Probability Density Function (PDF) methods

Both RANS and LES versions

For RANS, (LES)

Instead of developing the eqns for the average quantities,

eg, $\langle \underline{U} \rangle$, $\langle u_i u_j \rangle$, etc, or $\bar{U}_i$,

1. develop eqn for the PDF of $\underline{U}$, say $f(\underline{V};\underline{x},t)$ (or residual PDF)

where $\underline{V}$ are the values that $\underline{U}$ can take on

(sample space, composition space)

2. Compute averages given f or information about f.

Gained popularity for treating turbulent reacting flows

started by chemical engineers (Curl, 1963)

Avoids certain difficult closure assumptions,

eg, reaction rate term is closed (highly nonlinear)

more intuitive modeling

additional terms need to be modeled (Conservation of difficulty)

eg, mixing rate term

Dimensionality of eqns increases significantly

usually use Monte-Carlo method of solution

eg, axisymmetric jet: $f(u,v,r,x)$

instead of just (r,x) in eqns for $\langle \underline{U} \rangle$

much higher for reacting flows

(every unknown increases dimension by 1)

Basic idea (see chapter 12):

$$\begin{tikzcd}
\text{Eqns for physical system (unaveraged)} \arrow[r] \arrow[d, dashed, "\text{modeling}"] & \text{Eqns for PDF of unknowns closure problem} \arrow[d, "\text{modeling}"] \\
\text{Eqns for a modeled physical system (no averaging)} \arrow[r, dashed, shift right] & \text{Model eqn for PDF of unknown closed but difficult to solve directly.} \arrow[l, shift right]
\end{tikzcd}$$

To solve model eqn for PDF use Monte-Carlo method

Do it by solving eqns for modeled physical system

many times, and averaging {for LES all the  the points in averaging box

Important example - often used in modeling

Ornstein-Uhlenbeck process - Brownian motion

Physical system

(1) Langevin eqn: $dv(t) = \overbrace{-\alpha v(t)dt}^{\text{Stokes drag}} + \overbrace{dF(t)}^{\text{white noise}}$ velocity of small particle

PDF eqn for Langevin eqn

(2) Fokker-Planck eqn $\frac{\partial}{\partial t} f(u,t) = -\alpha \frac{\partial}{\partial u} f(u,t) + D \frac{\partial^2}{\partial u^2} f(u,t)$

where $\langle F(t_1) F(t_2) \rangle = 2D\delta(t_1 - t_2)$

Monte-Carlo

Instead of solving (2) directly,

which will be difficult or impossible for the turbulent case,

Solve (1) many times (easier),

and average over solutions.

PDF Method Applied to Turbulent, Reacting Flows (§12.7.4)

Consider the diffusion, reaction eqn for a reactive scalar $\phi(\underset{\sim}{x},t)$, i.e., { application to N-S — almost the same

(1) $$\frac{\partial \phi}{\partial t} + \underset{\sim}{U}\cdot\nabla\phi = S(\phi) + \Gamma\nabla^2\phi$$

$\underset{\sim}{U}(\underset{\sim}{x},t)$ - turbulent velocity field whose statistics are found in some other way (don't need to do this, but then would have to bring in the N-S)

$S(\phi)$ - chemical source term, a highly nonlinear function of ϕ; e.g., exponential

Usually there are many species + temperature (internal energy), each with a highly nonlinear source term.

We assume 1 specie here for simplicity; this has the basic features of interest

Note that averaging this eqn, with $\phi = \langle\phi\rangle + \phi'$ gives

(2) $$\frac{\partial}{\partial t}\langle\phi\rangle + \langle \underset{\sim}{U}\rangle\cdot\nabla\langle\phi\rangle = \langle S(\phi)\rangle + \Gamma\nabla^2\langle\phi\rangle \underbrace{- \nabla\cdot\langle\phi'\underset{\sim}{u}\rangle}_{\text{turbulent transport}}$$

A major problem is closing the source term.

For example, if $S(\phi) = A e^{-\phi_0/\phi}$,

A, ϕ_0 are constants

ϕ - could be temperature in a Arrhenius reaction,

Then $\langle S(\phi)\rangle = A\langle e^{-\phi_0/[\langle\phi\rangle+\phi']}\rangle$

$= A\langle \exp\left\{\frac{-\phi_0}{\langle\phi\rangle}\frac{1}{[1+\phi'/\langle\phi\rangle]}\right\}\rangle$ (expanding in $\phi'/\langle\phi\rangle$)

$= A \exp\left[\left\{\frac{-\phi_0}{\langle\phi\rangle}\right\}\left\{1+\frac{\phi_0}{\langle\phi\rangle}\frac{\langle\phi'\rangle}{\langle\phi\rangle}\right.\right.$

$+\frac{\phi_0}{\langle\phi\rangle}\left[\frac{\phi_0}{\langle\phi\rangle}-2\right]\frac{1}{2}\frac{\langle\phi'^2\rangle}{\langle\phi\rangle^2} + \cdots\Big]$ (all powers of ϕ')

(there is no reason to truncate the series; many new unknowns)

clearly very complicated and difficult to model.

The PDF approach side steps this issue.

To develop the PDF eqn for ϕ consider the fine-grained PDF for $\phi(\underline{x},t)$, i.e., $\left\{\begin{array}{l}\text{for a given realization of the flow field, with } \phi \\ \text{known at } \underline{x},t, \text{ this is the PDF.}\end{array}\right.$

(3) $\hat{f}_\phi(\psi;\underline{x},t) = \delta[\phi(\underline{x},t)-\psi]$ (approach introduced by Hopf, 1952; Lundgren, 1969)

$\hat{f}_\phi$ is a random fn of $\psi, \underline{x}, t$

consider this as definition

Note that

(4) $\langle \hat{f}_\phi(\psi;\underline{x},t)\rangle = \langle\delta[\phi(\underline{x},t)-\psi]\rangle = \int_{-\infty}^{\infty}\delta[\psi'-\psi]f_\phi(\psi';\underline{x},t)\,d\psi'$

$= f_\phi(\psi;\underline{x},t)$ (take care in working w. δ fns; see Appendix C)

So the fine-grained PDF is a way to get to the PDF.

Note that

$$\frac{\partial}{\partial t}\hat{f}_\phi = \frac{\partial}{\partial t}\delta[\phi(\underline{x},t)-\psi] = \overbrace{\delta'[\phi(\underline{x},t)-\psi]}^{-\frac{\partial}{\partial\psi}\delta[\psi-\psi] = -\frac{\partial}{\partial\psi}\hat{f}}\frac{\partial\phi}{\partial t} = -\frac{\partial}{\partial\psi}\left(\hat{f}_\phi\frac{\partial\phi}{\partial t}\right)$$

since $\frac{\partial\phi}{\partial t}$ is independent of ψ. Similarly

$$\frac{\partial}{\partial x_i}\hat{f}_\phi = -\frac{\partial}{\partial\psi}\left(\hat{f}_\phi\frac{\partial\phi}{\partial x_i}\right)$$, and hence

$$\frac{D}{Dt}\hat{f}_\phi = -\frac{\partial}{\partial\psi}\left(\hat{f}_\phi\frac{D\phi}{Dt}\right)$$

Note that care has to be taken when taking any derivative of a delta function (see Appendix C). They are defined in a limited way.

Therefore, using (1),

(5) $$\underbrace{\frac{D}{Dt}\hat{f}_\phi}_{\text{no physics}} = -\frac{\partial}{\partial\psi}\left(\hat{f}_\phi \frac{D\phi}{Dt}\right) = \overbrace{-\frac{\partial}{\partial\psi}\left[\hat{f}_\phi\left(S(\phi)+\underbrace{\Gamma\nabla^2\phi}_{m}\right)\right]}^{\text{physics}}$$

Averaging this equation gives the following:

$$\left\langle \frac{\partial}{\partial t}\hat{f}_\phi\right\rangle = \left\langle \frac{\partial}{\partial t}\delta[\phi(x,t)-\psi]\right\rangle = \frac{\partial}{\partial t}f_\phi(\psi;x,t) \qquad \int^{\infty}\delta(\psi'-\psi)\,d\psi'$$

$$\left\langle U_i\frac{\partial}{\partial x_i}\hat{f}_\phi\right\rangle \overset{\text{incompressibility}}{=} \frac{\partial}{\partial x_i}\left\langle U_i\,\delta[\phi(x,t)-\psi]\right\rangle = \frac{\partial}{\partial x_i}\int_{-\infty}^{\infty}u_i\, f_{U\phi}(u_i,\psi;x,t)\,du_i$$

$$= \frac{\partial}{\partial x_i}\int_{-\infty}^{\infty}u_i\, f_{U|\phi}(u_i|\psi;x,t)\, f_\phi(\psi;x,t)\,du_i$$

$$= \frac{\partial}{\partial x_i}\left[\langle U_i|\psi\rangle f_\phi\right]$$ – this is not closed.

$$-\left\langle\frac{\partial}{\partial\psi}\left(\hat{f}_\phi S(\phi)\right)\right\rangle = -\frac{\partial}{\partial\psi}\int_{-\infty}^{\infty}\delta(\psi'-\psi)\,S(\psi')\,f_\phi(\psi';x,t)\,d\psi'$$

$$= -\frac{\partial}{\partial\psi}\left[S(\psi)\,f_\phi(\psi)\right]$$

Note that this term is closed; it does not present a closure problem. Finally

$$-\frac{\partial}{\partial\psi}\left[\langle\hat{f}_\phi\underbrace{\Gamma\nabla^2\phi}_{m}\rangle\right] = -\frac{\partial}{\partial\psi}\left\{\iint\delta(\psi'-\psi)\,m'\,f_{\phi m}(\psi',m';x,t)\,d\psi'\,dm'\right\}$$

$$= -\frac{\partial}{\partial\psi}\int_{-\infty}^{\infty}m'\,f_{\phi m}(\psi,m';x,t)\,dm'$$

$$= -\frac{\partial}{\partial\psi}\int_{-\infty}^{\infty}m'\,f_m(m'|\psi;x,t)\,f_\phi(\psi;x,t)\,dm'$$

$$= -\frac{\partial}{\partial\psi}\left[\langle\nabla^2\phi|\psi\rangle f_\phi\right]$$

numerous – there [illegible] eqns – made out 400 models – various models for this term – present forms of eqn.

This term, a molecular mixing term, is now not closed.

underlying homogeneous test [illegible] modeling in [illegible] eqn.

Combining the above gives, for $f_\phi(\psi;x,t)$,

(6) $$\frac{\partial}{\partial t}f_\phi + \frac{\partial}{\partial x_i}\left[\langle U_i|\psi\rangle f_\phi\right] = -\frac{\partial}{\partial\psi}\left(S(\phi)f_\phi\right) - \frac{\partial}{\partial\psi}\left[\langle\Gamma\nabla^2\phi|\psi\rangle f_\phi\right]$$

Note that: $\langle U_i | \psi \rangle = \langle \langle U_i \rangle + u_i | \psi \rangle = \langle U_i \rangle + \langle u_i | \psi \rangle$

Also, since $\frac{\partial}{\partial x_i} \hat{f}_\phi = \frac{\partial}{\partial x_i} \delta[\phi(\underset{\sim}{x},t) - \psi] = -\frac{\partial}{\partial \psi}\left(\hat{f}_\phi \frac{\partial \phi}{\partial x_i}\right)$, then

$$\frac{\partial^2}{\partial x_i^2} \hat{f}_\phi = -\frac{\partial}{\partial x_i}\left[\frac{\partial}{\partial \psi}\left(\hat{f}_\phi \frac{\partial \phi}{\partial x_i}\right)\right] = -\frac{\partial}{\partial \psi}\left(\hat{f}_\phi \frac{\partial^2 \phi}{\partial x_i^2}\right) + \frac{\partial^2}{\partial \psi^2}\left[\hat{f}_\phi \frac{\partial \phi}{\partial x_i} \frac{\partial \phi}{\partial x_i}\right]$$

so taking the average,

$$\frac{\partial^2}{\partial x_i^2} f_\phi = -\frac{\partial}{\partial \psi}\left[\langle \nabla^2 \phi | \psi \rangle f_\phi\right] + \frac{\partial^2}{\partial \psi^2}\left[\langle \nabla\phi \cdot \nabla\phi | \psi \rangle f_\phi\right]$$

Using these relationships in (6) gives

(7) $$\frac{\bar{D}}{Dt} f_\phi = \Gamma \nabla^2 f_\phi - \frac{\partial}{\partial \psi}\left(S(\psi) f_\phi\right)$$

$$- \frac{\partial}{\partial x_i}\left[\langle u_i | \psi \rangle f_\phi\right] - \frac{\partial^2}{\partial \psi^2}\left[\langle \Gamma \nabla\phi \cdot \nabla\phi | \psi \rangle f_\phi\right]$$

scalar dissipation rate

work mainly w this form

[illegible] to find eqn for $\langle\phi\rangle$

In particular, the last two terms need to now be modeled.

A gradient diffusion model is almost always used for the first term:

turb. diffusivity - modeled, e.g., in terms of k, ε

$$-\langle u_i | \psi \rangle f_\phi = \Gamma_T \frac{\partial}{\partial x_i} f_\phi,$$ so that the term becomes:

(8) $$-\frac{\partial}{\partial x_i}\left[\langle u_i | \psi \rangle f_\phi\right] = \frac{\partial}{\partial x_i}\left(\Gamma_T \frac{\partial f_\phi}{\partial x_i}\right)$$

insight will be obtained by averaging eqn

The second term, the mixing term, has received considerable attention in the past. We will discuss it in some detail.

Note that, with (7), employing (8), we can determine the equation for $\langle\phi\rangle$. Multiplying (7) by ψ and integrating over ψ gives, on a term-by-term basis:

$$\frac{\partial}{\partial t} \int \psi f_\phi(\psi; \underset{\sim}{x}, t)\, d\psi = \frac{\partial}{\partial t} \langle \phi(\underset{\sim}{x}, t) \rangle$$

$$\langle \underset{\sim}{U} \rangle \cdot \nabla \int \psi f_\phi(\psi; \underset{\sim}{x}, t)\, d\psi = \langle \underset{\sim}{U} \rangle \cdot \nabla \langle \phi \rangle$$

molecular diffusion

turbulent diffusion

$$\frac{\partial}{\partial x_i}\left\{(\Gamma + \Gamma_T) \frac{\partial}{\partial x_i} \int \psi f_\phi(\psi; x, t)\, d\psi \right\} = \frac{\partial}{\partial x_i}\left[(\Gamma + \Gamma_T) \frac{\partial}{\partial x_i} \langle \phi \rangle\right]$$

$$-\int_{-\infty}^{\infty}\psi\frac{\partial}{\partial\psi}[S(\psi)f_\phi]\,d\psi = -\psi S(\psi)f_\phi(\psi;\underline{x},t)\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}S(\psi)f_\phi(\psi;\underline{x},t)\,d\psi$$

$= \langle S[\phi(\underline{x},t)]\rangle$, assuming f_ϕ goes to 0 fast enough.

$$-\int_{-\infty}^{\infty}\psi\frac{\partial^2}{\partial\psi^2}\left[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi;\underline{x},t)\right]d\psi$$

$$= -\psi\frac{\partial}{\partial\psi}\left[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi\right]\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}\frac{\partial}{\partial\psi}\left[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi\right]d\psi$$

$$= \langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi;\underline{x},t)\Big|_{-\infty}^{\infty} = 0$$

again assuming f_ϕ, $\frac{\partial f_\phi}{\partial\psi}$ goes to 0 fast enough. So

(9) $$\frac{D}{Dt}\langle\phi\rangle = \nabla\cdot\left[(\Gamma+\Gamma_T)\nabla\langle\phi\rangle\right] + \langle S(\phi)\rangle$$

This is what would be obtained by averaging the origin eqn for ϕ, using the turbulent diffusion model for $\langle u_i\phi'\rangle$.

The diffusion flux model for $\langle u_i|\psi\rangle f_\phi$ is consistent with the diffusion model for $\langle u_i\phi'\rangle$ (so are others)

We can obtain eqns for any averaged power of ϕ from the eqn for f_ϕ, eg, $\langle\phi\rangle$, $\langle\phi^2\rangle$, etc.

The PDF eqn contains much more info than the eqn for the average of any of the powers of ϕ.

The mixing term does not directly enter into this equation. But it would for $\langle\phi^2\rangle$

Consider again the mixing term: $-\frac{\partial^2}{\partial\psi^2}[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)]$

Note that $\chi = \langle\Gamma\nabla\phi\cdot\nabla\phi\rangle$ gives the rate of irreversible mixing on the molecular scale

E.g., for the mixing of two non premixed chemical species, it gives the rate of mixing of the 2 species at the molecular scale, necessary for the reaction to occur (irreversible)

Eg. for the ocean it gives the rate of mixing of salt (or heat) at the molecular scale to irreversibly modify the ambient density profile (subtle issues here; see general flux - Mike Gregg

Note that, even if the reaction rate is treated properly, if the mixing model is inaccurate, then the prediction of the overall reaction rate will be inaccurate (a weak link in the method.)

A common (and easy to implement) model for this term is:

(10) $$-\frac{\partial^2}{\partial\psi^2}\left[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi\right] = \frac{\partial}{\partial\psi}\left[f_\phi\left(\frac{1}{2}C_\phi\frac{\varepsilon}{k}(\psi-\langle\phi\rangle\right)\right]$$

no dependence on $S(\phi)$, which may be poor

called interaction by exchange with the mean (IEM)

or linear mean-square estimation

It will be easier to understand this model when we
(i) see its effect in the equation for $\langle\phi^2\rangle$ and
(ii) examine its corresponding Langevin equations. [phys. space]

Note that, to obtain an equation for $\langle\phi^2\rangle$, we can multiply (7) by ψ^2 and integrate, to obtain, with

$$-\int_{-\infty}^{\infty}\psi^2\frac{\partial}{\partial\psi}[S(\psi)f_\phi(\psi)]d\psi = -\psi^2 S(\psi)f_\phi(\psi)\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty}2\psi S(\psi)f_\phi(\psi)d\psi$$

$$= 2\langle\phi S(\phi)\rangle$$

skip some

$$-\int_{-\infty}^{\infty}\psi^2\frac{\partial^2}{\partial\psi^2}[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)]d\psi = -\psi^2\frac{\partial}{\partial\psi}[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)]\Big|_{-\infty}^{\infty}$$

$$+2\int_{-\infty}^{\infty}\psi\frac{\partial}{\partial\psi}[\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)]d\psi$$

$$= 2\psi\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)\Big|_{-\infty}^{\infty} - 2\int_{-\infty}^{\infty}\langle\Gamma\nabla\phi\cdot\nabla\phi|\psi\rangle f_\phi(\psi)d\psi$$

$$= -2\iint_{-\infty}^{\infty} m f_{\underbrace{\phi\,\Gamma\nabla\phi\cdot\nabla\phi}_{m}}(\psi,m;\underline{x},t)dm\,d\psi = -2\overbrace{\langle\Gamma\nabla\phi\cdot\nabla\phi\rangle}^{\chi},$$

like KE

production term

10-only schmidt

Sc and Pr

(11) $$\frac{\bar{D}}{Dt}\frac{1}{2}\langle\phi^2\rangle = \nabla\cdot\left[(\Gamma+\Gamma_T)\nabla\frac{1}{2}\langle\phi^2\rangle\right] + \langle\phi S(\phi)\rangle - \underbrace{\langle\Gamma\nabla\phi\cdot\nabla\phi\rangle}_{\Gamma\nabla\langle\phi\rangle\cdot\nabla\langle\phi\rangle + \underbrace{\Gamma\langle\nabla\phi'\cdot\nabla\phi'\rangle}_{\text{dominate term}}}$$

On the other hand, IEM gives

$$\int_{-\infty}^{\infty}\psi^2\frac{\partial}{\partial\psi}\left[f_\phi\cdot\frac{1}{2}C_\phi\frac{\varepsilon}{k}(\psi-\langle\phi\rangle\right)d\psi = \psi^2\left[f_\phi\frac{1}{2}C_\phi\frac{\varepsilon}{k}(\psi-\langle\phi\rangle)\right]\Big|_{-\infty}^{\infty}$$

$$-\frac{1}{2}C_\phi\frac{\varepsilon}{k}\int_{-\infty}^{\infty}2\psi(\psi-\langle\phi\rangle)f_\phi(\psi)d\psi$$

$$= -C_\phi\frac{\varepsilon}{k}\left[\langle\phi^2\rangle-\langle\phi\rangle^2\right] = -C_\phi\frac{\varepsilon}{k}\langle\phi'^2\rangle$$

With the constant $C_\phi = 2$ (as it is generally taken), the approximation in physical space reduces to:

$$2\Gamma(\nabla\langle\phi\rangle\cdot\nabla\langle\phi\rangle + \langle\nabla\phi'\cdot\nabla\phi'\rangle) \approx 2\frac{\varepsilon}{k}\langle\phi'^2\rangle$$

Usually $\langle\nabla\phi'\cdot\nabla\phi'\rangle \gg \nabla\langle\phi\rangle\cdot\nabla\langle\phi\rangle$. } depends on small scales

Furthermore, the inverse turbulent time scale is

$$\frac{1}{\tau} = \frac{\varepsilon}{k}$$ (this has been used often previously)

So we have

$$\Gamma\langle\nabla\phi'\cdot\nabla\phi'\rangle \approx \frac{\langle\phi'^2\rangle}{\tau}$$ } consistent with previous dissipation rate modeling - which is common to do in PDF modeling

With the models for the mixing term and the turbulent diffusion term, the PDF eqn is: } now closed

(12)
$$\frac{\bar D}{Dt} f_\phi = \nabla\cdot[(\Gamma+\Gamma_T)\nabla f_\phi] - \frac{\partial}{\partial\psi}[S(\psi)f_\phi] + \frac{1}{2}C_\phi\frac{\varepsilon}{k}\frac{\partial}{\partial\psi}[f_\phi(\psi-\langle\phi\rangle)]$$
} (need additional eqns, eg., k-ε model) (could also develop eqn for $f(\psi, u, \ldots)$ - see text)

How do we solve this? Same - x, t, ψ

This can be considered to be a generalized Fokker-Planck eqn. There is also a generalized Langevin system.

Consider the Lagrangian system: (Pope 12.56, p. 548)

Langevin eqn of position not velocity

(13)
$$d\underset{\sim}{X}^+(t) = \underset{\sim}{a}(\underset{\sim}{X}^+, t)\,dt + b(\underset{\sim}{X}^+, t)\,d\overset{\text{white noise}}{\underset{\sim}{W}(t)}$$ } Particle trajectory
$$d\phi^+ = c(\phi^+, X^+, t)\,dt$$ } Lagrangian scalar

Here $\underset{\sim}{X}^+(t)$ is a particle position at time t,

$\phi^+(t)$ is the value of the scalar ϕ for this particle at time t. (suppress $\underset{\sim}{X}(t, \underset{\sim}{Y})$ notation)

a, b, c are functions to be determined (to be consistent with gen-F-P eqn)

$\underset{\sim}{W}(t)$ is an isotropic Wiener process (white noise)

The joint PDF of $\underset{\sim}{X}^+$ and ϕ^+ can be obtained by the method used to obtain the Fokker-Planck equation (the Wiener term must be specially treated) and is: in combination with fine-grained PDF, i.e.

(14)
$$\frac{\partial}{\partial t} f^+_{\phi \underset{\sim}{X}} = -\frac{\partial}{\partial x_i}\left[f^+_{\phi \underset{\sim}{X}}\, a_i(\underset{\sim}{x},t)\right] + \overbrace{\frac{1}{2}\frac{\partial^2}{\partial x_i^2}\left[f^+_{\phi \underset{\sim}{X}}\, b(\underset{\sim}{x},t)\right]}^{\text{Wiener term, as in F-P eqn}}$$
$$-\frac{\partial}{\partial \psi}\left[f^+_{\phi \underset{\sim}{X}}\, c(\psi, \underset{\sim}{x}, t)\right]$$

with $f^+_{\phi \underset{\sim}{X}} = f^+_{\phi \underset{\sim}{X}}(\psi; \underset{\sim}{x}; t)$ $\;\;\Big\{$ ψ sample space of ϕ, $\underset{\sim}{x}$ sample space of $\underset{\sim}{X}^+$

The eqn for the PDF of $\underset{\sim}{X}^+(t)$ can be obtained by integrating this eqn over ψ (it should be the Fokker-Planck eqn), giving (now in terms of $\underset{\sim}{x}$, not u) in 3-D

(15)
$$\frac{\partial}{\partial t} f^+_{\underset{\sim}{X}} = -\frac{\partial}{\partial x_i}\left[f^+_{\underset{\sim}{X}}\, a_i(\underset{\sim}{x},t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_i}\left[f^+_{\underset{\sim}{X}}\, b(\underset{\sim}{x},t)\right]$$

Note that, if $f^+_{\underset{\sim}{X}}(0)$ is uniformly distributed over the sample space of $\underset{\sim}{X}^+(t)$, then

$$\frac{\partial}{\partial t} f^+_{\underset{\sim}{X}}\Big|_0 = f^+_{\underset{\sim}{X}}(0)\left\{-\nabla\cdot\underset{\sim}{a} + \frac{1}{2}\nabla^2 b\right\}\Big|_0$$

$\Big\{$ e.g., in a closed box, probability of initial position of particles is uniform so $f^+_{\underset{\sim}{X}}(\underset{\sim}{x},0) = \text{const}$, indep. of $\underset{\sim}{x}$.

(16) Therefore, if $-\nabla\cdot a + \frac{1}{2}\nabla^2 b = 0$ for all t, then

$$\frac{\partial}{\partial t} f^+_{\underset{\sim}{X}}(t) = 0,$$

$\Big\{$ formally can show $f^+_{\underset{\sim}{X}}(t) = f^+_{\underset{\sim}{X}}(0)$ satisfies eqn and IC, must be a solution.

and $\underset{\sim}{X}^+(t)$ remains uniformly distributed. ($f^+_{\underset{\sim}{X}}$ is a constant)

Furthermore,

$$f^+_{\phi}(\psi, t \mid \underset{\sim}{X}^+(t) = \underset{\sim}{x}) = f^+_{\phi \underset{\sim}{X}}(\psi; \underset{\sim}{x}; t) \Big/ f^+_{\underset{\sim}{X}}(\underset{\sim}{x}, t)$$

Note that $f^+_{\phi}(\psi, t \mid \underset{\sim}{X}^+(t) = \underset{\sim}{x}) = f_{\phi}(\psi; \underset{\sim}{x}, t)$, the previously defined Eulerian variable. So

$$f^+_{\phi \underset{\sim}{X}}(\psi, t; \underset{\sim}{x}, t) \propto f_{\phi}(\psi, \underset{\sim}{x}, t) \quad \text{since } f^+_{\underset{\sim}{X}}(\underset{\sim}{x}, t) = \text{const}$$

and eqn (14) becomes:

(17)
$$\frac{\partial}{\partial t} f_{\phi} = -\frac{\partial}{\partial x_i}\left[f_{\phi}\, a_i(\underset{\sim}{x},t)\right] + \frac{1}{2}\frac{\partial^2}{\partial x_i^2}\left[f_{\phi}\, b(\underset{\sim}{x},t)\right]$$
$$-\frac{\partial}{\partial \psi}\left[f_{\phi}\, c(\psi, \underset{\sim}{x}, t)\right]$$

Therefore, with the choices: (comparing (12) and (17))

(18) $$\underset{\sim}{a}(\underset{\sim}{x},t) = \langle \underset{\sim}{U} \rangle + \nabla(\Gamma_T + \Gamma) \qquad \Big\{ \nabla^2(f_\phi b) = \nabla\cdot\nabla(f_\phi b) = \underbrace{\nabla\circ\Big[b\nabla f_\phi}_{\text{gives } b} + \underbrace{f_\phi \nabla b\Big]}_{\text{in } \underset{\sim}{a} \text{ to cancel}}$$

$$b(x,t) = 2(\Gamma_T + \Gamma)$$

So $-\nabla\circ\underset{\sim}{a} + \frac{1}{2}\nabla^2 b = -\nabla\circ\langle \vec{\underset{\sim}{U}} \rangle - \nabla^2(\Gamma_T+\Gamma) + \frac{1}{2}\cdot 2\nabla^2(\Gamma_T+\Gamma) = 0$

$$c(\psi, \underset{\sim}{x}; t) = -\frac{1}{2} C_\phi \frac{\varepsilon}{k}\left[\psi - \langle \phi^+ | \underset{\sim}{x} \rangle\right] + S(\psi) \qquad \Big\{ \langle \phi^+(t) | \underset{\sim}{X}^+(t) = \underset{\sim}{x} \rangle = \langle \phi(\underset{\sim}{x}, t$$

giving the original eqn for $f_\phi(\psi; \underset{\sim}{x}, t)$ with the diffusion model and the IEM model.

Therefore, with (13) and (18), we have a generalized Langevin system:

(19) $$d\underset{\sim}{X}^+(t) = \langle \underset{\sim}{U} \rangle dt + \nabla(\Gamma + \Gamma_T) dt + 2(\Gamma + \Gamma_T) d\underset{\sim}{W}$$

$$d\phi^+(t) = S(\phi^+) dt - \frac{1}{2} C_\phi \frac{\varepsilon}{k}\left[\phi^+ - \langle \phi^+ | \underset{\sim}{x} \rangle\right] dt$$

) Lagrangian problem

corresponding to the generalized Fokker-Planck eqn:

(12) $$\frac{\overline{D}}{Dt} f_\phi = \nabla\circ\left[(\Gamma + \Gamma_T)\nabla f_\phi\right] - \frac{\partial}{\partial\psi}\left[S(\psi) f_\phi\right] + \frac{1}{2}\frac{\varepsilon}{k}\frac{\partial}{\partial\psi}\left[f_\phi(\psi - \langle\phi\rangle)\right]$$

Note that we started with

$$\begin{tikzcd} \text{original eqn for } \phi \arrow[r] & \text{original PDF eqn for } \phi \arrow[d, "\text{(thru modeling)}"'] \\ \text{model eqn for } \phi & \text{model eqn for PDF of } \phi \arrow[l] \end{tikzcd}$$

The modeling can be done either

(i) for the eqn for the PDF of ϕ, checking for consistency with the equations for $\langle\phi\rangle$, $\langle\phi^2\rangle$, etc., or

(ii) for the eqns for ϕ itself.

If the latter can be constructed to be a dynamically realizable system, at least in theory, then realizability is assured. (Some researchers so sought to model eq ϕ itself, Furthermore, modeling directly for ϕ can be much more intuitive than for the eqn for the PDF of ϕ.

eq. $d\phi^+(t) = \underbrace{-\frac{1}{2}C_\phi \frac{\varepsilon}{k}\left[\phi^+ - \langle\phi^+|\underline{x}\rangle\right]}_{\text{model for mixing}} dt + \underbrace{S(\phi^+)dt}_{\text{exact reaction}}$

If $\phi^+ > \langle\phi^+|\underline{x}\rangle$, then ϕ^+ decreases towards the mean, and vice-versa (interaction by exchange with the mean)
This will drive ϕ^+ towards the mean, which is what mixing does.

eq. For simplicity consider the case of homogeneous turbulence, so $\nabla(\Gamma+\Gamma_T) = \underline{0}$, and $\underline{X}^+(t)$ satisfies

$$d\underline{X}^+(t) = \langle\underline{U}\rangle dt + 2(\Gamma+\Gamma_T)\,d\underline{W}(t)$$

The Wiener term in the particle trajectory eqn corresponds to the diffusion term $(\Gamma+\Gamma_T)\nabla^2 f_\phi$ in the PDF eqn
"Random walk" is consistent with gradient diffusion.
(and gradient diffusion is sometimes modeled as a random walk, with Monte-Carlo methods.)

and in the equations for moments