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 course. But it does serve to motivate some general discussions we will have on PDF methods.

Look at a convection-diffusion-reaction equation:

\[ \frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} = D \frac{\partial^2 C}{\partial x^2} + \dot{w}_C \]

\[ \dot{w}_C = \text{rate of conversion (generation or consumption)} \]

\[ \dot{w}_C \text{ is usually a nonlinear function of other scalar values} \]

Consider a case where \( C \) is produced in a simple reaction:

\[ A + B \rightarrow C \]

And assume \( \dot{w}_C = k \overline{AB} \).

For \( k \) constant, we have

\[ \overline{\dot{w}_C} = k \overline{A} \overline{B} + a' b' \]

\( a' b' \) must be modeled.

How to do it?

More realistic:

\[ \dot{w}_C = kAB \quad \text{where} \quad k = k_0 e^{-Ta/T} \]
Then \( \overline{w}_c = (\overline{A} + a')(\overline{B} + b') e^{-(T_a/T + T')} \)

When \( T \) dependencies are important, the above approach is not practical.

And more realistic: \( \overline{w}_c = \kappa A^m B^m \)

\( \kappa = K_0(T, p) e^{-(T_a/T)} \)

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

For some scalar \( \phi \)

\[ \int_{-\infty}^{\infty} P_b(\psi; x, t) d\psi = 1 \]

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

Also \( \overline{\phi} = \int_{-\infty}^{\infty} \psi P(\psi) d\psi \)

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

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,

\[ P(\psi_n) = \text{probability that} \]

\[ \psi_1 < \phi_1 < \psi_1 + d\psi_1 \quad \psi_2 < \phi_2 < \psi_2 + d\psi_2 \quad \vdots \]

\[ \psi_n < \phi_n < \psi_n + d\psi_n \]

Then, from the properties of the pdf:

\[ \bar{\omega}_\alpha = \int \cdots \int \omega_\alpha P(\psi) d\psi_1 d\psi_2 \ldots d\psi_n \]

where \( \omega_\alpha = f(\phi_1, \phi_2, \ldots, \phi_n) \)

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. Gaussian, Beta, ...
Both the Gaussian & Beta are characterized
by their first two moments
\[ \bar{\phi}, \bar{\phi}^2 \]

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

A typical use for this is in reaction modeling

b) Evolution equation for PDF

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

Joint PDF \[ P_{\phi,v} (\phi', v'; x, t) \] we defined already

Conditional PDF
\[ P_{\phi|v} (\phi' | v') = \frac{P_{\phi,v} (\phi', v')}{P_v (v')} \] (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 \( \phi \) \& \( \nu \), \( g(\phi, \nu) \).

The conditional mean:

\[
\langle g(\phi, \nu) \mid \phi = \phi' \rangle = \int_{-\infty}^{\infty} g(\phi', \nu') P_{\phi'\nu} d\nu'
\]

mean value of \( g \) given that \( \phi = \phi' \)

Independence:

Assume the random variables \( \phi \) \& \( \nu \) are independent.

then \( P_{\phi\nu} = P_{\phi} P_{\nu} \)

Derivation of PDF transport equation (See Pope Appendix H)

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

\[
P_{V_i}(v_i'; x, t) = \delta(v_i(x, t) - v_i')
\]

Note that \( \langle P_{V_i}' \rangle = P_{V_i} \)

Proof (Pope, 702)

\[
\langle P_{V_i}' \rangle = \langle \delta(v_i(x, t) - v_i') \rangle
\]

\[
= \int \delta(v_i'' - v_i') P_V(v_i''; x, t) dV''
\]

\[
= P_{V_i}(v_i'; x, t)
\]
A final equality use

\[ \frac{\partial V_i}{\partial x_i} P'_i (V'_i; x, t) = \frac{\partial}{\partial x_i} \left( V_i (x, t) P'_i (V'_i; x, t) \right) \quad \text{incompressible} \]

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

\[ = V_i' \frac{\partial}{\partial x_i} \left( P'_i (V'_i; x, t) \right) \quad V_i' \text{ independent of } x \]

Using \( \ast, \ast, \ast, \ast \ast \) we can write

\[ \frac{\partial P'_i}{\partial t} + V_i' \frac{\partial P'_i}{\partial x_i} = -\frac{\partial}{\partial V_i'} \left( P'_i \frac{\partial V_i}{\partial t} \right) \]

Next take mean of this equation

\[ \frac{\partial P}{\partial t} + V_i \frac{\partial P}{\partial x_i} = -\frac{\partial}{\partial V_i} \left( P \langle \frac{\partial V_i}{\partial t} | V_i' \rangle \right) \quad \ast \ast \ast \ast \ast \]

look at proof a couple of pages back for;

\[ \langle \phi(x,t) P'_i \rangle = \langle \phi(x,t) | V_i (x,t) P'_i \rangle \]

\( \ast \ast \ast \ast \ast \) still doesn't give us information on the velocity evolution as there is no physics.

Next use Navier Stokes Equation

\[ \frac{D V_i}{D t} = v \nabla^2 V_i - \frac{1}{S} \frac{\partial P}{\partial x_i} \]

Plug this into \( \ast \ast \ast \ast \ast \ast \ast \ast \ast \ast \)

\[ \frac{\partial P}{\partial t} + V_i' \frac{\partial P}{\partial x_i} = -\frac{\partial}{\partial V_i'} \left( P \langle v \nabla^2 V_i - \frac{1}{S} \frac{\partial P}{\partial x_i} | V_i' \rangle \right) \]

Transport equation for velocity PDF
We also have

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

**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

\[
= \int \int \phi' \delta(v'' - v') P_{V_i}(v'', \phi'; x, t) dv'' d\phi'
\]

- definition of mean (correlation) of 2 random variables

\[
= \int \phi' P_{V_i}(v', \phi'; x, t) d\phi'
\]

- integration over dv'' & property of \( \delta \) function

\[
= \int \phi' P_{V}(v', x, t) P_{\phi|V_i}(\phi'|v''; x, t) d\phi'
\]

- using definition of conditional pdf

\[
= P_{V}(v'; x, t) \int \phi' P_{\phi|V_i}(\phi'|v''; x, t) d\phi'
\]

- since \( P_V \) independent of \( \phi' \)

\[
= P_{V}(v'; x, t) \langle \phi(x,t) | V(x,t) = v' \rangle
\]

- definition of conditional mean.
Finally we need some properties of derivatives of the fine gramed pdf

\[ P'_v(v'; t) = S(v(t) - v') \]

For some constant \( C \), the derivative of the delta function is an odd function

So we can write

\[
\frac{d}{dt} P'_v = \frac{d}{dv} P'_v \frac{dv}{dt} \quad \text{chain rule}
\]

\[
= \frac{d}{dv} S(v(t) - v') \frac{dv}{dt} \quad \text{definition of } P'_v
\]

\[
= \frac{d}{dv} S(v' - v(t)) \frac{dv}{dt} \quad S \text{ function is even}
\]

\[
= \frac{d}{dv} S(v' - v(t)) \frac{dv}{dt} \quad \text{call this } S'(v' - v(t)) = -S'(v - v')
\]

\[
= -\frac{d}{dv} S(v - v') \frac{dv}{dt} \quad \text{derivative of } S \text{ function is odd}
\]

\[
= -\frac{d P'_v}{dv} \frac{dv}{dt} \quad \text{definition of } P'_v
\]

\[
= -\frac{d P'_v}{dv} \frac{dV(t)}{dt} \quad V(t) \text{ independent from } V(t)
\]

Similarly

\[
\frac{\partial}{\partial x_i} P'_v(v'; x; t) = -\frac{d P'_v}{dv} \frac{dV_j(x; t)}{dx_i}
\]
Scalar PDF

We can do the same thing for the Scalar PDF start with

\[ \frac{\partial P_i}{\partial t} + \nabla_i \cdot \frac{\partial P_i}{\partial x_i} = - \frac{\partial}{\partial x} \left( P_i \left( \frac{\partial \phi}{\partial t} \right) \right) \]

For \( \frac{\partial \phi}{\partial t} = \nabla^2 \phi + \dot{\omega}_\phi \)

We have

\[ \langle \dot{\omega}_\phi (\phi) \rangle = \dot{\omega}(\phi) \]

Consider a homogeneous turbulent flow with no mean velocity:

\[ \frac{\partial P_i}{\partial t} = - \frac{\partial}{\partial x} \left( P_i \left( \langle \nabla^2 \phi \rangle + \langle \dot{\omega}_\phi \rangle \right) \right) \]

Observations:

- \( P_i \) changes due to reaction and "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

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

\( \psi \) = concentration before mixing

\( \psi^* \) = concentration after mixing

Say we have a mixing frequency \( \omega \) (every particle will mix in a time \( \frac{1}{\omega} \))

So for \( N \) total particles, in a time \( \Delta t \), \( N_p \) particles will mix, where

\[ N_p = \Delta t \omega N \]

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

\[ p(\psi; t+\Delta t) = p(\psi; t) + \frac{N_p}{N} \int p(\psi_a) p(\psi_b) \left[ -\delta (\psi - \psi_a) - \delta (\psi - \psi_b) \right. \]

\[ + \delta (\psi - \psi_a^*) \delta (\psi - \psi_b^*) \left. \right] d\psi_a d\psi_b \]

So what's going on here

\( N_p \) - mixed pairs in \( \Delta t \)

\[ \int p(\psi_a) d\psi_a \Rightarrow \text{selection of element with } \phi = \psi_a \]

\[ p(\psi_b) d\psi_b \Rightarrow \quad \phi = \psi_b \]

\[ - \delta (\psi - \psi_a) \Rightarrow \text{removal of element with } \psi = \psi_a \]

\[ - \delta (\psi - \psi_b) \Rightarrow \quad \psi = \psi_b \]

\[ + \delta (\psi - \psi_a^*) \Rightarrow \text{addition} \quad \psi = \psi_a^* (= \psi_b^*) \]

\[ + \delta (\psi - \psi_b^*) \Rightarrow \quad \psi = \psi_b^* (= \psi_a^*) \]
To obtain PDF evolution equation take \( \Delta t \) on previous pg.

1) Divide by \( \Delta t \)
2) Take limit as \( \Delta t \to 0 \)

and show you get

\[
\frac{\partial p}{\partial t} = -2wp + 2w \int_{-\infty}^{\infty} p(v_a)p(v_b) \delta \left( v - \frac{1}{2} (v_a + v_b) \right) dv_a \, dv_b
\]

Do this for homework.

For reaction, we add closed term

\[-\frac{\partial}{\partial \psi} (p \psi(t))\]

Compare to \( \Delta t \) on pg \( \text{pdf 9} \)

The r.h.s. of \( \Delta t \) (on this pg) is Curn'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:

\[
\frac{\partial p}{\partial t} = -2\beta \omega p + 2\beta \omega \int_{\mathbb{R}^d} p(\psi) p(\psi_b) K(\psi, \psi_a, \psi_b) d\psi_a d\psi_b
\]

\(\beta\) is a constant selected to give appropriate decay rate of scalar variance

\(\omega\) mixing frequency, usually modeled as \(\varepsilon/k\)

\(A\) is removal of scalar values contributing to \(p\)

\(B\) is addition of scalar values contributing to \(p\)

\(K(\psi, \psi_a, \psi_b)\) is a general kernel that distinguishes among the different C-D models

Modified Curl C-D model:

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

\[
\phi_a = (1 - \alpha) \phi_a + \frac{1}{2} \alpha (\phi_a + \phi_b)
\]

\[
\phi_b = (1 - \alpha) \phi_b + \frac{1}{2} \alpha (\phi_a + \phi_b)
\]

This can be represented in PDF transport form by specifying \(K\) as

\[
K(\psi, \psi_a, \psi_b) = \delta (\psi - (1 - \alpha) \psi_a - \frac{1}{2} \alpha (\psi_a + \psi_b))
\]

For any specified value of \(\alpha\), still get discontinuous PDFs.

(Note \(\alpha = 1\) gives Curl's Model)
To obtain continuous pdf's we noted that we can take $\alpha$ to be a random variable with pdf $A(\alpha)$

For this case, the kernel, $K$ is

$$K(v, v_a, v_b) = \int_0^1 A(\alpha) S \left( y - (1 - \alpha)v_a - \frac{1}{2} \alpha (v_a + v_b) \right) d\alpha$$

For details on this, see

Dopazo Phys. Fluids Vol 22 1979

Other discussion: Infinite moments

Age biasing (Pope, 1982)