MICROMIXING MODELS FOR TURBULENT REACTING FLOWS

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Small-Scale Turbulence: Theory, Phenomenology and Applications

Thursday (16/8) and Friday (17/8)

14:00–16:00

CAMBRIDGE SERIES IN CHEMICAL ENGINEERING

This book presents the current state of the art in computational models for turbulent reacting flows, and analyzes carefully the strengths and weaknesses of the various techniques described. The focus is on formulation of practical models as opposed to numerical issues arising from their solution. A theoretical framework based on the one-point, one-time joint probability density function (PDF) is developed. It is shown that all commonly employed models for turbulent reacting flows can be formulated in terms of the joint PDF of the chemical species and enthalpy. Models based on direct closures for the chemical source term, as well as transported PDF methods, are covered in detail. An introduction to the theory of turbulent and turbulent scalar transport is provided for completeness. The book is aimed at chemical, mechanical, and aerospace engineers in academia and industry, as well as developers of computational fluid dynamics codes for reacting flows.

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Computational Models for Turbulent Reacting Flows

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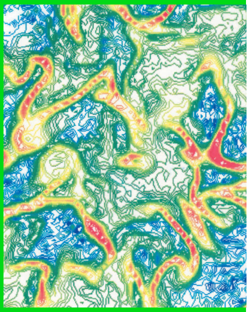

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Chapter 1

Background on Scalar Mixing

1.1 Transport Equations for Passive Scalars

Momentum balance:

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i}, \tag{1.1}$$

Chemical species mass balance:

$$\frac{\partial \phi_\alpha}{\partial t} + U_j \frac{\partial \phi_\alpha}{\partial x_j} = \Gamma_\alpha \frac{\partial^2 \phi_\alpha}{\partial x_j \partial x_j} + S_\alpha(\boldsymbol{\phi}). \tag{1.2}$$

Solution for velocity depends on Reynolds number (Re)

Solution for inert scalars depends on Re and Schmidt number (Sc $= \nu/\Gamma$)

Solution for reacting scalars also depends on Damköhler numbers (Da)

Modeling challenge: Direct-numerical simulations (DNS) are intractable for turbulent flows of interest, how can we use transport equations?

Turbulence Models

Reynolds-averaged transport equations are unclosed:

Mean momentum balance:

$$\frac{\partial \langle U_i \rangle}{\partial t} + \frac{\partial \langle U_j U_i \rangle}{\partial x_j} = \nu \frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} \tag{1.3}$$

Mean chemical species mass balance:

$$\frac{\partial \langle \phi_\alpha \rangle}{\partial t} + \frac{\partial \langle U_j \phi_\alpha \rangle}{\partial x_j} = \Gamma_\alpha \frac{\partial^2 \langle \phi_\alpha \rangle}{\partial x_j \partial x_j} + \langle S_\alpha(\boldsymbol{\phi}) \rangle \tag{1.4}$$

- Reynolds stresses: $\langle u_j u_i \rangle$
- Scalar fluxes: $\langle u_j \phi_\alpha \rangle$
- Mean chemical source term: $\langle S_\alpha(\boldsymbol{\phi}) \rangle$

CFD models for the Reynolds stresses and scalar fluxes are available and reasonably reliable (can be validated with PIV and PLIF)

Due to coupling with chemical time scales and nonlinear form, $\langle S_\alpha(\boldsymbol{\phi}) \rangle$ is much more difficult to model!

Similar remarks hold for large-eddy simulations (LES) because micromixing and chemical reactions occur at small scales!

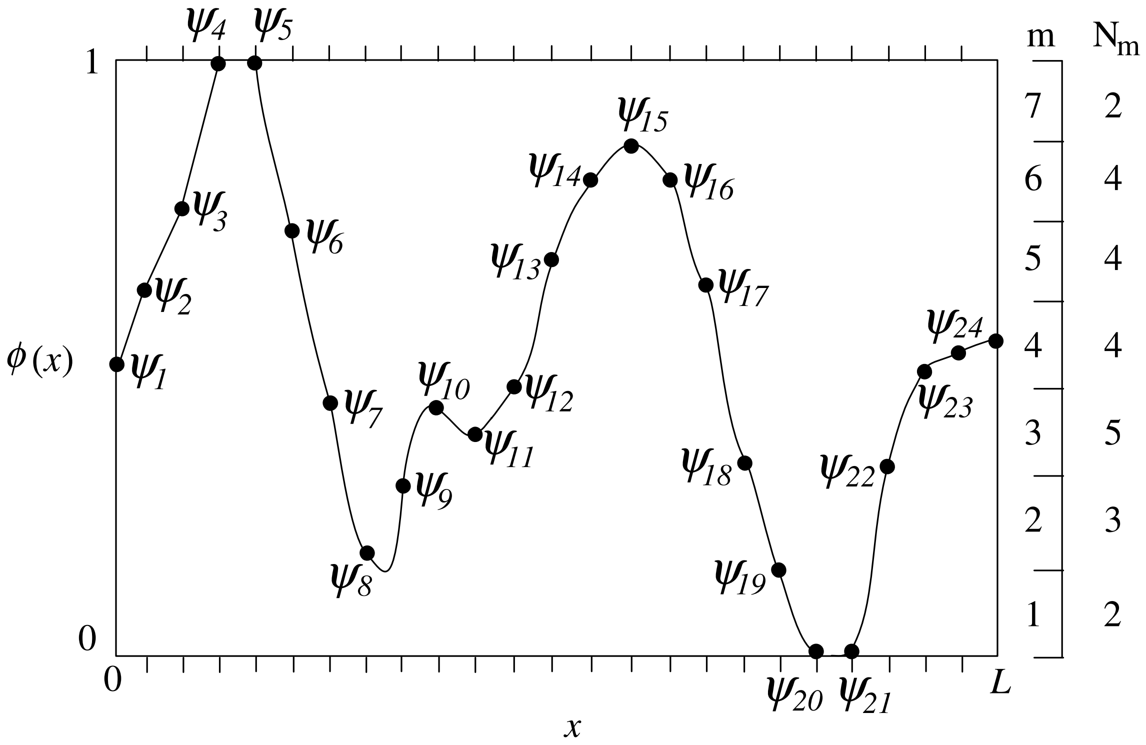
Chemical-Source Term

Chemical source term depends on *local* concentrations and temperature (not on gradients):

$$\mathbf{S}(\boldsymbol{\phi}) \quad \text{where} \quad \boldsymbol{\phi}^{\mathrm{T}} = (c_{\mathrm{A}}, c_{\mathrm{B}}, \ldots, T)$$

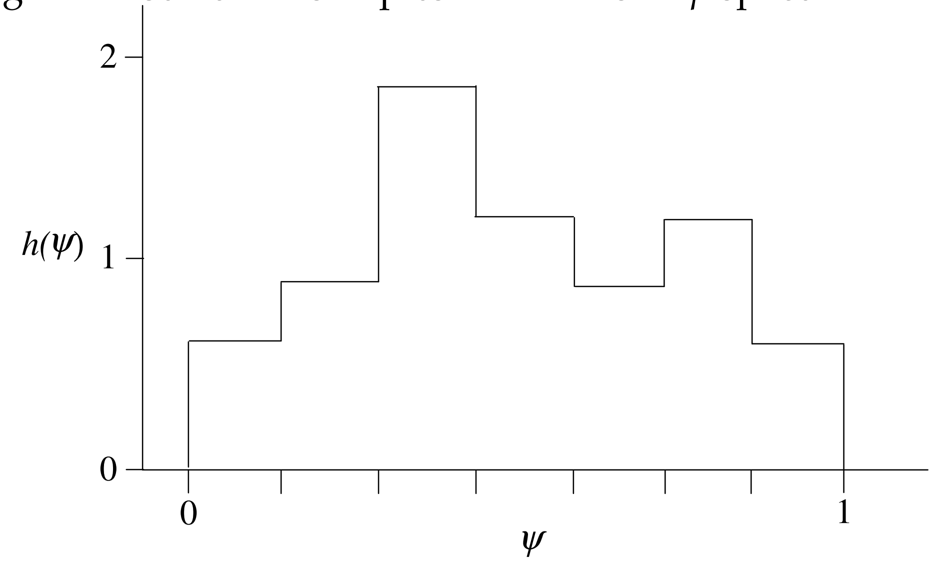
If we know the one-point, one-time composition probability density function (PDF) $f_{\boldsymbol{\phi}}(\boldsymbol{\psi}; \mathbf{x}, t)$, we can compute $\langle S_\alpha(\boldsymbol{\phi}) \rangle$!

For one scalar, $f_\phi(\psi; \mathbf{x}, t)$ can be approximated by a histogram of the subgrid-scale distribution of ϕ:



ψ_4
ψ_5
m
N_m
1
7
2
ψ_{15}
ψ_{14}
ψ_{16}
6
4
ψ_3
ψ_6
ψ_{13}
5
4
ψ_2
ψ_{17}
ψ_{24}
$\phi(x)$
ψ_1
4
4
ψ_{10}
ψ_{12}
ψ_7
ψ_{23}
ψ_{11}
3
5
ψ_{18}
ψ_{22}
ψ_9
2
3
ψ_8
ψ_{19}
1
2
0
0
ψ_{20}
ψ_{21}
L
x

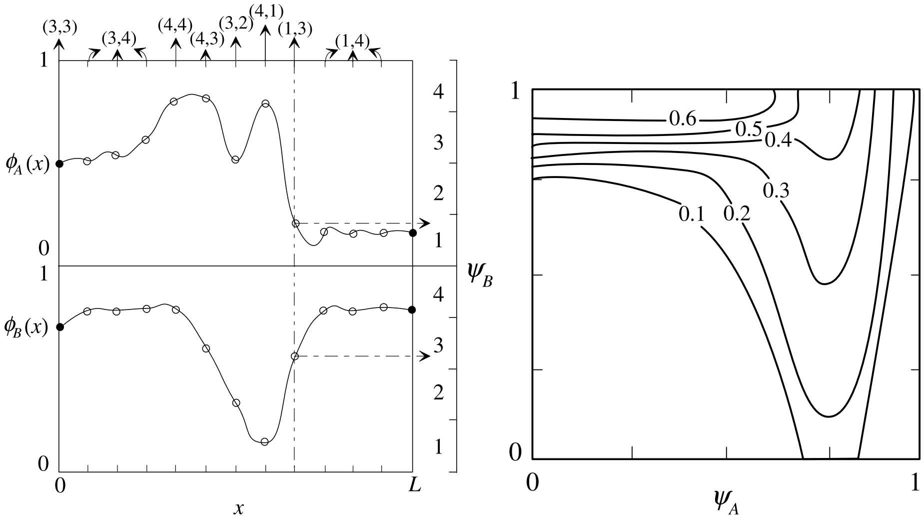
Sketch of histogram based on 24 samples and 7 bins in ϕ-space:



Taking a sufficiently large sample and small bins, the histogram converges to the PDF:

$$\lim_{N,M \to \infty} h(m\Delta) \to \hat{f}_{\phi}(\psi). \tag{1.5}$$

The same idea extends to two scalars ϕ_{A} and ϕ_{B}:



The bivariate PDF is represented by a contour plot

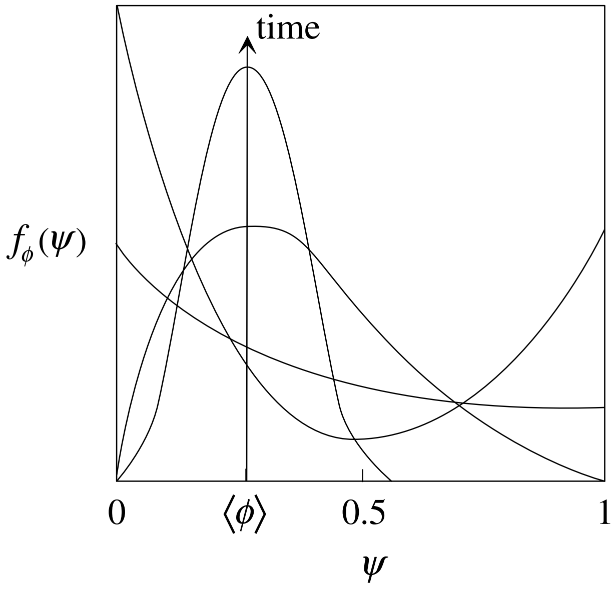
In summary, the statistical approach to turbulent mixing is based on finding appropriate models for the joint PDF (which can be directly measured experimentally)

Molecular Mixing

The one-point PDF approach introduces conditional quantities that must be modeled:

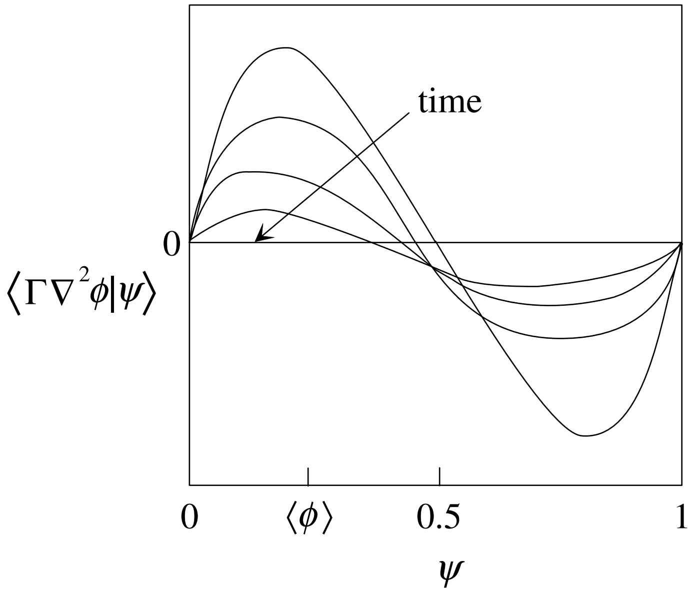
- Conditional diffusion: $\langle \Gamma \nabla^2 \phi | \psi \rangle$
- Conditional dissipation: $\langle \varepsilon_\phi | \psi \rangle = 2 \langle \Gamma \left| \nabla \phi \right|^2 | \psi \rangle$

The effect of molecular diffusion (micromixing) is to change the shape of the PDF:



Without diffusion ($\Gamma = 0$), $f_{\boldsymbol{\phi}}(\boldsymbol{\psi})$ will always be the same!

The effect of diffusion is contained explicitly in the conditional Laplacian:



$\langle \Gamma \nabla^2 \phi | \psi \rangle$ can be found from DNS

For example, the concentration in a Lagrangian fluid element is governed by

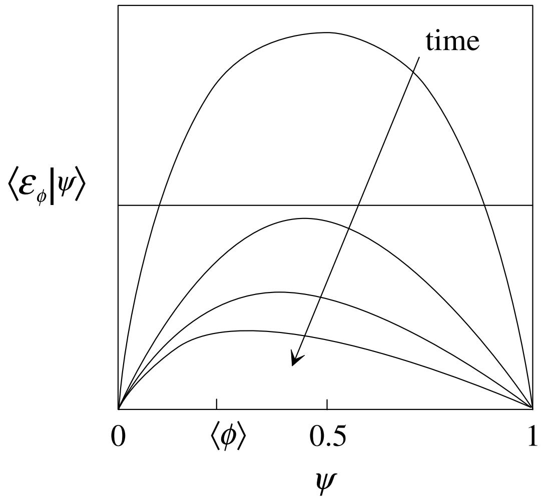
$$\frac{\mathrm{d}\phi_\alpha^*}{\mathrm{d}t} = \langle \Gamma_\alpha \nabla^2 \phi_\alpha | \boldsymbol{\phi} = \boldsymbol{\phi}^* \rangle + S_\alpha(\boldsymbol{\phi}^*) \tag{1.6}$$

A simple model for the conditional Laplacian is

$$\langle \Gamma_\alpha \nabla^2 \phi_\alpha | \boldsymbol{\phi} = \boldsymbol{\phi}^* \rangle = \frac{1}{\tau_\phi} \left(\langle \phi_\alpha \rangle - \phi_\alpha^* \right) \tag{1.7}$$

which is the interaction-by-exchange-with-the-mean (IEM) micromixing model

In other mixing models, the conditional scalar dissipation rate is needed:



$\langle \epsilon_\phi | \psi \rangle$ can be extracted from experiments or DNS to validate micromixing models

In summary, models for micromixing should be based on the underlying physics so that they can be validated experimentally or by using DNS

1.2 Turbulent Mixing

Basic question: If we introduce a "blob" of scalar with length scale l_ϕ into a fully-developed turbulent flow with Reynolds number Re_L and integral length scale L_u, how long will it take (on average) for ϕ to be completely mixed?

Length Scales of Turbulent Mixing

Integral scale:

Like velocity, a turbulent scalar field will have an integral length scale L_ϕ

In a transient mixing experiment, $L_\phi(t)$ depends on time: $L_\phi(0) = l_\phi$

However, due to turbulence advection, $L_\phi(t)$ will approach L_u on a time scale proportional to $\tau_u = k/\varepsilon$

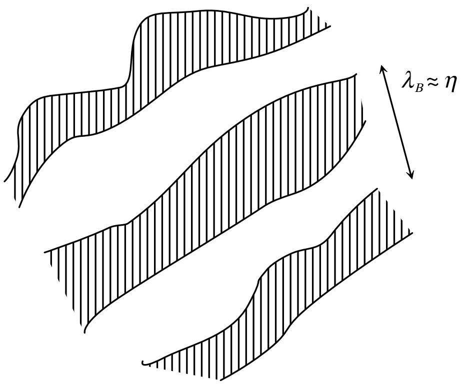
Batchelor scale:

For $\mathrm{Sc} = \nu/\Gamma > 1$, the Batchelor scale is defined by

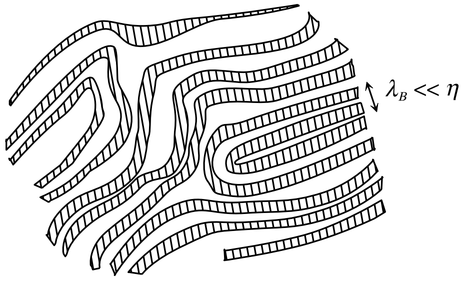
$$\lambda_B \equiv \mathrm{Sc}^{-1/2}\eta \tag{1.8}$$

λ_B is the characteristic length scale of the smallest diffusion layers in the scalar field

$\mathrm{Sc} = 1$



$\mathrm{Sc} \gg 1$



Scalar "eddies" of size λ_B *can be assumed to be completely micromixed*

Phenomenological Model for Turbulent Mixing

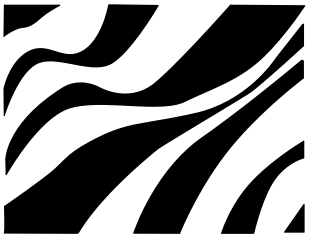
For $l_\phi \gg \lambda_B$, molecular diffusion is not effective and thus

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + U_i \frac{\partial \phi}{\partial x_i} = 0 \tag{1.9}$$

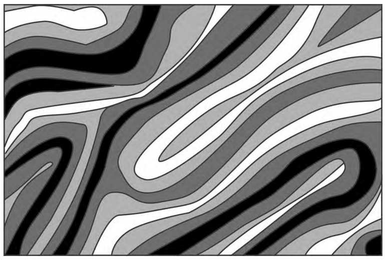
with initial conditions

$$\phi(\mathbf{x}, 0) = \begin{cases} 0 & \text{for } \mathbf{x} \in D \\ 1 & \text{for } \mathbf{x} \in D^c \end{cases} \tag{1.10}$$

Then for $t > 0$, the turbulence will reduce l_ϕ:



Until $t \gg 0$ where molecular diffusion starts to micromix the fluid:



Question: From turbulence theory, what is the rate $\gamma(l_\phi)$ at which l_ϕ decreases in size?

From spectral theory, convection rate through inertial range scales like $(\kappa\eta)^{2/3}$

We can use this rate for $l_\phi \geq \eta$:

$$\gamma(l_\phi) = \left(\frac{\varepsilon}{\nu}\right)^{1/2} \left(\frac{\eta}{l_\phi}\right)^{2/3} \quad \text{for} \quad \eta \leq l_\phi \leq L_u \tag{1.11}$$

For $l_\phi = L_u$, this yields

$$\gamma(L_u) = \frac{\varepsilon}{k} \tag{1.12}$$

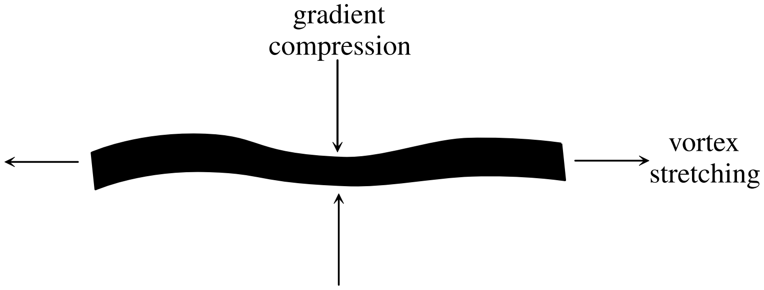
and for $l_\phi = \eta$

$$\gamma(\eta) = \left(\frac{\varepsilon}{\nu}\right)^{1/2} = \mathrm{Re}_L^{1/2}\gamma(L_u) \tag{1.13}$$

Thus, mixing rate increases greatly as scalar size decreases

Initial length scale fixes the rate-determining (slowest) step!

For $l_\phi < \eta$, vortex stretching reduces eddy size at a constant rate:



thus

$$\gamma(l_\phi) = \left(\frac{\varepsilon}{\nu}\right)^{1/2} \quad \text{for} \quad l_\phi \le \eta \tag{1.14}$$

Simple phenomenological model for mixing:

$$\frac{\mathrm{d}l_\phi}{\mathrm{d}t} = -\gamma(l_\phi)l_\phi \tag{1.15}$$

with $l_\phi(0) = L_\phi > \eta$

The total mixing time can be approximated by $l_\phi(t_{\text{mix}}) = \eta$:

$$t_{\text{mix}} \approx \frac{3}{2}\left(\frac{L_\phi}{L_u}\right)^{2/3}\tau_u + \frac{1}{2}\ln(\text{Sc})\tau_\eta \tag{1.16}$$

Remarks:

(a) Unless $\text{Sc} \gg 1$, the second term will be negligible for large Re

(b) The ratio L_ϕ:L_u (scalar-to-velocity integral-scale ratio) is a key parameter in scalar mixing

(c) If the scalar eddies are initially generated by turbulent velocity fluctuations acting on a mean scalar gradient, then $L_\phi \approx L_u$ and $t_{\mathrm{mix}} \approx \tau_u$ is determined entirely by the turbulent flow

(d) Model assumes fully developed high-Reynolds-number turbulence: A more accurate estimate can be found from the scalar spectrum as functions of $\mathrm{Re}_L = k^2/\nu\varepsilon$ and Sc

Scalar mixing time is more complicated to model than turbulence time scales (L_ϕ:$L_u \neq 1$, large Sc, *low* Re, *etc.)*

1.3 Statistical Description of Turbulent Mixing

Emphasis will be on how to describe scalar statistics and on how length and time scales change with Reynolds and Schmidt numbers

One-Point Velocity, Composition PDF

General theory starts with joint PDF:

$$f_{\mathbf{U},\phi}(\mathbf{V},\psi;\mathbf{x},t)\,\mathrm{d}\mathbf{V}\,\mathrm{d}\psi \equiv \mathrm{P}[\{\mathbf{V} \le \mathbf{U}(\mathbf{x},t) < \mathbf{V}+\mathrm{d}\mathbf{V}\} \cap \{\psi \le \phi(\mathbf{x},t) < \psi+\mathrm{d}\psi\}] \quad (1.17)$$

Composition PDF is defined by

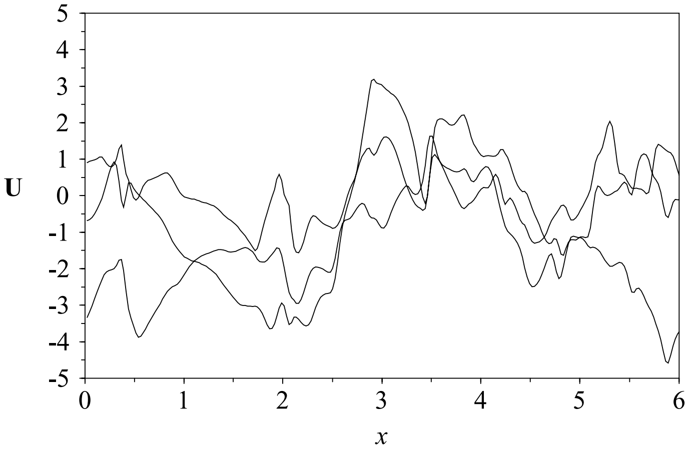
$$f_{\phi}(\psi;\mathbf{x},t)\,\mathrm{d}\psi \equiv \mathrm{P}[\psi \le \phi(\mathbf{x},t) < \psi+\mathrm{d}\psi] \quad (1.18)$$

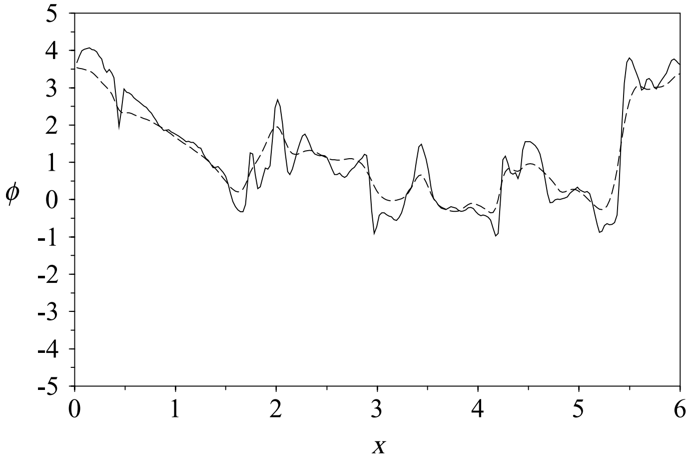
and be found by integrating out the velocity:

$$f_\phi(\psi;\mathbf{x},t) = \iiint\limits_{-\infty}^{+\infty} f_{\mathbf{U},\phi}(\mathbf{V},\psi;\mathbf{x},t)\,\mathrm{d}\mathbf{V} \tag{1.19}$$

Velocity and scalar statistics can be studied using direct-numerical simulation (DNS)

$\mathbf{U}(\mathbf{x}, t^*)$ and $\boldsymbol{\phi}(\mathbf{x}, t^*)$ as functions of $x = x_1$ with fixed $t = t^*$:

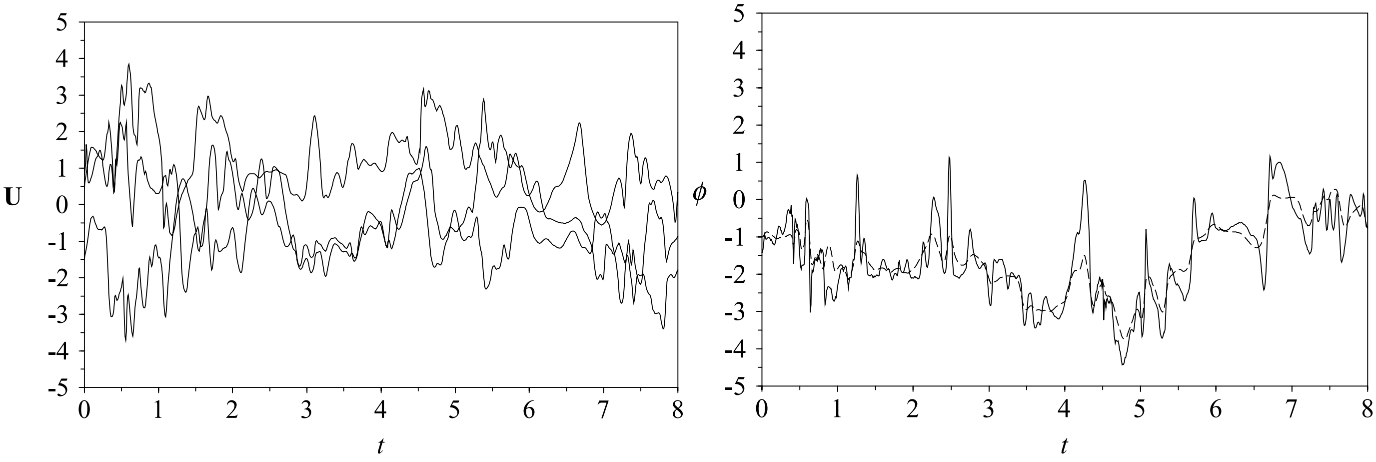




Dashed line: $\mathrm{Sc} = 1/8$ Solid Line: $\mathrm{Sc} = 1$

Low Sc *line is "smoother"* $\Rightarrow$ *Batchelor scale is larger*

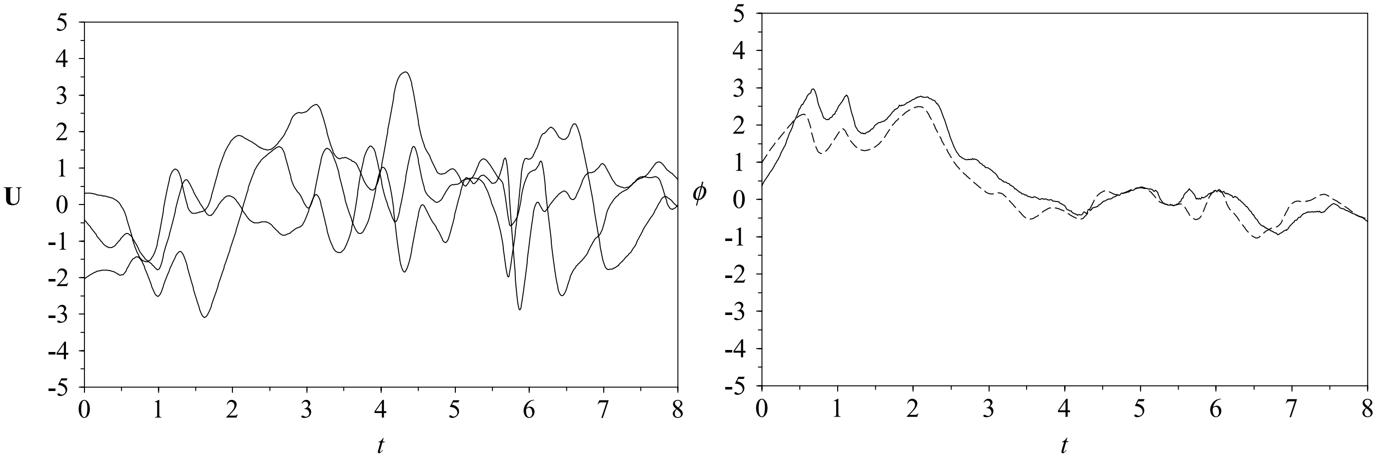
$\mathbf{U}(\mathbf{x}^*, t)$ and $\boldsymbol{\phi}(\mathbf{x}^*, t)$ as functions of t with fixed $\mathbf{x} = \mathbf{x}^*$:



Dashed line: $\mathrm{Sc} = 1/8$ Solid Line: $\mathrm{Sc} = 1$

Low Sc *line is "smoother"* $\Rightarrow$ *Eulerian time scale is larger*

Lagrangian velocity $\mathbf{U}^{+}(t)$ and scalars $\boldsymbol{\phi}^{+}(t)$ as functions of t:



Dashed line: $\mathrm{Sc} = 1/8$ Solid Line: $\mathrm{Sc} = 1$

Low Sc *line is "smoother"* $\Rightarrow$ *Lagrangian time scale is larger*

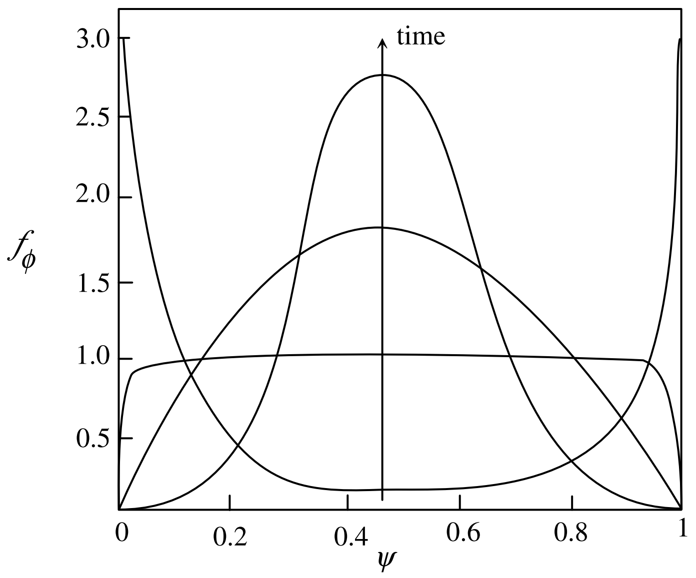
Nonpremixed composition PDF $f_\phi(\psi;t)$ starts from

$$f_\phi(\psi;0) = p_0\delta(\psi) + p_1\delta(\psi-1) \tag{1.20}$$

with mean value:

$$\langle\phi(\mathbf{x},0)\rangle = \int_{-\infty}^{+\infty} \psi f_\phi(\psi;0)\,\mathrm{d}\psi = p_1 \tag{1.21}$$

Due to molecular mixing, the variance decreases with time:



where the variance is defined by

$$\langle \phi'^2(\mathbf{x}, t) \rangle \equiv \int_{-\infty}^{+\infty} (\psi - \langle \phi \rangle)^2 f_\phi(\psi; t) \, \mathrm{d}\psi \tag{1.22}$$

At $t = \infty$, PDF is a delta function:

$$f_\phi(\psi;\infty) = \delta(\psi - p_1) \tag{1.23}$$

The micromixing model determines both the rate of variance decay and the shape of the PDF at each instant

We will see later how to write a transport equation for the PDF

Conditional Velocity and Scalar Statistics

Conditional statistics are used often in PDF methods (e.g., the micromixing model)

Example: scalar-conditioned velocity fluctuations (scalar dispersion)

$$\langle \mathbf{u} | \boldsymbol{\psi} \rangle \equiv \langle \mathbf{U} | \boldsymbol{\phi} = \boldsymbol{\psi} \rangle - \langle \mathbf{U} \rangle \tag{1.24}$$

Computed using the conditional PDF of velocity given scalar:

$$f_{\mathbf{U}|\boldsymbol{\phi}}(\mathbf{V}|\boldsymbol{\psi};\mathbf{x},t) \equiv \frac{f_{\mathbf{U},\boldsymbol{\phi}}(\mathbf{V},\boldsymbol{\psi};\mathbf{x},t)}{f_{\boldsymbol{\phi}}(\boldsymbol{\psi};\mathbf{x},t)} \tag{1.25}$$

$$\langle \mathbf{U}(\mathbf{x},t) | \boldsymbol{\psi} \rangle \equiv \iiint\limits_{-\infty}^{+\infty} \mathbf{V} f_{\mathbf{U}|\boldsymbol{\phi}}(\mathbf{V}|\boldsymbol{\psi};\mathbf{x},t) \, \mathrm{d}\mathbf{V} \tag{1.26}$$

Example: Conditional scalar dissipation rate (CSDR) of mixture fraction

$$\langle \epsilon_{\xi} | \zeta \rangle \equiv \left\langle 2\Gamma \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right| \xi = \zeta \right\rangle$$

This function is needed to close the mixing term in PDF models

Scalar dissipation is a random field:

$$\epsilon_\xi(\mathbf{x},t) \equiv 2\Gamma \frac{\partial \xi}{\partial x_i}\frac{\partial \xi}{\partial x_i} \tag{1.27}$$

so one-point joint PDF is defined by

$$f_{\epsilon_\xi,\xi}(z,\zeta;\mathbf{x},t)\,\mathrm{d}z\,\mathrm{d}\zeta \equiv \mathrm{P}[\{z \leq \epsilon_\xi(\mathbf{x},t) < z+\mathrm{d}z\} \cap \{\zeta \leq \xi(\mathbf{x},t) < \zeta+\mathrm{d}\zeta\}] \tag{1.28}$$

CSDR defined by

$$\langle \epsilon_\xi | \zeta \rangle \equiv \int_{-\infty}^{+\infty} z f_{\epsilon_\xi|\xi}(z|\zeta;\mathbf{x},t)\,\mathrm{d}z = \int_{-\infty}^{+\infty} z \frac{f_{\epsilon_\xi,\xi}(z,\zeta;\mathbf{x},t)}{f_\xi(\zeta;\mathbf{x},t)}\,\mathrm{d}z \tag{1.29}$$

This is needed in conditional moment closure (CMC) to model micromixing

Scalar Energy Spectrum (2-point statistic)

Scalar variance:

$$\langle \phi'^2 \rangle (t) = \int_0^\infty E_\phi(\kappa, t)\, \mathrm{d}\kappa \tag{1.30}$$

Scalar dissipation rate:

$$\varepsilon_\phi(t) = \int_0^\infty 2\Gamma \kappa^2 E_\phi(\kappa, t)\, \mathrm{d}\kappa = \int_0^\infty D_\phi(\kappa, t)\, \mathrm{d}\kappa \tag{1.31}$$

Scalar mixing time:

$$\tau_\phi(t) \equiv \frac{2\langle \phi'^2 \rangle}{\varepsilon_\phi} \tag{1.32}$$

Need expression for τ_ϕ as part of micromixing model

Model for Fully-Developed Scalar Spectrum

Model scalar spectrum for $E_\phi(\kappa)$ (*time independent*) can be used to determine effects of Re_L and Sc on equilibrium scalar mixing $\Rightarrow$ equilibrium model for τ_ϕ

However, must account for differences when $\mathrm{Sc} \ll 1$ and $\mathrm{Sc} \gg 1$

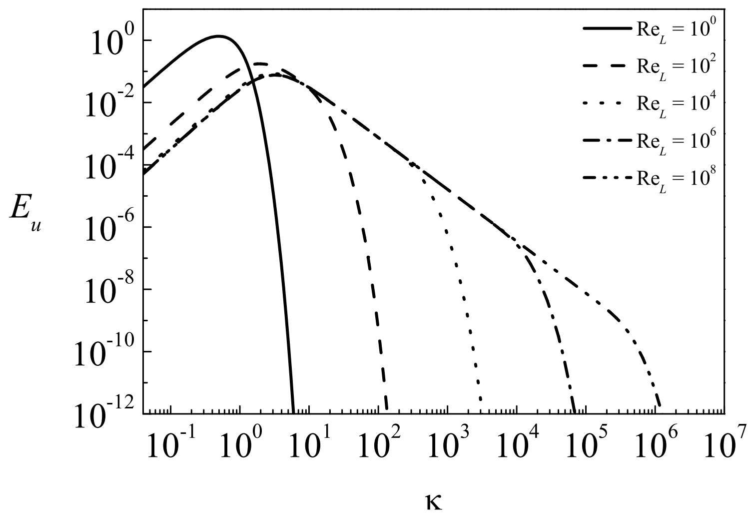
For $\mathrm{Sc} \ll 1$, two scalar dissipation wavenumbers can be defined:

$$\kappa_{c1} \equiv \mathrm{Sc}^{3/4} \kappa_{DI} \tag{1.33}$$

$$\kappa_{c2} \equiv \mathrm{Sc}^{3/4} \kappa_{\eta} \tag{1.34}$$

where κ_{DI} and κ_η are from turbulence energy spectrum (see Pope (2000) *Turbulent Flows*)

Model turbulence energy spectrum: (Pope 2000)



Extend this "correlation" to the scalar spectrum to account for Sc

Model scalar energy spectrum: (Fox 2003)

$$E_{\phi}(\kappa) = C_{OC}\varepsilon_{\phi}\varepsilon^{-3/4}\nu^{5/4}(\kappa\eta)^{-\beta(\kappa\eta)} f_L(\kappa L_u) f_B(\kappa\eta) \tag{1.35}$$

with exponent

$$\beta(\kappa\eta) \equiv 1 + \frac{2}{3}\left[7 - 6 f_D(\kappa\eta)\right] f_{\eta}(\kappa\eta) \tag{1.36}$$

where the cut-off functions f_L, f_{η}, f_D and f_B determine the sub-ranges

Diffusion-scale exponent cut off:

$$f_D(\kappa\eta) \equiv \left(1 + c_D \mathrm{Sc}^{-d(\kappa\eta)/2}\kappa\eta\right) \exp\left(-c_D \mathrm{Sc}^{-d(\kappa\eta)/2}\kappa\eta\right) \tag{1.37}$$

with $c_D = 2.59$ (fit to DNS) and

$$d(\kappa\eta) \equiv \frac{1}{2} + \frac{1}{4} f_{\eta}(\kappa\eta) \tag{1.38}$$

Batchelor-scale cut off:

$$f_B(\kappa\eta) \equiv \left(1 + c_d \mathrm{Sc}^{-d(\kappa\eta)}\kappa\eta\right) \exp\left(-c_d \mathrm{Sc}^{-d(\kappa\eta)}\kappa\eta\right) \tag{1.39}$$

Scalar-dissipation constant c_d is found by forcing

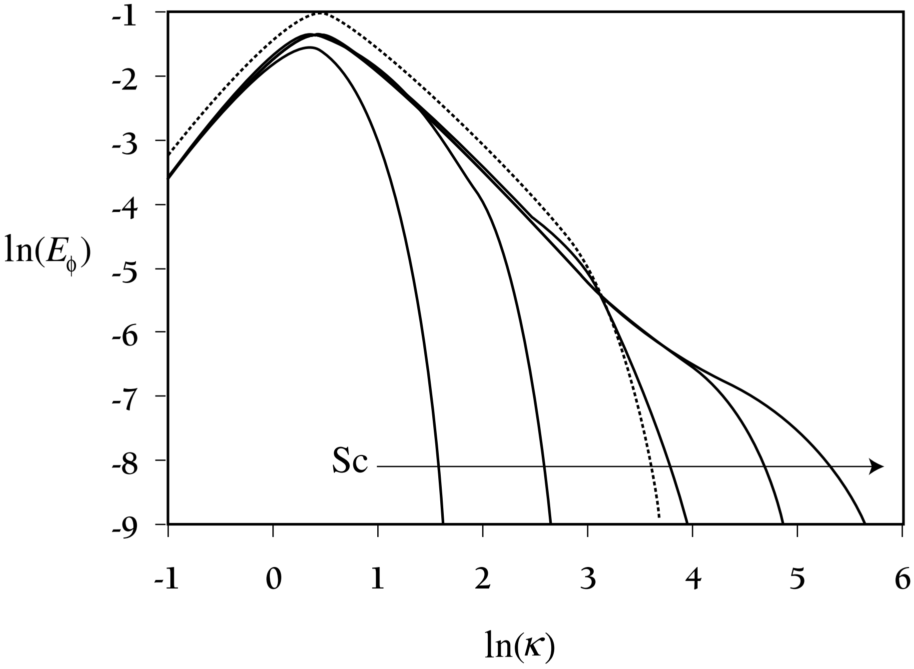
$$\varepsilon_\phi = \int_0^\infty 2\Gamma\kappa^2 E_\phi(\kappa)\,\mathrm{d}\kappa \tag{1.40}$$

or

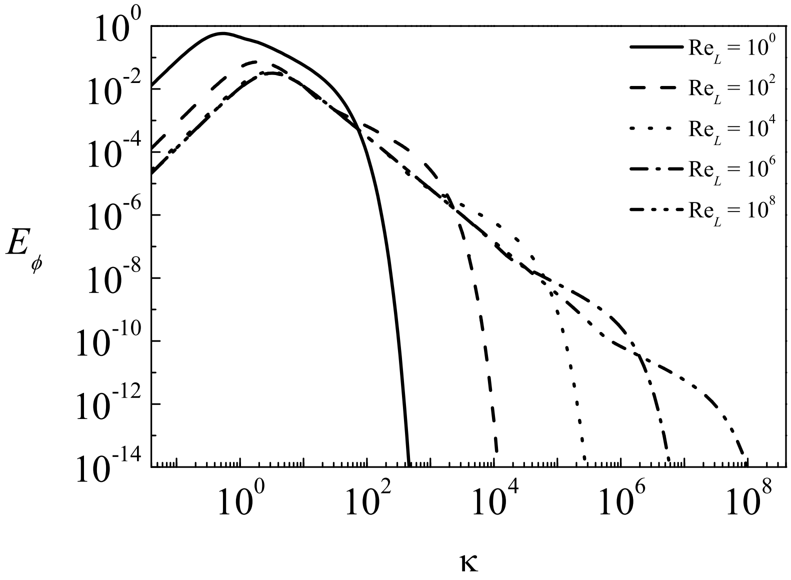
$$\int_0^\infty (\kappa\eta)^{2-\beta(\kappa\eta)} f_L(\kappa L_u) f_B(\kappa\eta)\,\mathrm{d}(\kappa\eta) = \frac{\mathrm{Sc}}{2C_{OC}} \tag{1.41}$$

For $\mathrm{Sc} > 1$, $c_d \approx 2$ for all values of Re_L

Model spectra for $R_\lambda = 500$ and $\mathrm{Sc} = 10^{-4}$ to $\mathrm{Sc} = 10^{4}$ in powers of 10^{2}:



Model spectra for $\mathrm{Sc} = 1000$:



1.4 Equilibrium Models for Scalar Mixing

Scalar-Variance Transport Equation

In order to account for micromixing in inhomogeneous flows, we need to compute the scalar variance

The RANS scalar-variance transport equation is

$$\frac{\partial \langle \phi'^2 \rangle}{\partial t} + \langle U_i \rangle \frac{\partial \langle \phi'^2 \rangle}{\partial x_i} + \frac{\partial \langle u_i \phi'^2 \rangle}{\partial x_i} = \Gamma \nabla^2 \langle \phi'^2 \rangle + \mathcal{P}_\phi - \varepsilon_\phi \tag{1.42}$$

where the production term is closed (assuming scalar flux is known)

The scalar-variance flux can be modeled by

$$\langle u_i \phi'^2 \rangle = -\Gamma_T \frac{\partial \langle \phi'^2 \rangle}{\partial x_i} \tag{1.43}$$

or (in the RSM context) by

$$\langle u_i \phi'^2 \rangle = -\frac{k}{\mathrm{Sc}_T \varepsilon} \langle u_i u_j \rangle \frac{\partial \langle \phi'^2 \rangle}{\partial x_j} \tag{1.44}$$

The SDR rate is usually modeled by the "equilibrium" model:

$$\varepsilon_\phi = C_\phi \frac{\varepsilon}{k} \langle \phi'^2 \rangle \tag{1.45}$$

with $C_\phi \approx 2$ (independent of Re and Sc)

Extended-Equilibrium Model for Scalar Dissipation

Many "practical" flows are not at high Reynolds

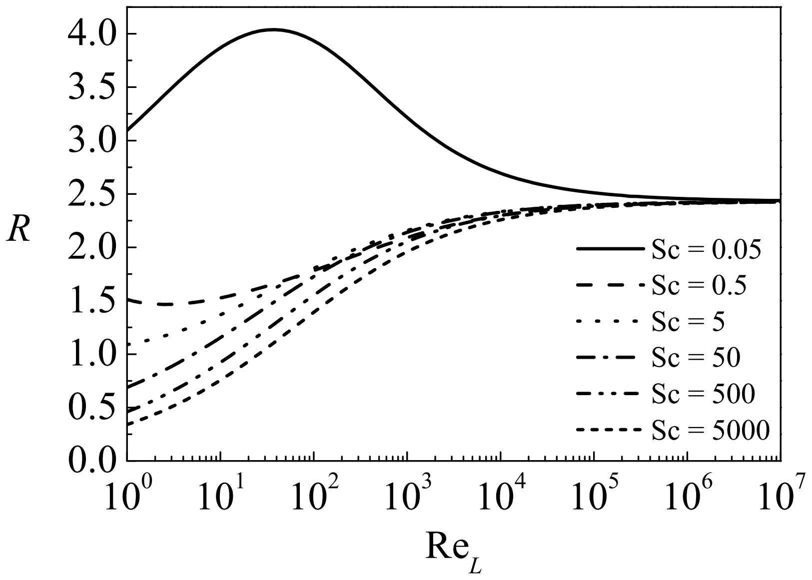
Following Corrsin (1964), we can use the model spectrum to compute Re and Sc dependence:

$$\varepsilon_\phi = C_\phi(\mathrm{Re}, \mathrm{Sc}) \frac{\varepsilon}{k} \langle \phi'^2 \rangle \tag{1.46}$$

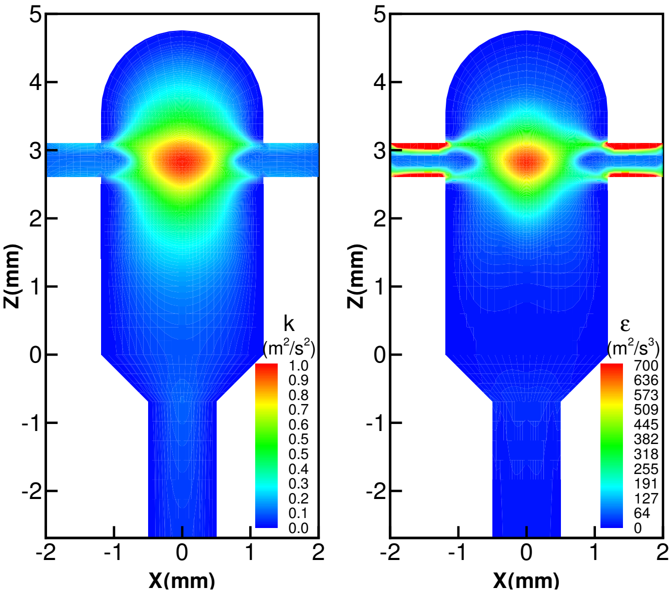
Local k and ε (and hence Re) found from turbulence model

Accounts for ***local*** *low-Reynolds-number effects that are common in many applications*

Mechanical-to-scalar time-scale ratio: $R = C_\phi(\mathrm{Re}_L, \mathrm{Sc})$

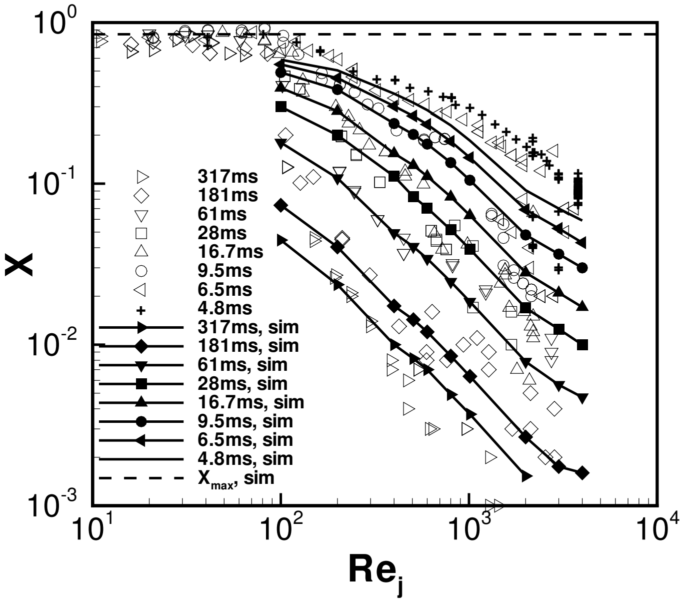


Example: Impinging-jet microreactor: Sc = 1000



Local values: $1 < \text{Re}_L < 100 \Rightarrow$ high Re model invalid

Comparison with experiments:



Reaction conversion X versus inlet jet Re

Summary: Small-scale equilibrium models assume that scalar spectrum is fully developed for a given set of large-scale flow statistics

Non-equilibrium models attempt to capture the evolution of the scalar spectrum starting from arbitrary initial conditions

Note: In both cases, models provide rate of mixing (not shape of PDF)

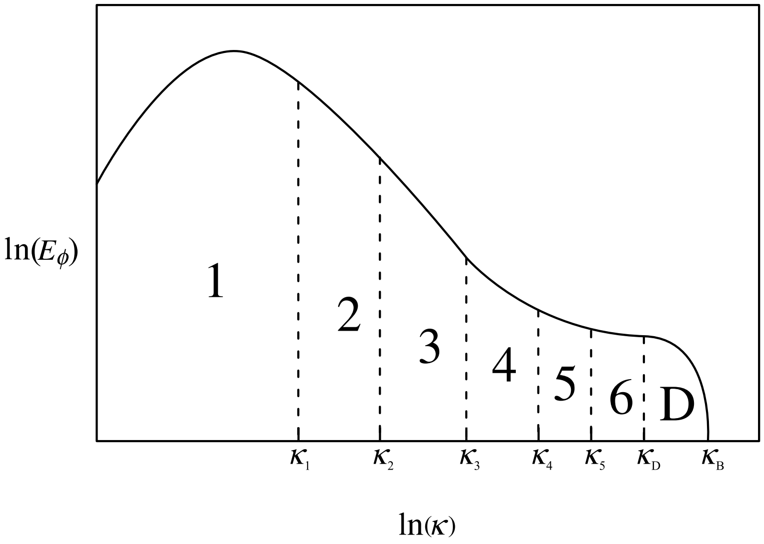
Chapter 2

Non-Equilibrium Models

2.1 Non-Equilibrium Models for Scalar Dissipation

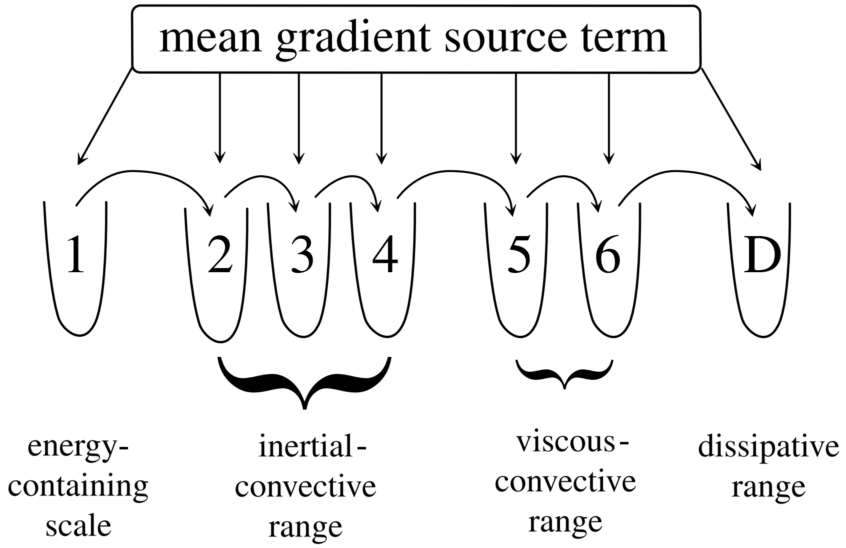
To account for initial conditions where the scalar spectrum is not in equilibrium with the velocity spectrum, a multi-scale model is needed

For a given Sc and Re_L, we can divide the scalar equilibrium spectrum into a finite set of wavenumber bands:



I.e., a highly simplified spectral model

We can then model the scalar variance in each range as a dynamic model with a source term due to mean gradients and dissipation



Spectral Relaxation Model (Fox 1995, 1997, 1999, 2003)

Example: $\mathrm{Sc} = 1$ and $\mathrm{Re}_\lambda = 90$

The cut-off wavenumbers are defined by

$$\kappa_0 \equiv 0 \tag{2.1}$$

$$\kappa_1 \equiv \mathrm{Re}_1^{-3/2} \kappa_\eta \tag{2.2}$$

$$\kappa_2 \equiv \left(\frac{3}{C_u \mathrm{Re}_1 + 2} \right)^{3/2} \kappa_u \tag{2.3}$$

$$\kappa_3 \equiv \mathrm{Sc}^{1/2} \kappa_u \tag{2.4}$$

where

$$\kappa_\eta \equiv \frac{1}{\eta} = \frac{\mathrm{Re}_1^{3/2}}{L_u} \tag{2.5}$$

and

$$\kappa_u \equiv C_u^{3/2} \kappa_\eta \tag{2.6}$$

with $C_u = (0.1)^{2/3} = 0.2154$

The scalar dissipation range starts at

$$\kappa_D \equiv \kappa_3 = \mathrm{Sc}^{1/2} \kappa_u \tag{2.7}$$

The scalar energy in each range is defined by

$$\langle \phi'^2 \rangle_n(t) \equiv \int_{\kappa_{n-1}}^{\kappa_n} E_\phi(\kappa, t)\, \mathrm{d}\kappa \tag{2.8}$$

These are modeled by ODEs with spectral transport, production, and dissipation:

$$\frac{\mathrm{d}\langle\phi'^2\rangle_1}{\mathrm{d}t} = \mathcal{T}_1 + \gamma_1\mathcal{P}_\phi \tag{2.9}$$

$$\frac{\mathrm{d}\langle\phi'^2\rangle_2}{\mathrm{d}t} = \mathcal{T}_2 + \gamma_2\mathcal{P}_\phi \tag{2.10}$$

$$\frac{\mathrm{d}\langle\phi'^2\rangle_3}{\mathrm{d}t} = \mathcal{T}_3 + \gamma_3\mathcal{P}_\phi \tag{2.11}$$

and

$$\frac{\mathrm{d}\langle\phi'^2\rangle_D}{\mathrm{d}t} = \mathcal{T}_D + \gamma_D\mathcal{P}_\phi - \varepsilon_\phi \tag{2.12}$$

The variance-production term $\mathcal{P}_\phi$ is known

The scalar variance is found by summing over all bands:

$$\langle \phi'^2 \rangle = \sum_{n=1}^{3} \langle \phi'^2 \rangle_n + \langle \phi'^2 \rangle_D \tag{2.13}$$

The sum of the transport is null, so that

$$\frac{\mathrm{d}\langle \phi'^2 \rangle}{\mathrm{d}t} = \mathcal{P}_\phi - \varepsilon_\phi \tag{2.14}$$

The model is closed by a small-scale equation for the SDR:

$$\frac{\mathrm{d}\varepsilon_\phi}{\mathrm{d}t} = \gamma_D \mathcal{P}_\phi \frac{\varepsilon_\phi}{\langle \phi'^2 \rangle_D} + C_D \left(\frac{\varepsilon}{\nu}\right)^{1/2} \mathcal{T}_\varepsilon + C_s \left(\frac{\varepsilon}{\nu}\right)^{1/2} \varepsilon_\phi - C_d \frac{\varepsilon_\phi}{\langle \phi'^2 \rangle_D} \varepsilon_\phi \tag{2.15}$$

where

$$C_D \equiv 2\Gamma \kappa_D^2 \left(\frac{\nu}{\varepsilon}\right)^{1/2} = 0.02 \tag{2.16}$$

Note that the right-hand side scales like $\mathrm{Re}_1 = k/(\varepsilon\nu)^{1/2}$

Spectral Transfer Rates

The spectral transfer rates determine the dynamics of the model

Based on DNS, the rates are assumed to be local: $\mathcal{T}_n(\langle \phi'^2 \rangle_{n-1}, \langle \phi'^2 \rangle_n, \langle \phi'^2 \rangle_{n+1})$

$$\mathcal{T}_1 = -(\alpha_{12} + \beta_{12})\langle \phi'^2 \rangle_1 + \beta_{21}\langle \phi'^2 \rangle_2 \tag{2.17}$$

$$\mathcal{T}_2 = (\alpha_{12} + \beta_{12})\langle \phi'^2 \rangle_1 - (\alpha_{23} + \beta_{23})\langle \phi'^2 \rangle_2 - \beta_{21}\langle \phi'^2 \rangle_2 + \beta_{32}\langle \phi'^2 \rangle_3 \tag{2.18}$$

$$\mathcal{T}_3 = (\alpha_{23} + \beta_{23})\langle \phi'^2 \rangle_2 - (\alpha_{3D} + \beta_{3D})\langle \phi'^2 \rangle_3 - \beta_{32}\langle \phi'^2 \rangle_3 + \beta_{D3}\langle \phi'^2 \rangle_D \tag{2.19}$$

$$\mathcal{T}_D = (\alpha_{3D} + \beta_{3D})\langle \phi'^2 \rangle_3 - \beta_{D3}\langle \phi'^2 \rangle_D \tag{2.20}$$

$$\mathcal{T}_\varepsilon = (\alpha_{3D} + \beta_{3D})\langle \phi'^2 \rangle_3 - \beta_\varepsilon \varepsilon_\phi \tag{2.21}$$

The forward-transfer parameters are fit to a fully developed velocity energy spectrum:

$$\alpha_{12} = R_0 \frac{\varepsilon}{k} \qquad \alpha_{23} = \frac{\alpha_{12}}{a} \qquad \alpha_{3D} = \frac{2C_u \mathrm{Re}_1 \alpha_{12}}{aC_u \mathrm{Re}_1 + 3(1 - \mathrm{Sc}^{-1/3})} \tag{2.22}$$

$$\beta_{12} = c_b \alpha_{12} \qquad \beta_{23} = c_b \alpha_{23} \qquad \beta_{3D} = c_b \alpha_{3D} \tag{2.23}$$

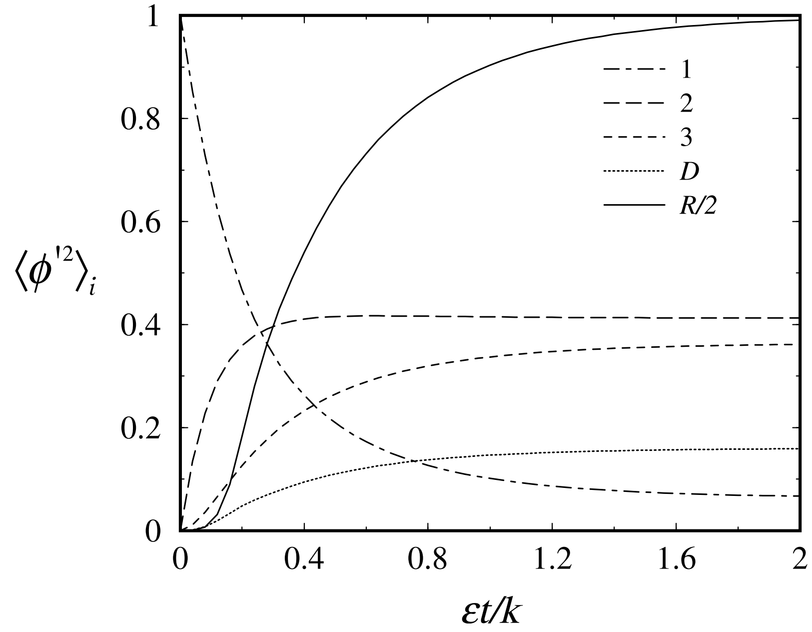
The backscatter parameters are fit to yield an equilibrium spectrum independent of c_b:

$$\beta_{21} = c_b(\alpha_{23} - \alpha_{12}) \qquad \beta_{32} = c_b(\alpha_{3D} - \alpha_{12}) \tag{2.24}$$

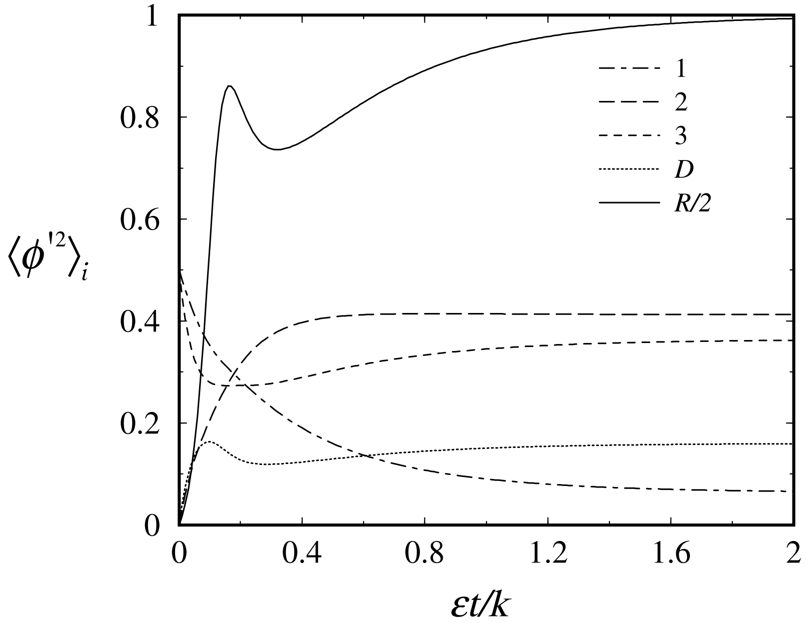
$$\beta_{D3} = c_b \alpha_{12} \mathrm{Sc}^{1/2}(1 - b)/b \qquad \beta_{\varepsilon} = c_b \mathrm{Sc}^{1/2}(1 - b) \tag{2.25}$$

The time evolution of $\langle \phi'^2 \rangle_n$ and mechanical-to-scalar time-scale ratio R depends on the initial scalar spectrum

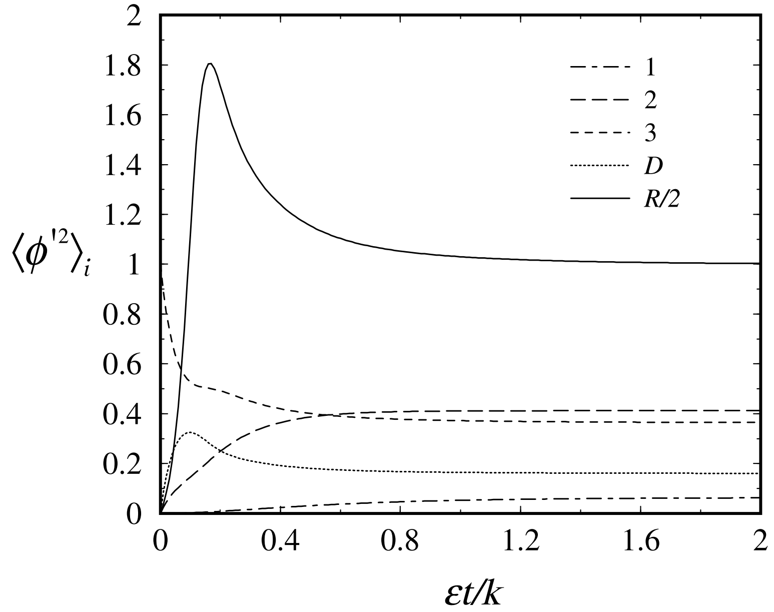
Example 1: $\langle\phi'^2\rangle_1 = 1$ and others $\langle\phi'^2\rangle_n = 0$ (all scalar energy in largest scales): micromixing is slower than equilibrium rate



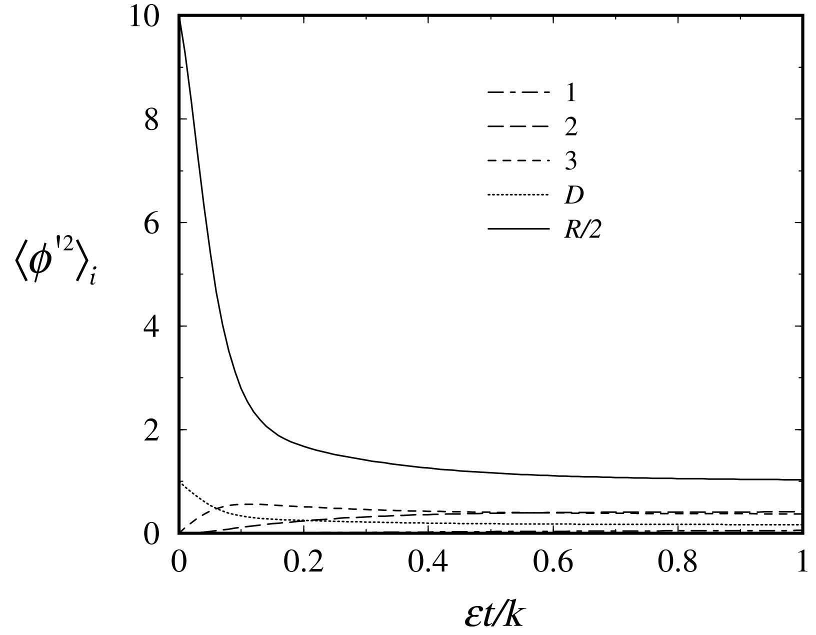
Example 2: $\langle \phi'^2 \rangle_1 = 1/2$, $\langle \phi'^2 \rangle_3 = 1/2$ and others $\langle \phi'^2 \rangle_n = 0$ (two length scales): micromixing rate is complicated



Example 3: $\langle\phi'^2\rangle_3 = 1$ and others $\langle\phi'^2\rangle_n = 0$ (all energy at small length scales): micromixing rate overshoots equilibrium



Example 4: $\langle \phi'^2 \rangle_D = 1$ and others $\langle \phi'^2 \rangle_n = 0$ (all energy at dissipation scales): micromixing rate higher than equilibrium



2.2 Differential Diffusion

Basic question: How do covariance and joint scalar dissipation rate depend on $\Gamma_\alpha \neq \Gamma_\beta$ for large Re?

For example, in combustion H_2 and small MW free radicals diffuse much faster than hydrocarbons

How does $\Gamma_\alpha \ll \Gamma_\beta$ change the structure of a turbulent diffusion flame?

This question cannot be answered without chemistry, so we will look at an easier problem of two inert scalars in homogeneous turbulence

First, since molecular diffusivity only has a *direct* effect on the dissipation range, we define a scalar-gradient correlation coefficient:

$$g_{\alpha\beta} \equiv \frac{\langle (\nabla \phi'_{\alpha}) \cdot (\nabla \phi'_{\beta}) \rangle}{\sqrt{\langle |\nabla \phi'_{\alpha}|^2 \rangle \langle |\nabla \phi'_{\beta}|^2 \rangle}} = \frac{\varepsilon_{\alpha\beta}}{\sqrt{\varepsilon_{\alpha\alpha}\varepsilon_{\beta\beta}}} \tag{2.26}$$

If scalar fields are correlated at the dissipative scales, $g_{\alpha\beta} = 1$

This occurs when initially $\langle \phi_{\alpha} \rangle = \langle \phi_{\beta} \rangle$ and $\Gamma_{\alpha} = \Gamma_{\beta}$

Differential diffusion will have an *indirect* effect on the energy-containing scales, which is measured by the scalar correlation coefficient:

$$\rho_{\alpha\beta} \equiv \frac{\langle \phi'_{\alpha} \phi'_{\beta} \rangle}{\sqrt{\langle \phi'^2_{\alpha} \rangle \langle \phi'^2_{\beta} \rangle}} \tag{2.27}$$

This is the correlation coefficient that can be measured experimentally

We would like to estimate the dependence of $\rho_{\alpha\beta}$ and $g_{\alpha\beta}$ on Re_L for turbulent mixing with and without mean scalar gradients

Homogeneous Turbulence

In stationary, homogeneous turbulence (i.e., $E_u(\kappa)$ is time independent), the scalar covariance and joint scalar dissipation rate reduce to

$$\frac{\mathrm{d}\langle \phi'_{\alpha}\phi'_{\beta}\rangle}{\mathrm{d}t} = -\langle u_i\phi_\alpha\rangle G_{i\beta} - \langle u_i\phi_\beta\rangle G_{i\alpha} - \gamma_{\alpha\beta}\varepsilon_{\alpha\beta} \tag{2.28}$$

and

$$\frac{\mathrm{d}\varepsilon_{\alpha\beta}}{\mathrm{d}t} = C_B \left(\frac{\epsilon}{\nu}\right)^{1/2} \varepsilon_{\alpha\beta} - C_d \gamma_{\alpha\beta} \frac{\varepsilon_{\alpha\beta}}{\langle {\phi'}_{\alpha} {\phi'}_{\beta} \rangle_D} \varepsilon_{\alpha\beta} \tag{2.29}$$

where

$$G_{i\alpha} \equiv \frac{\partial \langle \phi_\alpha \rangle}{\partial x_i} \tag{2.30}$$

are uniform (i.e., constant) scalar gradients

Although in DNS data sets $G_{i\alpha}$ and $G_{i\beta}$ are usually aligned in the same direction, they need no be so (e.g., they could be orthogonal)

Observing these equations, we see that the only effect of differential diffusion comes from

$$\gamma_{\alpha\beta} \equiv \frac{\Gamma_\alpha + \Gamma_\beta}{2\sqrt{\Gamma_\alpha \Gamma_\beta}} = \frac{1}{2}\left(\frac{\Gamma_\alpha}{\Gamma_\beta}\right)^{1/2} + \frac{1}{2}\left(\frac{\Gamma_\beta}{\Gamma_\alpha}\right)^{1/2} \tag{2.31}$$

which takes on values $1 \leq \gamma_{\alpha\beta}$

In limiting case of $\Gamma_\alpha = \Gamma_\beta$, $\gamma_{\alpha\beta} = 1$

We need a model for the scalar flux (gradient diffusion):

$$\langle u_i \phi_\alpha \rangle = -\Gamma_T G_{i\alpha} \tag{2.32}$$

where Γ_T is turbulent diffusivity (independent of molecular Sc)

We also need a model for the covariance in the dissipation range ($\mathrm{Re}_1^{-1} \equiv \mathrm{Re}_L^{-1/2}$):

$$\langle \phi'_\alpha \phi'_\beta \rangle_D = \frac{C_{\alpha\beta}}{\mathrm{Re}_1} \langle \phi'_\alpha \phi'_\beta \rangle \tag{2.33}$$

where $C_{\alpha\beta}$ has weak dependence on Sc but becomes constant at high Re_1 (shown using DNS)

The governing equations then reduce to

$$\frac{\mathrm{d}\langle \phi'_\alpha \phi'_\beta \rangle}{\mathrm{d}t} = 2\Gamma_T G_{i\alpha} G_{i\beta} - \gamma_{\alpha\beta}\varepsilon_{\alpha\beta} \tag{2.34}$$

and

$$\frac{\mathrm{d}\varepsilon_{\alpha\beta}}{\mathrm{d}t} = C_B \left(\frac{\epsilon}{\nu}\right)^{1/2} \varepsilon_{\alpha\beta} - \left(\frac{\mathrm{Re}_1 C_d}{C_{\alpha\beta}}\right) \gamma_{\alpha\beta} \frac{\varepsilon_{\alpha\beta}}{\langle \phi'_\alpha \phi'_\beta \rangle} \varepsilon_{\alpha\beta} \tag{2.35}$$

which will be our starting point for studying $\rho_{\alpha\beta}$ and $g_{\alpha\beta}$

Mean Scalar Gradients

We first consider the case with mean gradients (production term for covariance)

For this case, the statistics reach a steady state where

$$\varepsilon_{\alpha\beta} = 2\Gamma_T \frac{G_{i\alpha} G_{i\beta}}{\gamma_{\alpha\beta}} \tag{2.36}$$

and

$$\langle {\phi'}_{\alpha} {\phi'}_{\beta} \rangle = \left(\frac{k C_d}{\varepsilon C_B} \right) \left(\frac{\gamma_{\alpha\beta} \varepsilon_{\alpha\beta}}{C_{\alpha\beta}} \right) \tag{2.37}$$

These steady-state values can be used to find the correlation coefficients:

$$g_{\alpha\beta} = \frac{1}{\gamma_{\alpha\beta}} \frac{G_{i\alpha} G_{i\beta}}{|G_\alpha||G_\beta|} = \frac{\cos(\theta_{\alpha\beta})}{\gamma_{\alpha\beta}} \tag{2.38}$$

where $\theta_{\alpha\beta}$ is the angle between the mean scalar gradients, and

$$\rho_{\alpha\beta} = \left(\frac{\sqrt{C_{\alpha\alpha} C_{\beta\beta}}}{C_{\alpha\beta}} \right) \gamma_{\alpha\beta} g_{\alpha\beta} = \left(\frac{\sqrt{C_{\alpha\alpha} C_{\beta\beta}}}{C_{\alpha\beta}} \right) \cos(\theta_{\alpha\beta}) \tag{2.39}$$

Thus, for very large Re we find

$$\rho_{\alpha\beta} \rightarrow \cos(\theta_{\alpha\beta}) \tag{2.40}$$

$$g_{\alpha\beta} = \frac{\cos(\theta_{\alpha\beta})}{\gamma_{\alpha\beta}} \tag{2.41}$$

so that only $g_{\alpha\beta}$ depends on differential diffusion (i.e., energy-containing scales are independent of molecular diffusion)

Overall, differential diffusion has a very small effect in the case of mean scalar gradients (which is the case closest to inhomogeneous mixing)

Decaying Scalars

This case is more subtle because there are no production terms to drive the process

Correlation coefficients depend on small differences in decay rates

Using the definitions of the correlation coefficients, from Eqs. (2.34) and (2.35) we can derive

$$\frac{\mathrm{d}\rho_{\alpha\beta}}{\mathrm{d}t} = -\frac{1}{2}\left(2\frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\langle \phi'_{\alpha}\phi'_{\beta}\rangle} - \frac{\varepsilon_{\alpha\alpha}}{\langle \phi'^{2}_{\alpha}\rangle} - \frac{\varepsilon_{\beta\beta}}{\langle \phi'^{2}_{\beta}\rangle}\right) \tag{2.42}$$

and

$$\frac{\mathrm{d}g_{\alpha\beta}}{\mathrm{d}t} = -\frac{\mathrm{Re}_1 C_d}{2}\left(\frac{2}{C_{\alpha\beta}}\frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\langle \phi'_{\alpha}\phi'_{\beta}\rangle} - \frac{1}{C_{\alpha\alpha}}\frac{\varepsilon_{\alpha\alpha}}{\langle \phi'^{2}_{\alpha}\rangle} - \frac{1}{C_{\beta\beta}}\frac{\varepsilon_{\beta\beta}}{\langle \phi'^{2}_{\beta}\rangle}\right) \tag{2.43}$$

Note that these equations contain only the dissipation terms (production terms cancel)

The vortex-stretching term appears in the scalar time-scales equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\langle {\phi'}_{\alpha}{\phi'}_{\beta}\rangle}\right) = \left(\frac{\varepsilon}{\nu}\right)^{1/2}\left[C_B - \left(C_d - \frac{C_{\alpha\beta}}{\mathrm{Re}_1}\right)\frac{k\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\varepsilon C_{\alpha\beta}\langle {\phi'}_{\alpha}{\phi'}_{\beta}\rangle}\right]\frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\langle {\phi'}_{\alpha}{\phi'}_{\beta}\rangle} \tag{2.44}$$

where $\mathrm{Re}_1 C_d > C_{\alpha\beta}$

Note that the time scale equation has characteristic rate of $(\varepsilon/\nu)^{1/2}$ and thus quickly reaches a quasi-steady state at high Re:

$$\frac{k\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\varepsilon C_{\alpha\beta}\langle {\phi'}_{\alpha}{\phi'}_{\beta}\rangle} = \frac{C_B}{C_d - C_{\alpha\beta}/\mathrm{Re}_1} \tag{2.45}$$

Thus, in the limit of large (but finite) Reynolds numbers:

$$\frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{C_{\alpha\beta}\langle {\phi'}_{\alpha}{\phi'}_{\beta}\rangle} = \frac{\varepsilon C_B}{k C_d}\left[1 + \frac{C_{\alpha\beta}}{C_d}\mathrm{Re}_1^{-1} + \mathcal{O}(\mathrm{Re}_1^{-2})\right] \tag{2.46}$$

where lowest-order term is independent of Sc

This result can be used in Eqs. (2.42) and (2.43) to find

$$\frac{\mathrm{d}\rho_{\alpha\beta}}{\mathrm{d}t} = -\frac{\varepsilon C_B}{2kC_d}\left(2C_{\alpha\beta} - C_{\alpha\alpha} - C_{\beta\beta}\right) \tag{2.47}$$

and

$$\frac{\mathrm{d}g_{\alpha\beta}}{\mathrm{d}t} = \frac{\mathrm{d}\rho_{\alpha\beta}}{\mathrm{d}t} \tag{2.48}$$

where we have kept only the lowest-order terms

We can conclude that

1. Both correlation coefficients change at the same rate proportional to ε/k

2. De-correlation will occur only if $0 < C_{\alpha\alpha} + C_{\beta\beta} \leq 2C_{\alpha\beta}$ (From DNS, this is the observed behavior)

3. At high Re the value of $C_{\alpha\beta}$ approaches a Sc-independent constant, thus de-correlation becomes very, very slow

4. Whether or not $\rho_{\alpha\beta} \rightarrow 0$ for large t will depend on the evolution of $C_{\alpha\beta} \Rightarrow$ difficult to study with DNS due to long simulation times

Differential diffusion for reacting scalars is likely to scale in a similar manner to inert scalars Thus, reaction products produced at small scales will be more sensitive to differential diffusion than reactants introduced at large scales

2.3 Multiscale Model for Differential Diffusion

Only DNS resolves the diffusive scales (and thus can treat differential diffusion exactly) ⇒ A multi-scale model is needed in LES/RANS methods

Multi-Variate SR Model

Defining the average diffusivity by

$$\Gamma_{\alpha\beta} \equiv \frac{\Gamma_\alpha + \Gamma_\beta}{2} \tag{2.49}$$

the model equations for the cospectrum $\langle {\phi'}_\alpha {\phi'}_\beta \rangle$ and joint dissipation $\varepsilon_{\alpha\beta}$ are exactly the same!

The covariance is found by summing:

$$\langle {\phi'}_\alpha {\phi'}_\beta \rangle = \sum_{n=1}^{3} \langle {\phi'}_\alpha {\phi'}_\beta \rangle_n + \langle {\phi'}_\alpha {\phi'}_\beta \rangle_D \tag{2.50}$$

The covariance at dissipation scales obeys

$$\frac{\mathrm{d}\langle {\phi'}_\alpha {\phi'}_\beta \rangle_D}{\mathrm{d}t} = \mathcal{T}_D + \gamma_D \mathcal{P}_{\alpha\beta} - \gamma_{\alpha\beta}\varepsilon_{\alpha\beta} \tag{2.51}$$

De-correlation at small scales is due to molecular diffusion:

$$\frac{\mathrm{d}\varepsilon_{\alpha\beta}}{\mathrm{d}t} = \mathcal{P}_\varepsilon + C_D \left(\frac{\varepsilon}{\nu}\right)^{1/2} \mathcal{T}_\varepsilon + C_s \left(\frac{\varepsilon}{\nu}\right)^{1/2} \varepsilon_{\alpha\beta} - C_d \frac{\gamma_{\alpha\beta}\varepsilon_{\alpha\beta}}{\langle {\phi'}_\alpha {\phi'}_\beta \rangle_D} \varepsilon_{\alpha\beta} \tag{2.52}$$

wherein the covariance-dissipation-production term $\mathcal{P}_\varepsilon$ is defined by

$$\mathcal{P}_\varepsilon \equiv -\frac{\gamma_D}{\gamma_{\alpha\beta}} \left(\frac{\varepsilon_\alpha}{\langle {\phi'}^2_\alpha \rangle_D} \langle u_i \phi_\alpha \rangle \frac{\partial \langle \phi_\beta \rangle}{\partial x_i} + \frac{\varepsilon_\beta}{\langle {\phi'}^2_\beta \rangle_D} \langle u_i \phi_\beta \rangle \frac{\partial \langle \phi_\alpha \rangle}{\partial x_i} \right) \tag{2.53}$$

For differential diffusion, $\gamma_{\alpha\beta} \geq 1$

The dissipation transfer rate:

$$\mathcal{T}_\varepsilon = \gamma_{\alpha\beta}^{-1}(\alpha_{3D} + \beta_{3D})\langle {\phi'}_\alpha {\phi'}_\beta \rangle_3 - \beta_\varepsilon \varepsilon_\phi \tag{2.54}$$

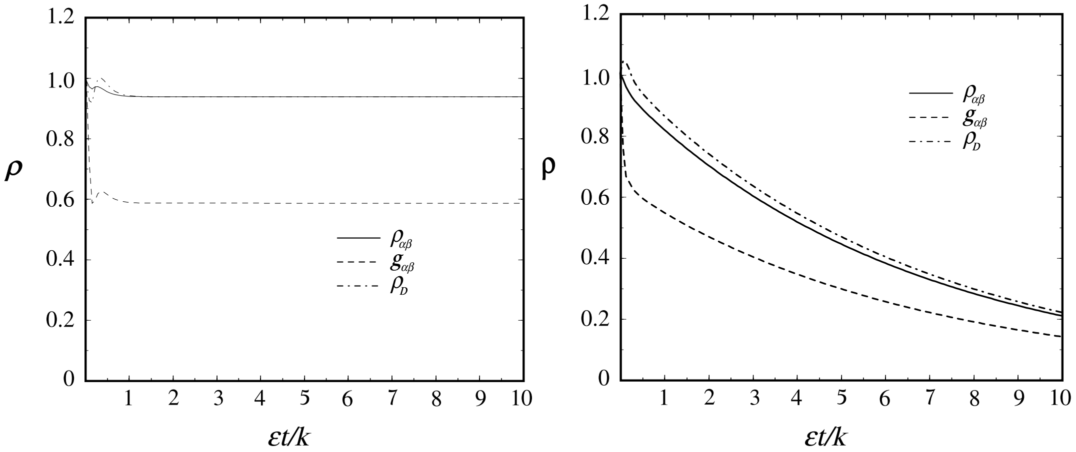
will depend on the Schmidt number through $\gamma_{\alpha\beta}$ and β_ε

The SR model can be solved with different initial conditions to determine how the correlation coefficients $\rho_{\alpha\beta}$ and $g_{\alpha\beta}$ depend on Sc and Re

Decaying Scalars

No backscatter (Left) $c_b = 0$: non-zero asymptotes

Backscatter (Right) $c_b = 1$: zero asymptotes (consistent with DNS)



De-correlation "leaks" from small scales to large scales due to backscatter

Chapter 3

PDF Description of Turbulent Mixing

We will now consider methods to find the joint PDF

These methods are called *transported PDF methods*

3.1 Introduction

We consider *one-point* velocity, composition PDFs:

- The joint PDF contains no information concerning local velocity and/or scalar gradients. (A two-point description would be required to describe the gradients)
- All non-linear terms involving spatial gradients require transported PDF *closures*. Examples of such terms are viscous dissipation, pressure fluctuations and scalar dissipation (micromixing)

Or one-point composition PDFs:

- There is no direct information on the velocity field, and thus a turbulence model is required to provide this information.
- There is no direct information on scalar transport due to velocity fluctuations. A PDF scalar-flux model is required to describe turbulent scalar transport.
- There is no information on the instantaneous scalar dissipation rate and its coupling to the turbulence field. A transported PDF micromixing model is required to determine the effect of molecular diffusion on both the shape of the PDF and the rate of scalar variance decay.

Velocity, Composition PDF

Formally, the one-point velocity, composition PDF is defined by

$$f_{\mathbf{U},\boldsymbol{\phi}}(\mathbf{V},\boldsymbol{\psi};\mathbf{x},t)\,\mathrm{d}\mathbf{V}\,\mathrm{d}\boldsymbol{\psi} \equiv \\ \mathrm{Prob}\left\{(\mathbf{V} < \mathbf{U}(\mathbf{x},t) < \mathbf{V}+\mathrm{d}\mathbf{V}) \cap (\boldsymbol{\psi} < \boldsymbol{\phi}(\mathbf{x},t) < \boldsymbol{\psi}+\mathrm{d}\boldsymbol{\psi})\right\} \quad (3.1)$$

We are interested in this PDF because:

If $f_{\mathbf{U},\boldsymbol{\phi}}(\mathbf{V},\boldsymbol{\psi};\mathbf{x},t)$ were known, then all one-point statistics of $\mathbf{U}$ and $\boldsymbol{\phi}$ would also be known

Formally, the statistics are found by integration:

$$\langle Q(\mathbf{U},\boldsymbol{\phi})\rangle = \iint\limits_{-\infty}^{+\infty} Q(\mathbf{V},\boldsymbol{\psi}) f_{\mathbf{U},\boldsymbol{\phi}}(\mathbf{V},\boldsymbol{\psi};\mathbf{x},t)\,\mathrm{d}\mathbf{V}\,\mathrm{d}\boldsymbol{\psi} \quad (3.2)$$

and some of the most widely used are

$$\langle \mathbf{U} \rangle \quad \text{mean velocity,}$$

$$\langle \boldsymbol{\phi} \rangle \quad \text{mean composition,}$$

$$\langle u_i u_j \rangle \quad \text{Reynolds stresses,}$$

$$\langle {\phi'}_\alpha {\phi'}_\beta \rangle \quad \text{composition covariances,}$$

$$\langle u_i {\phi'}_\alpha \rangle \quad \text{scalar fluxes,}$$

and

$$\langle \mathbf{S}(\boldsymbol{\phi}) \rangle \quad \text{mean chemical source term.}$$

Moreover, higher-order statistics are also available, e.g.,

$$\langle u_i u_j u_k \rangle \quad \text{triple correlations.}$$

Thus, solutions to the PDF transport equation will provide more information than is available from RANS and LES models without the problem of closing the chemical source term

Note, however, that non-linear gradient statistics remain unclosed:

$$\left\langle \frac{\partial \phi'}{\partial x_i} \frac{\partial \phi'}{\partial x_i} \right\rangle$$

Closure models will be required for such terms

Composition PDF

For reacting flows, the chemical source term involves only $\boldsymbol{\phi}$

Thus, in principal, we need only consider the composition PDF:

$$f_{\boldsymbol{\phi}}(\boldsymbol{\psi};\mathbf{x},t) = \int_{-\infty}^{+\infty} f_{\mathbf{U},\boldsymbol{\phi}}(\mathbf{V},\boldsymbol{\psi};\mathbf{x},t)\,\mathrm{d}\mathbf{V} \tag{3.3}$$

However, since it will require us to use a gradient-diffusion model for the velocity fluctuations, the composition PDF should only be used with turbulent-viscosity-based and LES models

With Reynolds-stress (second-order) models, the velocity, composition PDF provides a consistent closure

3.2 Velocity, Composition PDF Transport Equation

Starting from the Navier-Stokes equation:

$$\frac{DU_i}{Dt} \equiv \frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = A_i \tag{3.4}$$

where

$$A_i \equiv \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + g_i \tag{3.5}$$

and the scalar transport equation:

$$\frac{D\phi_\alpha}{Dt} \equiv \frac{\partial \phi_\alpha}{\partial t} + U_j \frac{\partial \phi_\alpha}{\partial x_j} = \Theta_\alpha \tag{3.6}$$

where

$$\Theta_\alpha \equiv \Gamma_\alpha \frac{\partial^2 \phi_\alpha}{\partial x_j \partial x_j} + S_\alpha(\boldsymbol{\phi}) \tag{3.7}$$

We can derive a transport equation for the joint velocity, composition PDF

There are at least two methods that can be used

1. starting from "fine-grained" PDF (Pope 2000, *Turbulent Flows*)

2. starting from an arbitrary function of $\mathbf{U}$ and $\boldsymbol{\phi}$ (Pope 1985)

The first method is more "formal" and requires manipulation of delta functions

The second method better reveals the assumptions that are made along the way

Joint PDF Transport Equation: Final Form

$$\frac{\partial f_{\mathbf{U},\boldsymbol{\phi}}}{\partial t} + V_i \frac{\partial f_{\mathbf{U},\boldsymbol{\phi}}}{\partial x_i} = -\frac{\partial}{\partial V_i}\left[\langle A_i | \mathbf{V}, \boldsymbol{\psi} \rangle f_{\mathbf{U},\boldsymbol{\phi}}\right] - \frac{\partial}{\partial \psi_i}\left[\langle \Theta_i | \mathbf{V}, \boldsymbol{\psi} \rangle f_{\mathbf{U},\boldsymbol{\phi}}\right] \tag{3.8}$$

From this expression, it can be seen that the joint PDF evolves by transport in

(i) real space due to the fluctuating velocity field $\mathbf{V}$,

(ii) velocity phase space due to the conditional acceleration term $\langle A_i | \mathbf{V}, \boldsymbol{\psi} \rangle$,

(iii) composition phase space due to the conditional reaction/diffusion term $\langle \Theta_i | \mathbf{V}, \boldsymbol{\psi} \rangle$.

NOTE: This procedure can be applied to find the transport equation for any set of random fields

Conditional Fluxes: The Unclosed Terms

The conditional acceleration comes from the NS equation:

$$\langle A_i|\mathbf{V},\boldsymbol{\psi}\rangle = \left\langle \left(\nu\frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{1}{\rho}\frac{\partial p'}{\partial x_i}\right)|\mathbf{V},\boldsymbol{\psi}\right\rangle - \frac{1}{\rho}\frac{\partial\langle p\rangle}{\partial x_i} + g_i \tag{3.9}$$

Gravity and mean pressure effects are closed, but viscosity and pressure fluctuations require a model

The conditional diffusion and reaction term comes from the scalar equation:

$$\langle \Theta_\alpha|\mathbf{V},\boldsymbol{\psi}\rangle = \left\langle \Gamma_\alpha\frac{\partial^2 \phi_\alpha}{\partial x_j \partial x_j}|\mathbf{V},\boldsymbol{\psi}\right\rangle + S_\alpha(\boldsymbol{\psi}) \tag{3.10}$$

The most important reason for using PDF methods is now obvious: The chemical source term is closed!

3.3 Composition PDF Transport Equation

The transport equation for the composition PDF can be found from that for the joint PDF

Derivation of Transport Equation

Integrating out the velocity:

$$\int_{-\infty}^{+\infty} \left\{ \frac{\partial f_{\mathbf{U},\boldsymbol{\phi}}}{\partial t} + V_i \frac{\partial f_{\mathbf{U},\boldsymbol{\phi}}}{\partial x_i} = -\frac{\partial}{\partial V_i} \left[\langle A_i | \mathbf{V}, \boldsymbol{\psi} \rangle f_{\mathbf{U},\boldsymbol{\phi}} \right] - \frac{\partial}{\partial \psi_i} \left[\langle \Theta_i | \mathbf{V}, \boldsymbol{\psi} \rangle f_{\mathbf{U},\boldsymbol{\phi}} \right] \right\} \mathrm{d}\mathbf{V} \quad (3.11)$$

yields

$$\frac{\partial f_{\boldsymbol{\phi}}}{\partial t} + \langle U_i \rangle \frac{\partial f_{\boldsymbol{\phi}}}{\partial x_i} + \frac{\partial}{\partial x_i}\left[\langle u_i | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}}\right] = \\ - \frac{\partial}{\partial \psi_i}\left[\langle \Gamma_i \nabla^2 {\phi'}_i | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}}\right] - \frac{\partial}{\partial \psi_i}\left[\left(\Gamma_i \nabla^2 \langle \phi_i \rangle + S_i(\boldsymbol{\psi})\right) f_{\boldsymbol{\phi}}\right] \quad (3.12)$$

This equation is the starting point for deriving PDF-based mixing models: (conditional PDF models, CMC model, multienvironment PDF, etc.)

It contains two unclosed terms:

1. Scalar-conditioned velocity fluctuations: $\langle u_i | \boldsymbol{\psi} \rangle$
2. Molecular mixing: $\langle \Gamma_i \nabla^2 {\phi'}_i | \boldsymbol{\psi} \rangle$

Models are required for both terms, but we will consider only the first for now

Scalar-Conditioned Velocity Fluctuations

Velocity fluctuations conditioned on the scalar(s) can be modeled in two forms

The first form holds when the velocity and scalars are both Gaussian:

$$\langle u_i | \boldsymbol{\psi} \rangle = \langle u_i \boldsymbol{\phi}^{\mathrm{T}} \rangle \langle \boldsymbol{\phi}' \boldsymbol{\phi}'^{\mathrm{T}} \rangle^{-1} (\boldsymbol{\psi} - \langle \boldsymbol{\phi} \rangle) \tag{3.13}$$

In general, this is rarely the case (especially for reacting scalars)

The second model invokes a gradient-diffusion hypothesis:

$$\langle u_i | \boldsymbol{\psi} \rangle = -\frac{\Gamma_T}{f_{\boldsymbol{\phi}}} \frac{\partial f_{\boldsymbol{\phi}}}{\partial x_i} \tag{3.14}$$

Although not exact, this model is more general and is consistent with using a gradient-diffusion model for the scalar flux

Using the gradient-diffusion model, the composition PDF follows:

$$\begin{aligned}\frac{\partial f_{\boldsymbol{\phi}}}{\partial t} + \langle U_i \rangle \frac{\partial f_{\boldsymbol{\phi}}}{\partial x_i} = \frac{\partial}{\partial x_i}\left[\Gamma_T \frac{\partial f_{\boldsymbol{\phi}}}{\partial x_i}\right] \\ - \frac{\partial}{\partial \psi_i}\left[\langle \Gamma_i \nabla^2 {\phi'}_i | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}}\right] - \frac{\partial}{\partial \psi_i}\left[\left(\Gamma_i \nabla^2 \langle \phi_i \rangle + S_i(\boldsymbol{\psi})\right) f_{\boldsymbol{\phi}}\right]\end{aligned} \quad (3.15)$$

where the turbulent diffusivity $\Gamma_T(\mathbf{x}, t)$ depends on the local values of k and ε and the molecular diffusion term $\Gamma_i \nabla^2 \langle \phi_i \rangle$ is negligible at high Reynolds numbers

In this equation, the chemical source term is closed (and thus exact)

However, a micromixing model must be developed for $\langle \Gamma_i \nabla^2 {\phi'}_i | \boldsymbol{\psi} \rangle$ before the equation can be solved to find $f_{\boldsymbol{\phi}}$

3.4 Models for Conditional Acceleration

PDF modeling is primarily concerned with closing the conditional fluxes

For the velocity field, the conditional acceleration must be modeled:

$$\langle A_i | \mathbf{V}, \boldsymbol{\psi} \rangle = \langle A_i' | \mathbf{V}, \boldsymbol{\psi} \rangle + \nu \frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + g_i \tag{3.16}$$

where the unclosed fluctuating component is defined by

$$\langle A_i' | \mathbf{V}, \boldsymbol{\psi} \rangle \equiv \left\langle \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \middle| \mathbf{V}, \boldsymbol{\psi} \right\rangle - \left\langle \frac{1}{\rho} \frac{\partial p'}{\partial x_i} \middle| \mathbf{V}, \boldsymbol{\psi} \right\rangle \tag{3.17}$$

The two unclosed terms are

1. fluctuating viscous forces

2. fluctuating pressure forces

The first term leads to turbulent energy dissipation and is relatively easy to model

The second term contributes to the complicated interactions between various velocity components and is difficult to model in a general way

Velocity PDF: Decoupling from the Scalar Field

For passive scalars, the acceleration does not depend on the scalars

This implies that

$$\langle A_i' | \mathbf{V}, \boldsymbol{\psi} \rangle = \langle A_i' | \mathbf{V} \rangle \tag{3.18}$$

We can thus integrate out the scalars, and consider first only the velocity PDF:

$$\frac{\partial f_{\mathbf{U}}}{\partial t} + V_i \frac{\partial f_{\mathbf{U}}}{\partial x_i} = -\frac{\partial}{\partial V_i}\left[\langle A_i | \mathbf{V} \rangle f_{\mathbf{U}}\right] \tag{3.19}$$

where closure requires a model for

$$\langle A_i' | \mathbf{V} \rangle \equiv \left\langle \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} \middle| \mathbf{V} \right\rangle - \left\langle \frac{1}{\rho} \frac{\partial p'}{\partial x_i} \middle| \mathbf{V} \right\rangle \tag{3.20}$$

In general, the PDF model can be formulated in terms of

$$\mathbf{V}, \quad \langle \mathbf{U} \rangle, \quad \langle u_i u_j \rangle, \quad \frac{\partial \langle \mathbf{U} \rangle}{\partial x_i}, \quad \text{and} \quad \varepsilon,$$

where ε can be treated as a deterministic variable, or modeled as a random process using a separate stochastic model

The PDF model must reproduce the known behavior of $f_{\mathbf{U}}$ and its statistics

For example, in homogeneous turbulence with uniform shear it is known that $f_{\mathbf{U}}$ becomes Gaussian with time-dependent Reynolds stresses

The conditional acceleration must therefore allow for a Gaussian $f_{\mathbf{U}}$

Velocity PDF Closures

The simplest models are based on a linear stochastic process:

$$\langle A_i' | \mathbf{V} \rangle = G_{ij} \left(V_j - \langle U_j \rangle \right) - \frac{C_0 \varepsilon}{2 f_{\mathbf{U}}} \frac{\partial f_{\mathbf{U}}}{\partial V_i} \tag{3.21}$$

where $G_{ij}(\mathbf{x}, t)$ is a second-order tensor which depends on

$$\langle u_i u_j \rangle, \quad \frac{\partial \langle \mathbf{U} \rangle}{\partial x_i}, \quad \text{and} \quad \varepsilon$$

All of the important physics that determine the Reynolds stresses must be contained in $\mathbf{G}$ (thus, most of the modeling work is still to come!)

A linear Fokker-Planck equation results:

$$\frac{\partial f_{\mathbf{U}}}{\partial t} + V_i \frac{\partial f_{\mathbf{U}}}{\partial x_i} + \left(\nu \frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_j} - \frac{1}{\rho} \frac{\partial \langle p \rangle}{\partial x_i} + g_i \right) \frac{\partial f_{\mathbf{U}}}{\partial V_i} = - \frac{\partial}{\partial V_i} \left[G_{ij} \left(V_j - \langle U_j \rangle \right) f_{\mathbf{U}} \right] + \frac{C_0 \varepsilon}{2} \frac{\partial^2 f_{\mathbf{U}}}{\partial V_i \partial V_i} \quad (3.22)$$

Linear Fokker-Planck equations admits a multi-variate Gaussian PDF as a solution

Generalized Langevin Model

A more complete acceleration model must account for the anisotropy tensor **b**

In practice, this is done by making stochastic versions of Reynolds stresses models

$$G_{ij} = \frac{\varepsilon}{k}\left(\alpha_1\delta_{ij} + \alpha_2 b_{ij} + \alpha_3 b^2_{ij}\right) + H_{ijkl}\frac{\partial\langle U_k\rangle}{\partial x_l} \tag{3.23}$$

where the fourth-order tensor **H** is a linear function of anisotropy tensor **b** and contains nine model parameters:

$$\begin{aligned} H_{ijkl} = {} & \beta_1\delta_{ij}\delta_{kl} + \beta_2\delta_{ik}\delta_{jl} + \beta_3\delta_{il}\delta_{jk} \\ & + \gamma_1\delta_{ij}b_{kl} + \gamma_2\delta_{ik}b_{jl} + \gamma_3\delta_{il}b_{jk} + \gamma_4\delta_{kl}b_{ij} + \gamma_5\delta_{jl}b_{ik} + \gamma_6\delta_{jk}b_{il} \end{aligned} \tag{3.24}$$

Pope and co-workers have made detailed comparisons between the GLM and turbulent flow data. In general, the agreement is good for flows where the corresponding Reynolds stress model performs adequately.

Despite the ability of the GLM to reproduce any realizable Reynolds stress model, it is not consistent with DNS data for homogeneous turbulent shear flow.

In order to overcome this problem and to incorporate the Reynolds-number effects observed in DNS, a stochastic model for the acceleration can be formulated

It remains to be seen how well such models will perform for more complex inhomogeneous flows

Chapter 4

Micromixing Models for Conditional Diffusion

The conditional diffusion term has the same form as the viscous term:

$$\langle \Gamma_\alpha \nabla^2 \phi_\alpha | \mathbf{V}, \boldsymbol{\psi} \rangle = \langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \mathbf{V}, \boldsymbol{\psi} \rangle + \Gamma_\alpha \nabla^2 \langle \phi_\alpha \rangle \tag{4.1}$$

However, it is much more difficult to model since the scalar fields are almost always non-Gaussian

In fact, because scalars fields are *bounded* and *correlated*, we cannot use a simple linear closure like the (linear) Langevin model

4.1 Some Useful Constraints

Before looking at particular closures, it is important to understand the constraints that they must satisfy

1. **Mass conservation:** averaging the model over all velocities and compositions should result in not net changes

$$\langle\langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \mathbf{U}, \boldsymbol{\phi} \rangle\rangle = \langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha \rangle = 0 \tag{4.2}$$

(I) *The molecular mixing model must leave the scalar mean unchanged*

2. **Covariance dissipation:** multiplying by the scalar fluctuation and averaging yields the scalar dissipation rate

$$\begin{aligned}\langle \phi'_\beta \langle \Gamma_\alpha \nabla^2 \phi'_\alpha | \mathbf{U}, \boldsymbol{\phi} \rangle \rangle &= \Gamma_\alpha \langle \phi'_\beta \nabla^2 \phi'_\alpha \rangle \\ &= -\Gamma_\alpha \langle (\boldsymbol{\nabla} \phi'_\alpha) \cdot (\boldsymbol{\nabla} \phi'_\beta) \rangle + \Gamma_\alpha \boldsymbol{\nabla} \cdot \langle \phi'_\beta \boldsymbol{\nabla} \phi'_\alpha \rangle\end{aligned} \tag{4.3}$$

or, because $\varepsilon_{\alpha\beta}$ is modeled separately,

$$\langle \phi'_\beta \Gamma_\alpha \nabla^2 \phi_\alpha \rangle = -\frac{1}{2}\sqrt{\frac{\Gamma_\alpha}{\Gamma_\beta}}\varepsilon_{\alpha\beta} + \Gamma_\alpha \boldsymbol{\nabla} \cdot \langle \phi'_\beta \boldsymbol{\nabla} \phi'_\alpha \rangle \tag{4.4}$$

(II) *The molecular mixing model must yield the correct joint scalar dissipation rate*

3. **Local anisotropy:** multiplying by the velocity fluctuation and averaging yields the small-scale velocity-scalar correlation

$$
\begin{aligned}
\langle u_i \langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \mathbf{U}, \boldsymbol{\phi} \rangle \rangle &= \Gamma_\alpha \langle u_i \nabla^2 {\phi'}_\alpha \rangle \\
&= -\Gamma_\alpha \langle (\boldsymbol{\nabla} u_i) \cdot (\boldsymbol{\nabla} {\phi'}_\alpha) \rangle + \Gamma_\alpha \boldsymbol{\nabla} \cdot \langle u_i \boldsymbol{\nabla} {\phi'}_\alpha \rangle .
\end{aligned}
\tag{4.5}
$$

Thus, local isotropy requires

$$
\langle u_i \Gamma_\alpha \nabla^2 {\phi'}_\alpha \rangle = 0, \tag{4.6}
$$

(III) *Molecular mixing model must be uncorrelated with velocity at high* Re

Note that this constraint implies that the mixing model should depend on the velocity **V** (which is usually not the case!)

Most micromixing models have been developed in the context of composition PDFs where conditioning is limited to scalars: $\left\langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \boldsymbol{\psi} \right\rangle$

Thus usually only constraints (I) and (II) are considered

4.2 Desirable Properties for Mixing Models

In addition to moment constraints, there are several desirable properties:

(i) Inert scalar PDF should relax to Gaussian form.
(ii) All scalars must remain in the allowable region.
(iii) Conserved linear combinations must be maintained.
(iv) Mixing should be local in composition space.
(v) Mixing rate should depend on scalar length scales.
(vi) Re, Sc, and Da dependencies should be taken into account.

4.3 Physical Basis for Desirable Properties

(i) Why Gaussian?

DNS studies of inert scalar mixing have shown that

- PDF of an inert scalar evolves through a series of “universal” shapes that are similar to a beta PDF
- scalar dissipation rate strongly depends on the initial scalar length-scale distribution (i.e., the initial scalar spectrum)
- limiting form of the scalar PDF is nearly Gaussian

These observations suggest that the development of molecular mixing models can proceed in two separate steps:

1. Generate a mixing model that predicts the correct joint scalar PDF shape for *a given scalar covariance matrix*, including the asymptotic collapse to a Gaussian
2. Couple it with a model for the *joint scalar dissipation rate* that predicts the correct scalar covariance matrix, including the effect of the initial scalar length-scale distribution

Most molecular mixing models concentrate on step 1. However, for "practical" reacting flow applications, step 2 can be very important

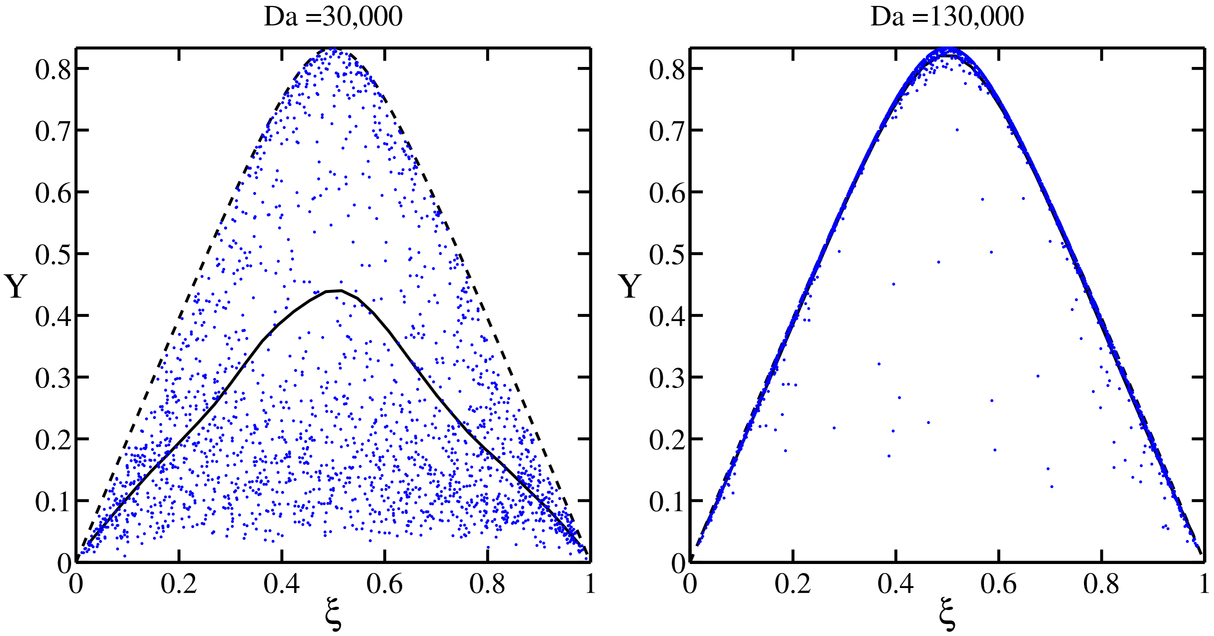
(ii) Why worry about the allowable region?

Consideration of the allowable region comes from the very nature of chemically reacting flows:

- All chemical species concentrations are, by definition, positive: $\boldsymbol{\phi} \geq \mathbf{0}$. Moreover, the maximum ($\boldsymbol{\phi}_{max}$) and minimum ($\boldsymbol{\phi}_{min}$) concentrations observed in a particular system will depend on the initial conditions, the extents of reaction, and the concentrations of other species

- Reaction-stoichiometry plus element-conservation constraints put non-trivial bounds on the composition vector $\boldsymbol{\phi}$. Interior of these bounds forms the allowable region

Example: nonpremixed one-step reaction $A + B \leftrightarrow Y$



(iii) Why linearity?

If the molecular diffusion coefficients are identical, chemical elements are conserved:

$$\mathbf{\Lambda S}_c = \mathbf{0} \tag{4.7}$$

the transport equations for the chemical species imply that

$$\frac{D\mathbf{c}_c}{Dt} = \Gamma \nabla^2 \mathbf{c}_c \tag{4.8}$$

where $\mathbf{c}_c$ is the (conserved) element “concentration” vector.

Thus, a viable mixing model must satisfy

$$\mathbf{\Lambda} \langle \Gamma \nabla^2 \mathbf{c} | \mathbf{c} \rangle = \langle \Gamma \nabla^2 \mathbf{c}_c | \mathbf{c}_c \rangle \tag{4.9}$$

In general, Eq. (4.9) will hold if the mixing model is linear in $\mathbf{c}$ and employs the same mixing time for every scalar (e.g., the IEM model)

$$\langle \Gamma \nabla^2 \mathbf{c} | \mathbf{c} \rangle = -\frac{1}{2\tau_\phi}(\boldsymbol{\phi} - \langle \boldsymbol{\phi} \rangle). \tag{4.10}$$

Non-linear variations of IEM have also been proposed (e.g., GIEM)

$$\langle \Gamma \nabla^2 \mathbf{c} | \mathbf{c}, \zeta \rangle = \alpha(\zeta, t)(\boldsymbol{\beta} - \mathbf{c}) \tag{4.11}$$

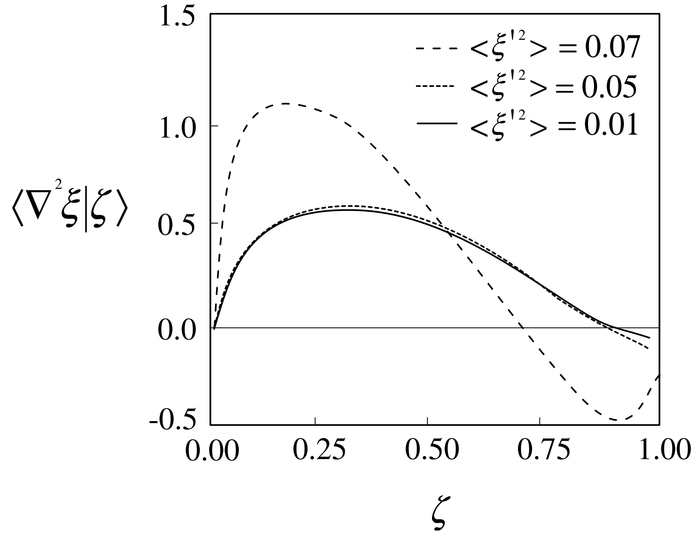
where $\boldsymbol{\beta}(t)$ is chosen to conserve the scalar means:

$$\boldsymbol{\beta}(t) \equiv \frac{\langle \alpha(\xi, t)\mathbf{c} \rangle}{\langle \alpha(\xi, t) \rangle} \tag{4.12}$$

GIEM models the mixture fraction using

$$\langle \Gamma \nabla^2 \xi | \zeta \rangle = \alpha(\zeta, t)(\beta_\xi - \zeta) \tag{4.13}$$

where $\beta_{\xi}(t)$ is the time-dependent intersection point with the ζ-axis, and $\alpha(\zeta, t)$ quantifies the deviations from linearity:



Thus, unlike IEM, the GIEM relaxes to a Gaussian PDF for mixture fraction

(iv) Why should mixing be local in composition space?

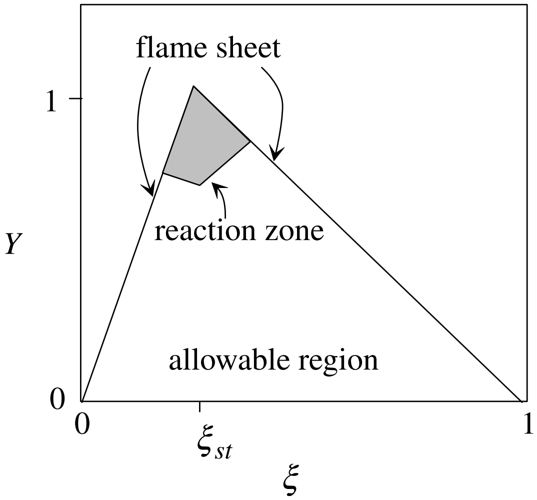
Local interactions refer to neighboring points in composition space

In general, since mixing in composition space is continuous, stochastic models that “jump” from point to point are not physical

The problems that occur due to non-local models is best illustrated with a “flame sheet” where

$$Y(\xi) = \min\left(\frac{\xi}{\xi_{st}}, \frac{1-\xi}{1-\xi_{st}}\right) \tag{4.14}$$

Flame sheet:



With fast chemistry, mixing moves along the flame sheet starting from 0 or 1

Non-local mixing generates points in allowable region away from flame sheet

IEM is non-local: homogeneous case

$$\frac{\mathrm{d}\xi}{\mathrm{d}t} = \frac{C_\phi \varepsilon}{2k} \left(\langle \xi \rangle - \xi \right) \tag{4.15}$$

$$\frac{\mathrm{d}Y}{\mathrm{d}t} = \frac{C_\phi \varepsilon}{2k} \left(\langle Y \rangle - Y \right) + S_Y(Y, \xi) \tag{4.16}$$

Mixture fraction follows

$$\xi(t) = \langle \xi \rangle + \left(\xi(0) - \langle \xi \rangle \right) \exp\left(-\frac{C_\phi \varepsilon}{2k} t \right). \tag{4.17}$$

Likewise, if $\langle Y \rangle(0)$ lies well below the reaction zone, the IEM model will collapse all points outside the reaction zone towards the mean values without passing through the reaction zone

(v) Why account for the scalar length-scale distribution?

DNS of inert scalars with different initial spectra show that the scalar dissipation rate is very dependent on the length-scale distribution

We have seen that the spectral relaxation (SR) model can account for the length-scale distribution using a multi-scale model

Accounting for the length-scale distribution is similar to accounting for dissipation fluctuations in the flamelet model

Fluctuations lead to local extinction (fast mixing) in reacting flows

(vi) Why include Re, Sc, and Da dependencies?

At very high Reynolds numbers, turbulent mixing theory predicts that the scalar dissipation rate will be independent of Re and Sc.

In general, the inclusion of dependencies on Re, Sc, or Da is difficult and mostly done on a case-by-case basis.

Examples where the Sc-dependence may be significant include liquid-phase reacting flows at moderate Reynolds for which the Schmidt number is very large and gas-phase reacting flows for which the molecular diffusion coefficients of some species differ by an order of magnitude

4.4 Three Simple Mixing Models

Rather than try to look at all proposed models, we will concentrate on 3 typical ones:

1. coalescence-dispersion model
2. interaction-by-exchange-with-the-mean model
3. Fokker-Planck model

CD Model

This model was first proposed to describe mixing of liquid droplets

It involves a jump process:

$$\begin{matrix} (\phi_{A1}, \phi_{B1})_1 \\ (\phi_{A2}, \phi_{B2})_2 \end{matrix} \xrightarrow{\text{coalescence}} \begin{pmatrix} \phi_A^* = (\phi_{A1} + \phi_{A2})/2 \\ \phi_B^* = (\phi_{B1} + \phi_{B2})/2 \end{pmatrix} \xrightarrow{\text{dispersion}} \begin{matrix} (\phi_A^*, \phi_B^*)_1 \\ (\phi_A^*, \phi_B^*)_2 \end{matrix}$$

where $(\cdot, \cdot)_1$ and $(\cdot, \cdot)_2$ are the compositions of fluid particle 1 and 2

The CD model is easy to program in Monte-Carlo simulations (randomly select two particles with a fixed probability)

In terms of the constraints, the CD model's behavior is

- **(I)** The mean concentration is the same before and after mixing
- **(II)** All scalars have the same dissipation rate, so joint scalar dissipation rate can not be completely controlled
- **(III)** Velocity is not included, so local anisotropy cannot be controlled

In terms of the desirable properites, the CD model's behavior is

- **(i)** The limiting PDF is *not* Gaussian
- **(ii)** All scalars remain in allowable region

- **(iii)** Linear combinations are conserved
- **(iv)** Scalar values jump, so CD model is *not* local
- **(v)** Length-scale distribution is not treated explicitly
- **(vi)** Re, Sc and Da are *not* accounted for

Despite its limitations, the CD model is still used for PDF simulations of turbulent reacting flows!

IEM Model

The IEM model uses a simple linear deterministic equation:

$$\langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \boldsymbol{\psi} \rangle = \frac{\varepsilon_\alpha}{2\langle \phi'^2_\alpha \rangle} (\langle \phi_\alpha \rangle - \psi_\alpha) \tag{4.18}$$

where ε_α is found from a separate model for the scalar dissipation rate

In most applications, a scale-similarity model is used:

$$\frac{\varepsilon_\alpha}{\langle \phi'^2_\alpha \rangle} = C_\phi \frac{\varepsilon}{k} \tag{4.19}$$

with $C_\phi \approx 2$

In terms of the constraints, the IEM model's behavior is

- **(I)** The mean concentration is conserved due to linear form
- **(II)** All scalars have the same dissipation rate, so joint scalar dissipation rate can not be completely controlled
- **(III)** Velocity is not included, so local anisotropy cannot be controlled unless velocity-conditioning is used:

$$\langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \mathbf{V}, \boldsymbol{\psi} \rangle = \frac{\varepsilon_\alpha}{2\langle \phi'^2_\alpha \rangle}(\langle \phi_\alpha | \mathbf{V} \rangle - \psi_\alpha) \tag{4.20}$$

  But this is difficult due to statistical noise when estimating $\langle \phi_\alpha | \mathbf{V} \rangle$

In terms of the desirable properties, the IEM model’s behavior is

- **(i)** The shape of the PDF does not change!
- **(ii)** All scalars remain in allowable region
- **(iii)** Linear combinations are conserved due to linear form
- **(iv)** Scalar values move continuously towards mean, so IEM model is *nearly* local
- **(v)** Length-scale distribution is not treated explicitly
- **(vi)** Re, Sc and Da are *not* accounted for

Due to constant shape, IEM does not work well for *homogeneous* mixing (i.e., without mean-scalar gradients)

IEM model is widely used for PDF simulations of turbulent reacting flows and the results for *inhomogeneous* cases are reasonable

FP Model

The Fokker-Planck model adds a nonlinear diffusion term to the IEM model in order to make the PDF shape relax to Gaussian

For a single scalar, conditional diffusion is related to the conditional dissipation rate:

$$\langle \Gamma \nabla^2 \phi' | \psi \rangle = \frac{1}{2 f_\phi} \frac{\partial}{\partial \psi} \left(\langle \epsilon_\phi | \psi \rangle f_\phi \right) \tag{4.21}$$

In principle, if $\langle \epsilon_\phi | \psi \rangle$ were known we could use this model for mixing

However, it leads to negative diffusion in phase space and is numerically unstable

The FP model 'regularizes' the diffusion process using

$$\begin{aligned}
\langle \Gamma \nabla^2 \phi' | \psi \rangle &= 2\langle \Gamma \nabla^2 \phi' | \psi \rangle - \langle \Gamma \nabla^2 \phi' | \psi \rangle \\
&= 2\langle \Gamma \nabla^2 \phi' | \psi \rangle - \frac{1}{2 f_\phi} \frac{\partial}{\partial \psi} \left(\langle \epsilon_\phi | \psi \rangle f_\phi \right) \\
&= \frac{\varepsilon_\phi}{\langle \phi'^2 \rangle} (\langle \phi \rangle - \psi) - \frac{1}{2 f_\phi} \frac{\partial}{\partial \psi} \left(\langle \epsilon_\phi | \psi \rangle f_\phi \right)
\end{aligned} \tag{4.22}$$

where the final form follows by using the IEM model for conditional scalar Laplacian The resulting Fokker-Planck equation for f_ϕ has the form of a non-linear diffusion process

$$\frac{\partial f_\phi}{\partial t} = \frac{\varepsilon_\phi}{\langle \phi'^2 \rangle} \frac{\partial}{\partial \psi} \left[(\psi - \langle \phi \rangle) f_\phi \right] + \frac{1}{2} \frac{\partial^2}{\partial \psi^2} \left(\langle \epsilon_\phi | \psi \rangle f_\phi \right) \tag{4.23}$$

Solution is well behaved, and shape of f_ϕ is determined by the choice of $\langle \epsilon_\phi | \psi \rangle$

Applying the same procedure for multiple (N_s) scalars, leads to an expression of the form

$$\sum_{\alpha=1}^{N_s} \frac{\partial}{\partial \psi_\alpha} \left[\langle \nabla^2 {\phi'}_\alpha | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}} \right] = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} \frac{1}{2\sqrt{\Gamma_\alpha \Gamma_\beta}} \frac{\partial^2}{\partial \psi_\alpha \partial \psi_\beta} \left(\langle \epsilon_{\alpha\beta} | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}} \right) \tag{4.24}$$

or

$$\langle \Gamma_\alpha \nabla^2 {\phi'}_\alpha | \boldsymbol{\psi} \rangle = -\frac{1}{2} \sum_{\beta=1}^{N_s} \left[M_{\alpha\beta} (\psi_\beta - \langle \phi_\beta \rangle) + \frac{1}{f_{\boldsymbol{\phi}}} \frac{\partial}{\partial \psi_\beta} \left(\langle \epsilon_{\alpha\beta} | \boldsymbol{\psi} \rangle f_{\boldsymbol{\phi}} \right) \right] \tag{4.25}$$

This yields a multi-variate Fokker-Planck equation for the composition PDF

However, the user must supply the conditional scalar dissipation rates $\langle \epsilon_{\alpha\beta} | \boldsymbol{\psi} \rangle$

If all scalar are Gaussian, then $\langle \epsilon_{\alpha\beta} | \boldsymbol{\psi} \rangle = \varepsilon_{\alpha\beta}$ is independent of $\boldsymbol{\psi}$

In general, $\langle \epsilon_{\alpha\beta} | \boldsymbol{\psi} \rangle$ will be hard to determine *a priori*

Coefficient matrix $\mathbf{M} \equiv [M_{\alpha\beta}]$ can be found using the covariance decay rate:

$$\begin{aligned}\frac{\mathrm{d}\langle \phi'_\alpha \phi'_\beta \rangle}{\mathrm{d}t} &= \langle \Gamma_\alpha \phi'_\beta \nabla^2 \phi'_\alpha \rangle + \langle \Gamma_\beta \phi'_\alpha \nabla^2 \phi'_\beta \rangle \\ &= -\gamma_{\alpha\beta} \varepsilon_{\alpha\beta}\end{aligned} \tag{4.26}$$

This yields the following expression for $\mathbf{M}$:

$$\mathbf{M} = (\mathbf{S}_\Gamma \boldsymbol{\varepsilon} \mathbf{S}_\Gamma^{-1} + \boldsymbol{\varepsilon}) \mathbf{C}^{-1} \tag{4.27}$$

where the matrices on the right-hand side are defined by

$$\mathbf{S}_\Gamma \equiv \mathbf{diag}\left(\sqrt{\Gamma_1}, \dots, \sqrt{\Gamma_{N_s}} \right) \quad \text{and} \quad \boldsymbol{\varepsilon} \equiv \left[\varepsilon_{\alpha\beta} \right] \tag{4.28}$$

and $\mathbf{C} \equiv \langle \boldsymbol{\phi}' \boldsymbol{\phi}'^{\mathrm{T}} \rangle$ is the scalar covariance matrix.

In order to see if the FP model satisfies the constraints and desirable properties, we need to express it as a *random process*

$$\mathrm{d}\boldsymbol{\phi} = -\frac{1}{2}\mathbf{M}(\boldsymbol{\phi} - \langle\boldsymbol{\phi}\rangle)\,\mathrm{d}t + \mathbf{B}(\boldsymbol{\phi})\,\mathrm{d}\mathbf{W}(t) \tag{4.29}$$

where $\mathrm{d}\mathbf{W}(t)$ in a multi-variate Wiener process

The diffusion matrix $\mathbf{B}(\boldsymbol{\phi})$ is related to $\langle\boldsymbol{\epsilon}|\boldsymbol{\phi}\rangle \equiv [\langle\epsilon_{\alpha\beta}|\boldsymbol{\phi}\rangle]$ by

$$\mathbf{B}(\boldsymbol{\phi})\mathbf{B}(\boldsymbol{\phi})^{\mathrm{T}} = \langle\boldsymbol{\epsilon}|\boldsymbol{\phi}\rangle \tag{4.30}$$

In terms of the constraints, the FP model's behavior is

- **(I)** The mean concentration is conserved due to linear form of drift term
- **(II)** The matrix $\mathbf{M}$ is defined to yield the correct joint scalar dissipation rates
- **(III)** Velocity is not included, so local anisotropy cannot be controlled unless velocity-conditioning is added (problematic due to statistical noise)

In terms of the desirable properties, the FP model's behavior is

- **(i)** The shape of the PDF approaches joint Gaussian due to form of $\langle \boldsymbol{\epsilon} | \boldsymbol{\psi} \rangle$
- **(ii)** All scalars remain in allowable region if $\langle \boldsymbol{\epsilon} | \boldsymbol{\psi} \rangle$ is defined to have zero flux on boundaries

- **(iii)** Linear property applies only with diffusion coefficients are equal:

  $$\mathrm{d}\boldsymbol{\phi} = -\boldsymbol{\varepsilon}\mathbf{S}_{\phi}^{-1}\mathbf{U}_{\rho}\mathbf{S}_{\rho}\mathbf{U}_{\rho}^{\mathrm{T}}\mathbf{S}_{\phi}^{-1}(\boldsymbol{\phi} - \langle\boldsymbol{\phi}\rangle)\,\mathrm{d}t + \mathbf{S}_{g}(\boldsymbol{\phi})\mathbf{C}_{g}(\boldsymbol{\phi})\,\mathrm{d}\mathbf{W}(t) \tag{4.31}$$

  Linearity holds if $\langle\boldsymbol{\epsilon}|\boldsymbol{\psi}\rangle$ transforms correctly

- **(iv)** Scalar values move continuously towards mean, so FP model is *nearly* local

- **(v)** Length-scale distribution is treated explicitly using SR model for $\boldsymbol{\varepsilon}$

- **(vi)** Re and Sc are accounted for explicitly (Da effect must be added to SR model)

Example: Bivariate FP model for mixture-fraction vector $\boldsymbol{\xi} = [\xi_1, \xi_2]$

The allowable region is defined by a right triangle: $0 \leq \xi_1 + \xi_2 \leq 1$

The 3 sides of the triangle have normal vectors defined by

$$\mathbf{n}(0, \zeta_2^*) = \begin{bmatrix} 1 \\ \\ 0 \end{bmatrix} \quad \mathbf{n}(\zeta_1^*, 0) = \begin{bmatrix} 0 \\ \\ 1 \end{bmatrix} \quad \mathbf{n}(\zeta_1^*, \zeta_2^*) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \\ 1 \end{bmatrix} \tag{4.32}$$

The stochastic model has the form

$$\mathrm{d}\boldsymbol{\xi} = -\boldsymbol{\varepsilon}\mathbf{C}_{\xi}^{-1}(\boldsymbol{\xi} - \langle\boldsymbol{\xi}\rangle)\,\mathrm{d}t + \mathbf{S}_g(\boldsymbol{\xi})\mathbf{C}_g(\boldsymbol{\xi})\,\mathrm{d}\mathbf{W}(t) \tag{4.33}$$

where the covariance matrix is $\mathbf{C}_{\xi} = [\langle \xi_i' \xi_j' \rangle]$

For this example, the conditional scalar dissipation rate matrix has three unknown components:

$$\langle \boldsymbol{\epsilon}_{\xi} | \zeta_1, \zeta_2 \rangle = \begin{bmatrix} \langle \epsilon_{11} | \zeta_1, \zeta_2 \rangle & \langle \epsilon_{12} | \zeta_1, \zeta_2 \rangle \\ \langle \epsilon_{12} | \zeta_1, \zeta_2 \rangle & \langle \epsilon_{22} | \zeta_1, \zeta_2 \rangle \end{bmatrix} \tag{4.34}$$

The functional forms of the 3 components must satisfy 3 moment conditions:

$$\begin{aligned} \langle \langle \epsilon_{11} | \xi_1, \xi_2 \rangle \rangle &= \varepsilon_{11} \\ \langle \langle \epsilon_{12} | \xi_1, \xi_2 \rangle \rangle &= \varepsilon_{12} \\ \langle \langle \epsilon_{22} | \xi_1, \xi_2 \rangle \rangle &= \varepsilon_{22} \end{aligned} \tag{4.35}$$

and 6 boundary conditions:

$$\begin{aligned}
\langle \epsilon_{11} | 0, \zeta_2^* \rangle &= 0 \quad \text{for all } \zeta_2^* \\
\langle \epsilon_{12} | 0, \zeta_2^* \rangle &= 0 \quad \text{for all } \zeta_2^* \\
\langle \epsilon_{12} | \zeta_1^*, 0 \rangle &= 0 \quad \text{for all } \zeta_1^* \\
\langle \epsilon_{22} | \zeta_1^*, 0 \rangle &= 0 \quad \text{for all } \zeta_1^* \\
\langle \epsilon_{11} | \zeta_1^*, \zeta_2^* \rangle + \langle \epsilon_{12} | \zeta_1^*, \zeta_2^* \rangle &= 0 \quad \text{for all } \zeta_1^* + \zeta_2^* = 1 \\
\langle \epsilon_{12} | \zeta_1^*, \zeta_2^* \rangle + \langle \epsilon_{22} | \zeta_1^*, \zeta_2^* \rangle &= 0 \quad \text{for all } \zeta_1^* + \zeta_2^* = 1
\end{aligned} \tag{4.36}$$

The last 6 constrain the diffusion to be zero in the direction of the normal vectors: $\langle \boldsymbol{\epsilon}_{\xi} | \zeta_1, \zeta_2 \rangle \mathbf{n} = \mathbf{0}$

If we postulate that (like the beta PDF) that the coefficients can depend only on the first and second moments, then they must have the form:

$$\begin{aligned}
\langle \epsilon_{11} | \zeta_1, \zeta_2 \rangle &= a_0 + a_1\zeta_1 + a_2\zeta_2 + a_3\zeta_1^2 + a_4\zeta_1\zeta_2 + a_5\zeta_2^2 \\
\langle \epsilon_{12} | \zeta_1, \zeta_2 \rangle &= b_0 + b_1\zeta_1 + b_2\zeta_2 + b_3\zeta_1^2 + b_4\zeta_1\zeta_2 + b_5\zeta_2^2 \\
\langle \epsilon_{22} | \zeta_1, \zeta_2 \rangle &= c_0 + c_1\zeta_1 + c_2\zeta_2 + c_3\zeta_1^2 + c_4\zeta_1\zeta_2 + c_5\zeta_2^2
\end{aligned} \tag{4.37}$$

where the coefficients must satisfy the constraints

Applying the constraints, we can express coefficients in terms of moments:

$$\begin{aligned}
\langle \epsilon_{11} | \zeta_1, \zeta_2 \rangle &= \alpha \zeta_1 (1 - \zeta_1 - \zeta_2) - \beta \zeta_1 \zeta_2 \\
\langle \epsilon_{12} | \zeta_1, \zeta_2 \rangle &= \beta \zeta_1 \zeta_2 \\
\langle \epsilon_{22} | \zeta_1, \zeta_2 \rangle &= \gamma \zeta_2 (1 - \zeta_1 - \zeta_2) - \beta \zeta_1 \zeta_2
\end{aligned} \tag{4.38}$$

where

$$\alpha = \frac{\varepsilon_{11} + \varepsilon_{12}}{\langle \xi_1 (1 - \xi_1 - \xi_2) \rangle} \quad \beta = \frac{\varepsilon_{12}}{\langle \xi_1 \xi_2 \rangle} \quad \gamma = \frac{\varepsilon_{22} + \varepsilon_{12}}{\langle \xi_2 (1 - \xi_1 - \xi_2) \rangle} \tag{4.39}$$

We can *define* the bivariate beta PDF to be the stationary solution to the FP equation with this diffusion matrix.

It is remarkable that this result can be extended to N components by inspection:

$$
\begin{aligned}
\langle \epsilon_{ii} | \boldsymbol{\zeta} \rangle &= \alpha_i \zeta_i \left(1 - \sum_j \zeta_j \right) - \sum_j \beta_{ij} \zeta_i \zeta_j \\
\langle \epsilon_{ij} | \boldsymbol{\zeta} \rangle &= \beta_{ij} \zeta_i \zeta_j
\end{aligned}
\tag{4.40}
$$

where the coefficients α_i and β_{ij} are determined by the constraints $\langle \langle \epsilon_{ij} | \boldsymbol{\xi} \rangle \rangle = \varepsilon_{ij}$

We can thus *define* the multi-variate beta PDF to be the stationary solution to the FP model with this diffusion matrix

4.5 Prospects for Mixing Model Improvements

For reactive scalars, in a PDF context the key unknown terms are the conditional scalar dissipations $\langle \boldsymbol{\epsilon} | \boldsymbol{\phi} \rangle$, which depend on Da and premixed/non-premixed, etc.

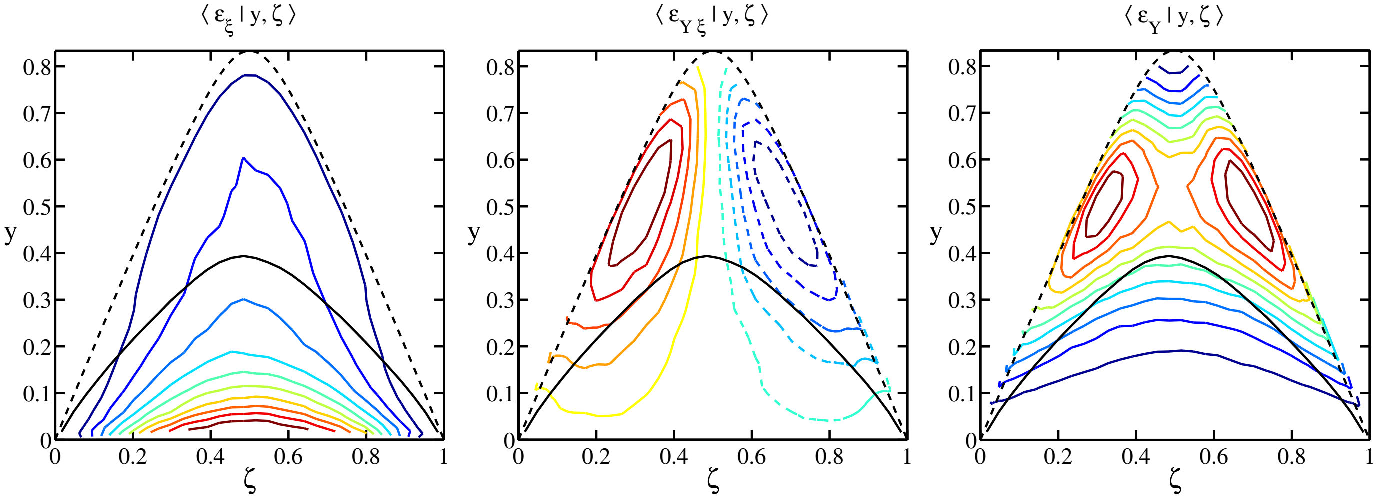
Unlike for inert scalars (e.g. mixture fraction), the functional dependence of $\langle \boldsymbol{\epsilon} | \boldsymbol{\phi} \rangle$ on $\boldsymbol{\phi}$ can be quite complex

The modeling challenge for reacting scalars is to find approximate forms for $\langle \boldsymbol{\epsilon} | \boldsymbol{\phi} \rangle$

For nonpremixed flows, it is useful to decompose $\langle \boldsymbol{\epsilon} | \boldsymbol{\phi} \rangle$ into mixture fraction ξ and reaction-progress variable Y (zero at inlets)

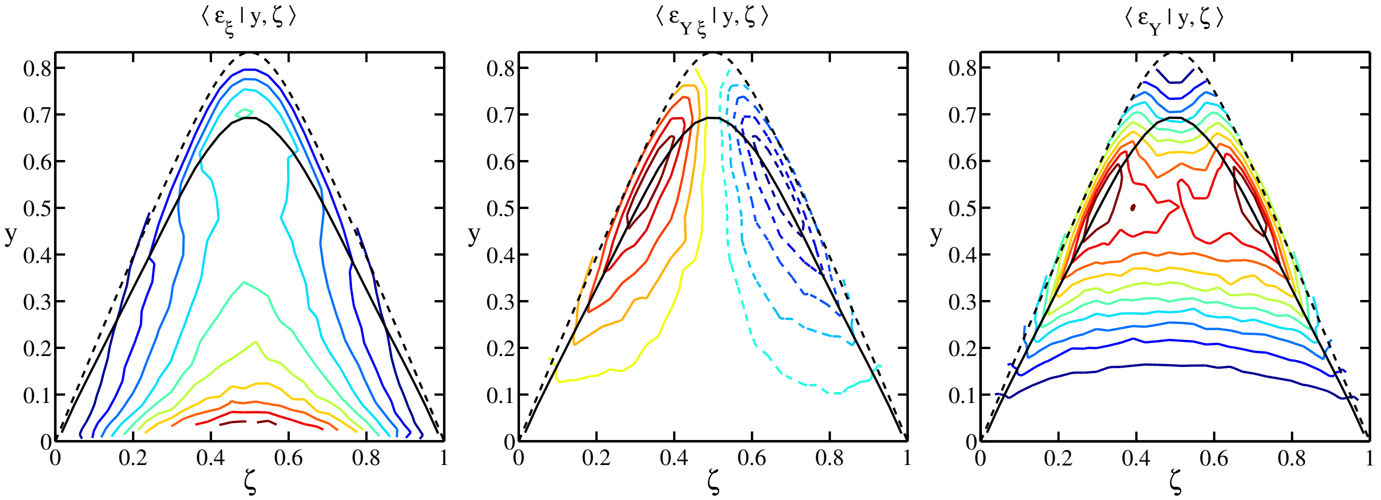
One-step reaction: $A + B \leftrightarrow Y$ where Y is product (temperature)

$Da = 3 \times 10^4$**:**



Y is bounded above due to chemistry (element balances) $\Rightarrow$ shapes of $\langle \epsilon | y, \zeta \rangle$

$Da = 8 \times 10^4$**:**



Y is strongly correlated with mixture fraction $\xi \Rightarrow$ use conditional model where Y statistics depend on $\xi = \zeta$, e.g., $\langle Y|\zeta \rangle$ is the conditional mean of Y

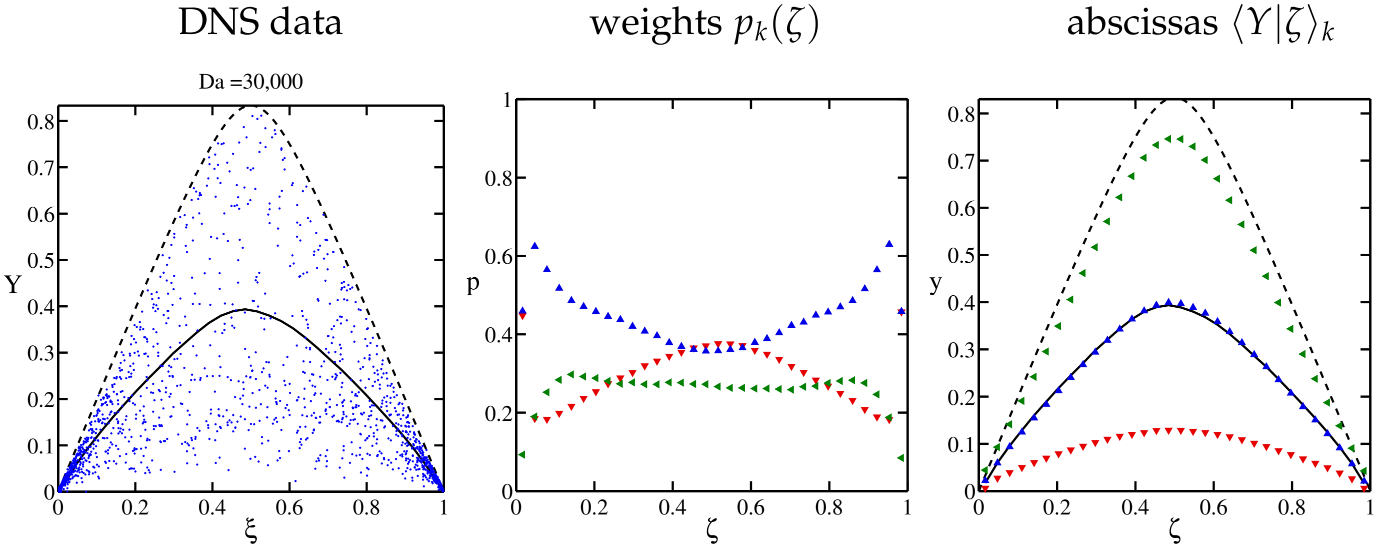
Use PDF transport equation for $f_\xi(\zeta)$ (i.e. PDF of mixture fraction) and quadrature to model conditional PDF $f_{Y|\xi}(y|\zeta)$:

$$f_{Y|\xi}(y|\zeta) \approx \sum_{k=1}^{N} p_k(\zeta)\delta(y - \langle Y|\zeta\rangle_k) \tag{4.41}$$

where weights p_k and abscissas $\langle Y|\zeta\rangle_k$ are found from conditional moments:

$$\langle Y^\alpha|\zeta\rangle = \sum_{k=1}^{N} p_k(\zeta)\langle Y|\zeta\rangle_k^\alpha \quad \alpha = 0, 1, \ldots, 2N-1 \tag{4.42}$$

As in other conditional models, $f_\xi(\zeta)$ and $\langle \epsilon_\xi|\zeta\rangle$ are assumed to be known



DNS data

weights $p_k(\zeta)$

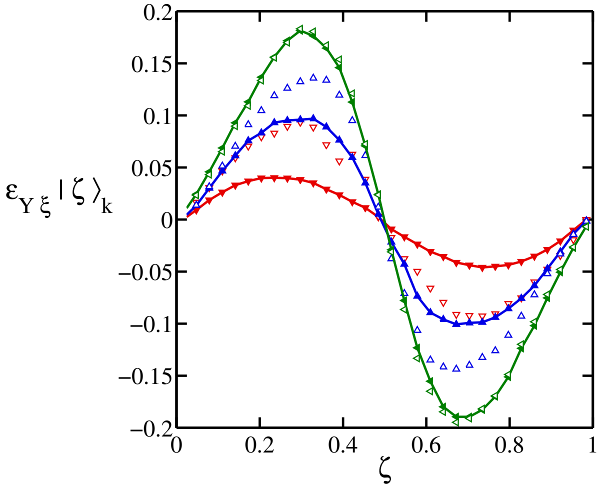
abscissas $\langle Y|\zeta\rangle_k$

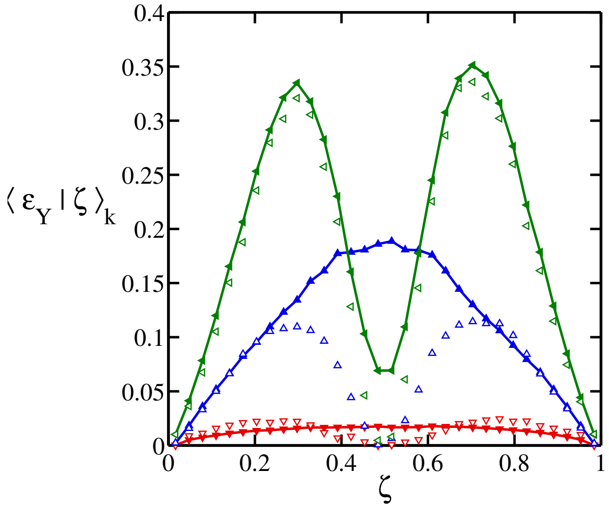
Provides models for the conditional dissipations:

$$\langle \epsilon_{Y\xi}|y,\zeta\rangle f_{Y|\xi} \approx \sum_{k=1}^{N} p_k(\zeta)\delta(y-\langle Y|\zeta\rangle_k)\langle \epsilon_{Y\xi}|\zeta\rangle_k \tag{4.43}$$

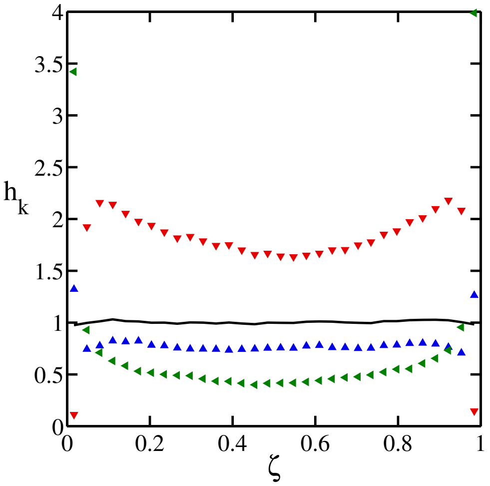
where

$$\langle \epsilon_{Y\xi}|\zeta\rangle_k = \langle \epsilon_\xi|\zeta\rangle h_k(\zeta)\frac{\partial\langle Y|\zeta\rangle_k}{\partial\zeta} \quad \langle \epsilon_Y|\zeta\rangle_k = \langle \epsilon_\xi|\zeta\rangle h_k(\zeta)\left(\frac{\partial\langle Y|\zeta\rangle_k}{\partial\zeta}\right)^2 + \mathcal{E}_k \tag{4.44}$$





where scalar dissipation fluctuations are modeled by h_k:



Model has the form of multiple "flamelets" with interaction terms:

$$\frac{\partial \langle Y|\zeta\rangle_k}{\partial t} = \frac{1}{2}\langle \epsilon_\xi|\zeta\rangle h_k \frac{\partial^2 \langle Y|\zeta\rangle_k}{\partial \zeta^2} + S_Y(\langle Y|\zeta\rangle_k, \zeta) + M_k \tag{4.45}$$

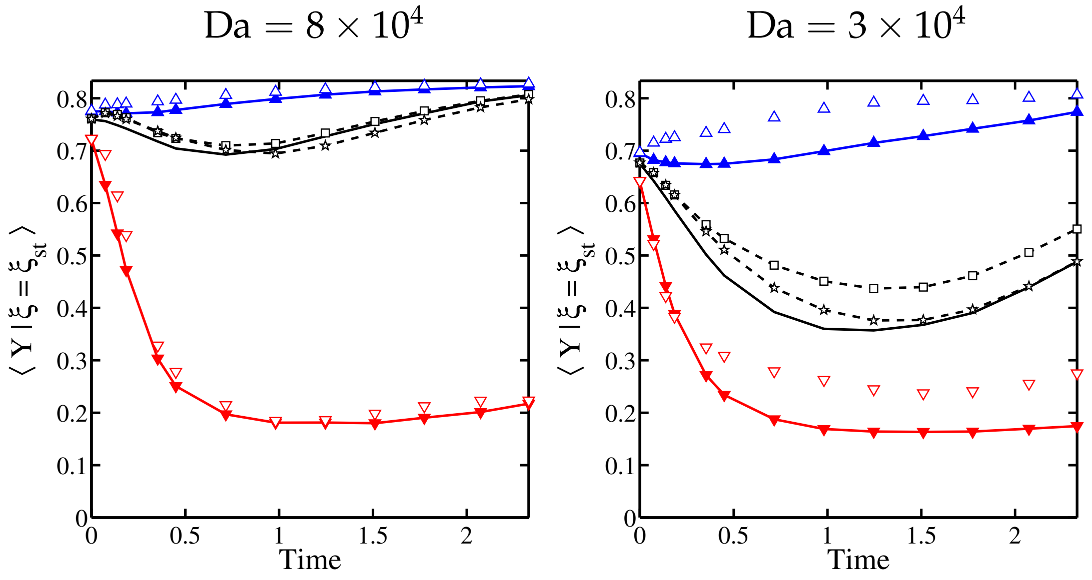
and

$$\frac{\partial p_k f_\xi}{\partial t} = -\frac{1}{2}\frac{\partial^2}{\partial \zeta^2}\left(\langle \epsilon_\xi | \zeta \rangle h_k p_k f_\xi\right) + G_k f_\xi \tag{4.46}$$

where $\langle \epsilon_\xi | \zeta \rangle$ and f_ξ are known (e.g. beta PDF)

The conditional micromixing model is represented by M_k and G_k, and controls the rate of "exchange" between the N environments ⇒ DNS suggests IEM + "engulfment", depending on Da

Structure of model allows for coexistence of "burning" and "extinguished" environments due to fluctuations in scalar dissipation rate (i.e. h_k), which are required to correctly predict partial extinction and re-ignition:


Da = 8×10^4

Da = 3×10^4

Extinction/re-ignition increases with decreasing Da

General Conclusion: *Micromixing models for multiple scalars must contain information about small-scale correlations between scalar gradients*

This is especially important for combusting flows where fluctuations in scalar dissipation lead to local extinction
Models that do not account for variations in ϵ_ξ (e.g. $\langle \epsilon_\xi \rangle_k$) cannot predict local extinction; however, just adding a fluctuating scalar dissipation term is not enough!

The (implied) model for $\langle \boldsymbol{\epsilon} | \boldsymbol{\phi} \rangle$ describes the small-scale correlations $\Rightarrow$ it is important to choose it carefully!