - \frac{1}{\rho}\frac{\partial p}{\partial x_i}\middle| V_i'\right\rangle\right)$$

Transport equation for velocity PDF

We also have

$$\langle \phi(x,t)\, P'_{V_i}(V'_i;x,t)\rangle = \langle \phi(x,t) \mid V_i(x,t)\rangle\, P_{V_i}(V'_i;x,t)$$

Proof (Pope Pg. 703)

$$\langle \phi(x,t)\, P'_{V_i}(V'_i;x,t)\rangle = \langle \phi(x,t)\, \delta(V_i(x,t)-V'_i)\rangle$$

definition of fine grained pdf

$$= \int\int_{-\infty}^{\infty} \phi'\, \delta(V''-V')\, P_{V\phi}(V''_i;\phi';x,t)\, dV''\, d\phi'$$

definition of mean (correlation) of 2 random variables

$$= \int_{-\infty}^{\infty} \phi' P_{V\phi}(V';\phi';x,t)\, d\phi'$$

integration over dV'' & property of δ function

$$= \int_{-\infty}^{\infty} \phi'\, P_V(V';x,t)\, P_{\phi|V}(\phi'|V';x,t)\, d\phi'$$

using definition of conditional pdf

$$= P_V(V';x,t) \int_{-\infty}^{\infty} \phi'\, P_{\phi|V}(\phi'|V';x,t)\, d\phi'$$

since P_V independent of ϕ'

$$= P_V(V';x,t)\,\langle \phi(x,t) \mid V(x,t) = V'\rangle$$

definition of conditional mean.

Finally we need some properties of derivatives of the fine grained pdf

$$P_v'(v';t) = \delta(v(t)-v')$$

For some constant c, the derivative of the delta function is an odd function

So we can write

$$\frac{\partial}{\partial t} P_v' = \frac{\partial}{\partial v} P_v' \frac{dv}{dt} \qquad \text{chain rule}$$

$$= \frac{\partial}{\partial v} \delta(v(t)-v') \frac{dv}{dt} \qquad \text{definition of } P_v'$$

$$= \frac{\partial}{\partial v} \delta(v'-v(t)) \frac{dv}{dt} \qquad \delta \text{ function is even}$$

$$= \frac{\partial}{\partial v'} \delta(v'-v) \frac{dv}{dt}$$

call this $\delta'(v'-v) = -\delta'(v-v')$

$$= -\left(\frac{\partial}{\partial v'} \delta(v-v')\right) \frac{dv}{dt} \qquad \text{derivative of } \delta \text{ function is odd}$$

$$= -\frac{\partial P_v'}{\partial v'} \frac{dv}{dt} \qquad \text{definition of } P_v' \qquad \star$$

$$= -\frac{\partial}{\partial v'}\left(P_v'(v';t)\frac{dv(t)}{dt}\right) \qquad v(t) \text{ independent from } v'(t)$$

Similarly

$$\frac{\partial}{\partial x_i} P_v'(v';x,t) = -\frac{\partial P_v'}{\partial v_j'} \frac{\partial v_j(x,t)}{\partial x_i} \qquad \star\star$$

Scalar PDF

We can do the same thing for the scalar PDF

Start with

$$\frac{\partial P_\phi}{\partial t} + v_i' \frac{\partial P_\phi}{\partial x_i} = -\frac{\partial}{\partial \psi}\left(P_\phi \left\langle \frac{D\phi}{Dt} \middle| \psi \right\rangle \right)$$

For $\frac{D\phi}{Dt} = D\nabla^2\phi + \dot{\omega}_\phi$

We have

$$'' \qquad = -\frac{\partial}{\partial \psi}\left(P_\phi\left(\langle D\nabla^2\phi | \psi \rangle + \dot{\omega}_\psi \right)\right)$$

$$\langle \dot{\omega}(\phi) | \phi = \psi \rangle = \dot{\omega}(\psi)$$

Consider a homogeneous turbulent flow with no mean velocity:

$$\frac{\partial P_\phi}{\partial t} = -\frac{\partial}{\partial \psi}\left(P_\phi\left(\langle D\nabla^2\phi | \psi \rangle + \dot{\omega}_\psi \right)\right) \quad \star$$

Observations:

P_ϕ changes due to reaction & "conditional diffusion

In PDF transport, reaction occurs in closed form, It is a single point statistic.

Conditional diffusion, which represents molecular mixing, must be modeled!

Models of this type constitute a class of mixing models.

Curl's Mixing Model in PDF Equation

Recall two particles mix such that

$$\psi_a^* = \psi_b^* = \frac{1}{2}(\psi_a + \psi_b)$$

ψ = concentration before mixing

ψ^* = concentration after mixing

Say we have a mixing frequency ω (every particle will mix in a time $= 1/\omega$

So for N total particles, in a time Δt, N_p particles will mix, where

$$N_p = \Delta t\, \omega N$$

To see how a PDF mixing model can be obtained consider the following

$$p(\psi; t+\Delta t) = p(\psi, t) + \frac{N_p}{N}\int_{-\infty}^{\infty}\!\!\int p(\psi_a)p(\psi_b)\big[-\delta(\psi-\psi_a) - \delta(\psi-\psi_b) + \delta(\psi-\psi_a^*) + \delta(\psi-\psi_b^*)\big]\, d\psi_a\, d\psi_b$$

So what's going on here

N_p – mixed pairs in Δt

$\int p(\psi_a)\, d\psi_a \rightarrow$ selection of element with $\phi = \psi_a$

$p(\psi_a)\, d\psi_b \rightarrow$ " " " " $\phi = \psi_b$

$-\delta(\psi-\psi_a) \rightarrow$ removal of element with $\psi = \psi_a$

$-\delta(\psi-\psi_b) \rightarrow$ " " " " $\psi = \psi_b$

$+\delta(\psi-\psi_a^*) \rightarrow$ addition " " " $\psi = \psi_a^*$ $(= \psi_b^*)$

$+\delta(\psi-\psi_b^*) \rightarrow$ " " " " $\psi = \psi_b^*$ $(= \psi_a^*)$

To obtain PDF evolution equation take ☆ on previous pg

1) Divide by Δt

2) take limit as $\Delta t \to 0$

and show you get

$$\frac{\partial P}{\partial t} = -2\omega P + 2\omega \int\int_{-\infty}^{\infty} P(\psi_a) P(\psi_b) \delta\left(\psi - \tfrac{1}{2}(\psi_a - \psi_b)\right) d\psi_a \, d\psi_b \qquad ☆$$

Do this for homework.

For reaction, we add closed term

$$-\frac{\partial}{\partial \psi}\left(P \dot{\omega}(\psi)\right)$$

Compare to ☆ on pg <u>pdf 9</u>

The r.h.s. of ☆ (on this pg) is Curl's CD model in pdf equation.

Suggests equivalence between pdf transport equation & stochastic Lagrangian particle methods

More general

The C-D model in PDF form can be written in a more general form:

$$\frac{\partial p}{\partial t} = \underset{\text{Ⓐ}}{-2\beta\omega p} + \underset{\text{Ⓑ}}{2\beta\omega \int\int_{-\infty}^{\infty} p(\psi_a)p(\psi_b)\, K(\psi,\psi_a,\psi_b)\, d\psi_a\, d\psi_b} \quad (*)$$

β is a constant selected to give appropriate decay rate of scalar variance

ω mixing frequency, usually modeled as ε/k

Ⓐ is removal of scalar values contributing to p

Ⓑ is addition " " " " " p

$K(\psi,\psi_a,\psi_b)$ is a general Kernel that distinguishes among the different CD models

Modified Curl C-D model:

Recall from earlier discussion we can modify Curl's model to control extent of mixing:

$$\phi_a^* = (1-\alpha)\phi_a + \tfrac{1}{2}\alpha(\phi_a+\phi_b)$$

$$\phi_b^* = (1-\alpha)\phi_b + \tfrac{1}{2}\alpha(\phi_a+\phi_b)$$

This can be represented in pdf transport form by specifying K as

$$K(\psi,\psi_a,\psi_b) = \delta\left(\psi - (1-\alpha)\psi_a - \tfrac{1}{2}\alpha(\psi_a+\psi_b)\right)$$

For any specified value of α, still get discontinuous pdfs.

(Note $\alpha = 1$ gives Curl's Model)

To obtain continuous pdf's we noted that we can take α to be a random variable with pdf $A(\alpha)$

For this case, the kernel, K is

$$K(\psi, \psi_a, \psi_b) = \int_0^1 A(\alpha)\,\delta\left(\psi - (1-\alpha)\psi_a - \tfrac{1}{2}\alpha(\psi_a + \psi_b)\right) d\alpha$$

For details on this, see

Dopazo Phys. Fluids Vol 22 1979

Janicka et al. J. Non Eq. Thermo, Vol 4 1979

Pope Comb. Sci. Tech Vol 28, 1982

Other discussion: infinite moments

Age biasing (Pope, 1982)