Mass Transfer in Turbulent Flow

ChEn 6603

References:

- S. B. Pope. Turbulent Flows. Cambridge University Press, New York, 2000.
- D. C. Wilcox. Turbulence Modeling for CFD. DCW Industries, La Caada CA, 2000.
- H. Tennekes and J. L. Lumley. A First Course in Turbulence. MIT Press, Cambridge, MA, 1972.
- R. O. Fox. Computational Models for Turbulent Reacting Flows. Cambridge University Press, 2003.

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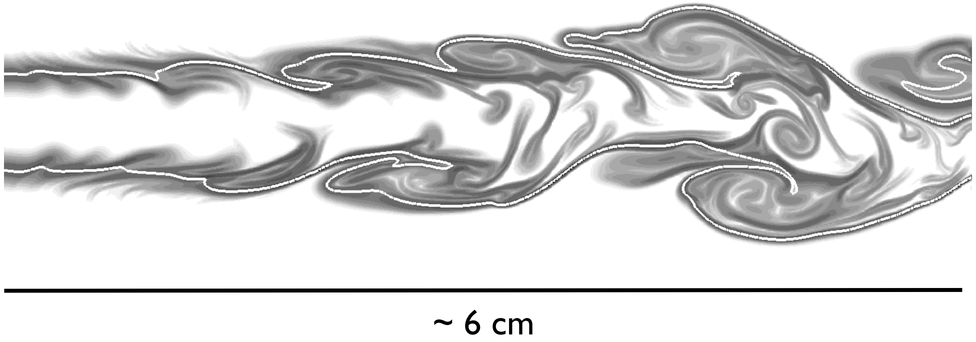
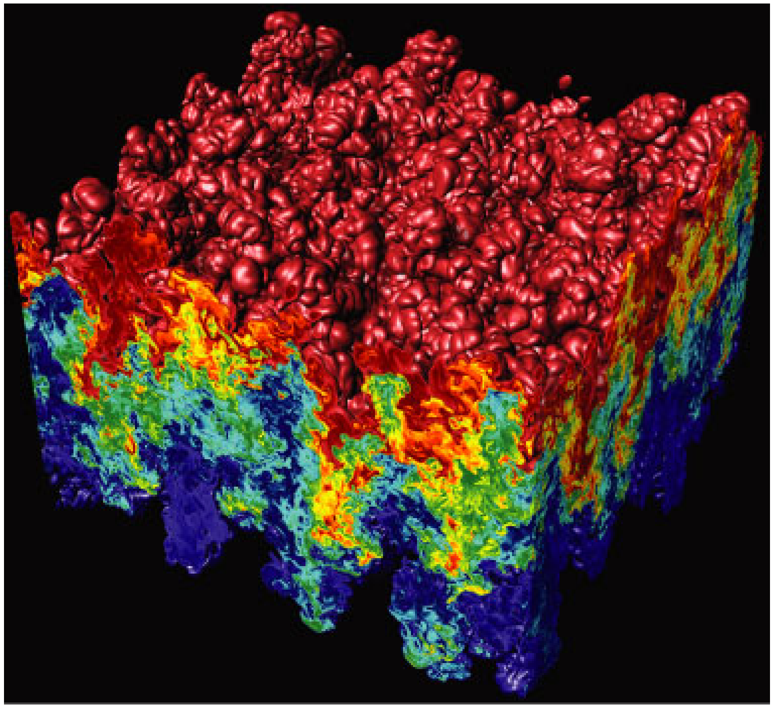
Mixing in reacting flow (DNS)



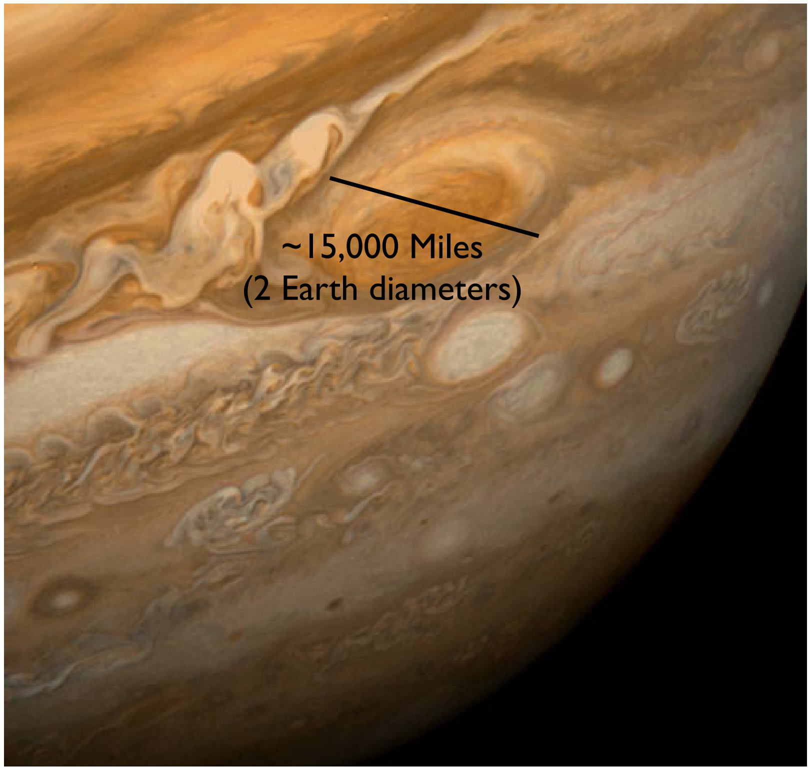
Methane pool fire

Rayleigh-Taylor instability (DNS calculation)



William H. Cabot and Andrew W. Cook
Nature Physics 2, 562 - 568 (2006)

Photograph of Jupiter from Voyager



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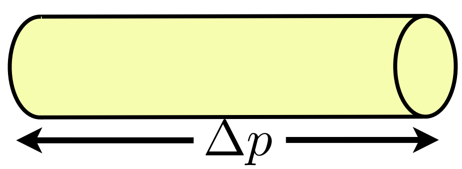
Origins of Turbulence

Energy balance perspective.

- Consider steady, isothermal, fully developed turbulent flow in a horizontal pipe
  - Increasing pressure drop does not increase flow rate proportionally. Why? Where is the energy going? How?
  - Work done by pressure forces balanced by work done by viscous forces
- Energy provided at "large" scales, dissipated at "small" scales.
  - Length scales reduce to meet demand of energy balance.
  - Smaller length scales ⇒ steeper gradients ⇒ more dissipation.



Kinetic energy equation:

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho k \mathbf{v}) = -\mathbf{v} \cdot \nabla \cdot \tau - \mathbf{v} \cdot \nabla p + \rho \sum_{i=1}^{n} \omega_i \mathbf{v} \cdot \mathbf{f}_i$$

What assumptions?

$$0 = \underbrace{\boxed{\mathbf{v} \cdot \nabla p}}_{\text{pressure work}} + \underbrace{\boxed{\mathbf{v} \cdot \nabla \cdot \tau}}_{\text{viscous dissipation}}$$

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Velocity Length Scales

L - largest length scale (m)
η - smallest length scale (m)
U - velocity at L-scale (m/s)

ν - kinematic viscosity (m^2/s) = μ/ρ
ε - kinetic energy dissipation rate (m^2/s$^2 \cdot$ s^{-1})

Most kinetic energy is contained in "large" length scales (L). It is dissipated primarily at "smallest" (Kolmogorov) length scales (η) by molecular viscosity (ν).

Can we form a length scale from ε and ν?

$$\eta \propto \left(\frac{\nu^3}{\epsilon}\right)^{1/4}$$

$$\epsilon \propto \frac{UU}{L/U}$$

kinetic energy

"integral" or "large" time scale

Note: ϵ doesn't depend on ν. ν just determines the smallest length scale in the flow.

$$\begin{aligned}\eta &\propto \left(\frac{\nu^3}{\epsilon}\right)^{1/4} \\ &\propto L^{1/4}\left(\frac{\nu}{U}\right)^{3/4}\end{aligned}$$

$$\boxed{\frac{L}{\eta} \propto \left(\frac{LU}{\nu}\right)^{3/4} = \mathrm{Re}^{3/4}}$$

Key result! Tells us how length-scales separate!

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Scalar Length Scales

ℓ_B - smallest scalar length scale (Batchelor scale)

$$\mathrm{Sc} \equiv \frac{\nu}{D}$$

Sc > 1

"mixing paint" - $\ell_B < \eta$ - scalar only feels straining from smallest velocity scales.
(mass diffuses slower than momentum)

$$\begin{aligned}
\ell_B^2 &\propto Dt \\
\ell_B &\propto D^{1/2}\left(\frac{\nu}{\epsilon}\right)^{1/4} \\
\frac{\ell_B}{\eta} &\propto D^{1/2}\left(\frac{\nu}{\epsilon}\right)^{1/4}\left(\frac{\nu^3}{\epsilon}\right)^{-1/4} \\
&\propto \left(\frac{D}{\nu}\right)^{1/2} = \mathrm{Sc}^{-1/2}
\end{aligned}$$

Form a time scale from the "Kolmogorov" time scale (*i.e.* from ν and ε).

$$\boxed{\frac{L}{\ell_B} = \frac{L}{\eta}\frac{\eta}{\ell_B} \propto \mathrm{Re}^{3/4}\mathrm{Sc}^{1/2}}$$

Sc < 1

$\ell_B > \eta$ - at ℓ_B, there are still velocity fluctuations, but the scalar field is uniform
(mass diffuses faster than momentum)

$$\begin{aligned}
\ell_B &\propto \left(\frac{D^3}{\epsilon}\right)^{1/4} \\
\frac{\ell_B}{\eta} &\propto \left(\frac{D}{\epsilon}\right)^{1/4}\left(\frac{\nu^3}{\epsilon}\right)^{-1/4} \\
&\propto \left(\frac{D}{\nu}\right)^{3/4} = \mathrm{Sc}^{-3/4}
\end{aligned}$$

Relevant parameters are D, ε.
(ν only dominant near η).

$$\boxed{\frac{L}{\ell_B} = \frac{L}{\eta}\frac{\eta}{\ell_B} \propto \mathrm{Re}^{3/4}\mathrm{Sc}^{3/4}}$$

Gases: $\mathrm{Sc} \approx 1$, Liquids: $\mathrm{Sc} \sim 10^3$.

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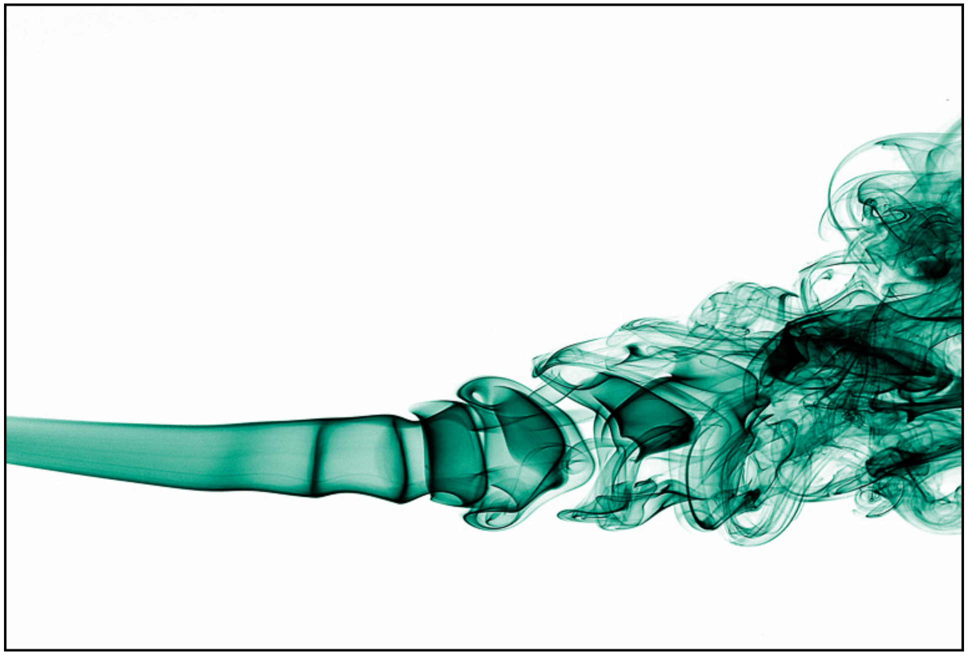
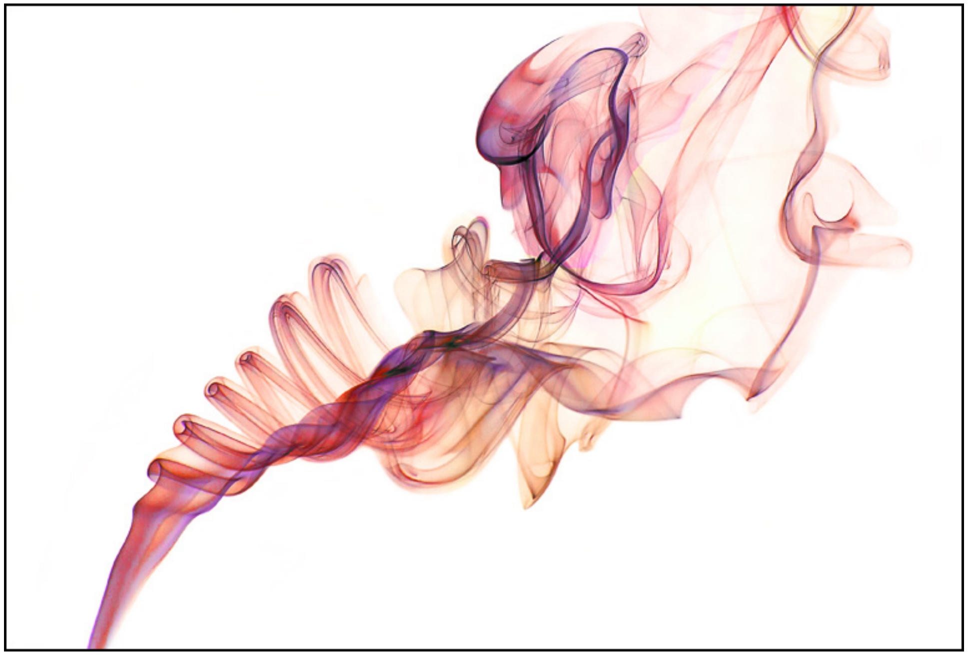
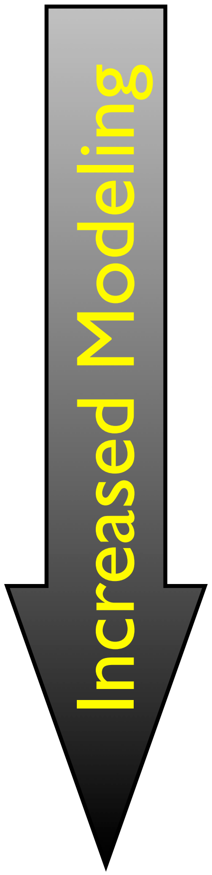
$Sc \rightarrow \infty$





http://sensitivelight.com/smoke2

Solution Options



- Direct Numerical Simulation (DNS)
  - Resolve all time/length scales by solving the governing equations directly.
  - Restricted to small problems.
  - Cost scales as Re^3 for turbulence alone! (Species with $\mathrm{Sc}>1$, and/or complex chemistry could further increase cost)
    - ($L/\eta \sim \mathrm{Re}^{3/4}$, 3D, time)
- Large Eddy Simulation (LES)
  - Resolve "large" spatial & temporal scales
  - Model "small" (unresolved) time/space scales
- Reynolds-Averaged Navier Stokes (RANS)
  - Time-averaged.
  - Describes only mean features of the flow.
- Model all effects of the flow field
  - Useful only for some classes of problems (usually interfaces like walls)
  - Commonly done in heat transfer & mass transfer (also for some problems involving aerodynamics)

Time/Ensemble Averaging (RANS)

Constant density, viscosity:
$$\begin{aligned}\nabla\cdot\mathbf{v} &= 0\\ \frac{\partial\mathbf{v}}{\partial t} &= -\nabla\cdot(\mathbf{v}\otimes\mathbf{v}) - \tfrac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v}\end{aligned}$$

$\langle\phi\rangle$ - ensemble average of ϕ.
$\langle\nabla\phi\rangle = \nabla\langle\phi\rangle$

$$\bar{\phi} = \langle\phi\rangle$$

Continuity:
$$\begin{aligned}\langle\nabla\cdot\mathbf{v}\rangle &= \langle 0\rangle\,,\\ \nabla\cdot\langle\mathbf{v}\rangle &= 0,\\ \nabla\bar{\mathbf{v}} &= 0\end{aligned}$$

Momentum:
$$\begin{aligned}\left\langle\frac{\partial\mathbf{v}}{\partial t}\right\rangle &= \left\langle -\nabla\cdot\mathbf{v}\mathbf{v} - \frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v}\right\rangle,\\ \frac{\partial\langle\mathbf{v}\rangle}{\partial t} &= -\nabla\cdot\langle\mathbf{v}\mathbf{v}\rangle - \frac{1}{\rho}\nabla\langle p\rangle + \nu\nabla^2\langle\mathbf{v}\rangle\,,\\ \frac{\partial\bar{\mathbf{v}}}{\partial t} &= -\nabla\cdot\overline{\mathbf{v}\mathbf{v}} - \frac{1}{\rho}\nabla\bar{p} + \nu\nabla^2\bar{\mathbf{v}}\end{aligned}$$

index (Einstein) notation:
$$\frac{\partial}{\partial x_j}\boxed{\overline{v_i v_j}} + \frac{1}{\rho}\frac{\partial\bar{p}}{\partial x_i} - \nu\frac{\partial}{\partial x_j}\frac{\partial\bar{v}_j}{\partial x_i} = 0$$

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The Closure Problem

$\phi' \equiv \phi - \bar{\phi}$ "Fluctuating" component

$$\begin{aligned}\overline{v_i v_j} &= \overline{(\bar{v}_i + v_i')(\bar{v}_j + v_j')} \\ &= \overline{\bar{v}_i \bar{v}_j} + \overline{\bar{v}_i v_j'} + \overline{v_i' \bar{v}_j} + \overline{v_i' v_j'}\end{aligned}$$

$$\bar{\phi}' = 0 \qquad \overline{\bar{\phi}\varphi'} = 0 \qquad \bar{\bar{\phi}} = \bar{\phi}$$

$$\overline{v_i v_j} = \bar{v}_i \bar{v}_j + \overline{v_i' v_j'}$$

$$\frac{\partial}{\partial x_j}\left(\bar{v}_i \bar{v}_j\right) + \frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - \nu \frac{\partial}{\partial x_j}\frac{\partial \bar{v}_j}{\partial x_i} + \boxed{\frac{\partial}{\partial x_j}\left(\overline{v_i' v_j'}\right)} = 0$$

Model this term using a "gradient diffusion" model.

$$\frac{\partial}{\partial x_j}\left(\overline{v_i' v_j'}\right) \approx -\frac{\mu_t}{\rho}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\bar{v}_j$$

$$\frac{\partial}{\partial x_j}\left(\bar{v}_i \bar{v}_j\right) + \frac{1}{\rho}\frac{\partial \bar{p}}{\partial x_i} - (\nu + \nu_t)\frac{\partial}{\partial x_j}\frac{\partial \bar{v}_j}{\partial x_i} = 0$$

For large Re, $\mu_t \gg \mu$ (molecular viscosity is negligible).

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Time-Averaged Species Equations

constant properties & density...

$$\nabla \cdot \overline{\omega_i \mathbf{v}} + \frac{1}{\rho} \nabla \cdot \bar{\mathbf{j}}_i = \boxed{\bar{s}_i}/\rho$$

A very difficult problem...

$$\nabla \cdot (\bar{\omega}_i \bar{\mathbf{v}}) + \frac{1}{\rho} \nabla \cdot \bar{\mathbf{j}}_i + \nabla \cdot \left(\overline{\omega_i' \mathbf{v}'} \right) = \bar{s}_i/\rho$$

$$\nabla \cdot (\bar{\omega}_i \bar{\mathbf{v}}) + \frac{1}{\rho} \nabla \cdot \left(\bar{\mathbf{j}}_i + \mathbf{j}_{i,\mathrm{turb}} \right) = \bar{s}_i/\rho$$

MODEL for turbulent species diffusive flux:

$$\mathbf{j}_{i,\mathrm{turb}} = -\rho D^\circ_{\mathrm{turb}} \nabla \bar{\omega}_i$$

$$\mathrm{Sc}_{\mathrm{turb}} = \frac{\nu_{\mathrm{turb}}}{D^\circ_{\mathrm{turb}}} = \frac{\mu_{\mathrm{turb}}}{\rho D^\circ_{\mathrm{turb}}}$$

- D°_{turb} - turbulent diffusivity (for mass flux relative to mass avg. velocity)
- μ_{turb} - eddy viscosity
- Typically, $\mathrm{Sc}_{\mathrm{turb}}$ is specified.

@ Large Re, $\mathbf{j}_{i,\mathrm{turb}} \gg \mathbf{j}_i$
(molecular diffusion is negligible)

$$\nabla \cdot (\bar{\omega}_i \bar{\mathbf{v}}) + \frac{1}{\rho} \nabla \cdot \mathbf{j}_{i,\mathrm{turb}} = \bar{s}_i/\rho$$

Multicomponent effects are irrelevant at sufficiently high Re.

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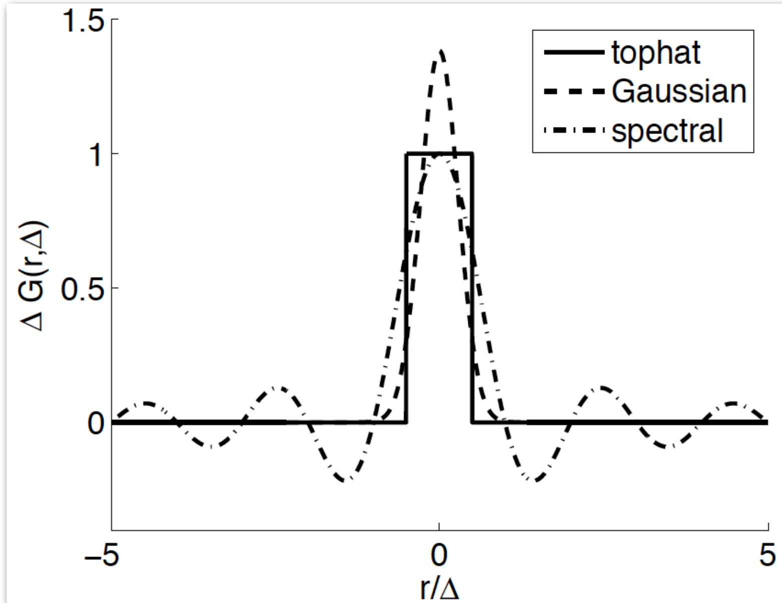
Spatial Averaging (LES)

$$\bar{\phi} \equiv \int_{-\infty}^{\infty} \phi(\mathbf{x}) G(\mathbf{x}) \mathrm{d}\mathbf{x}$$

$G(\mathbf{x})$ - filter kernel function

removes "high wavenumber" components of ϕ.

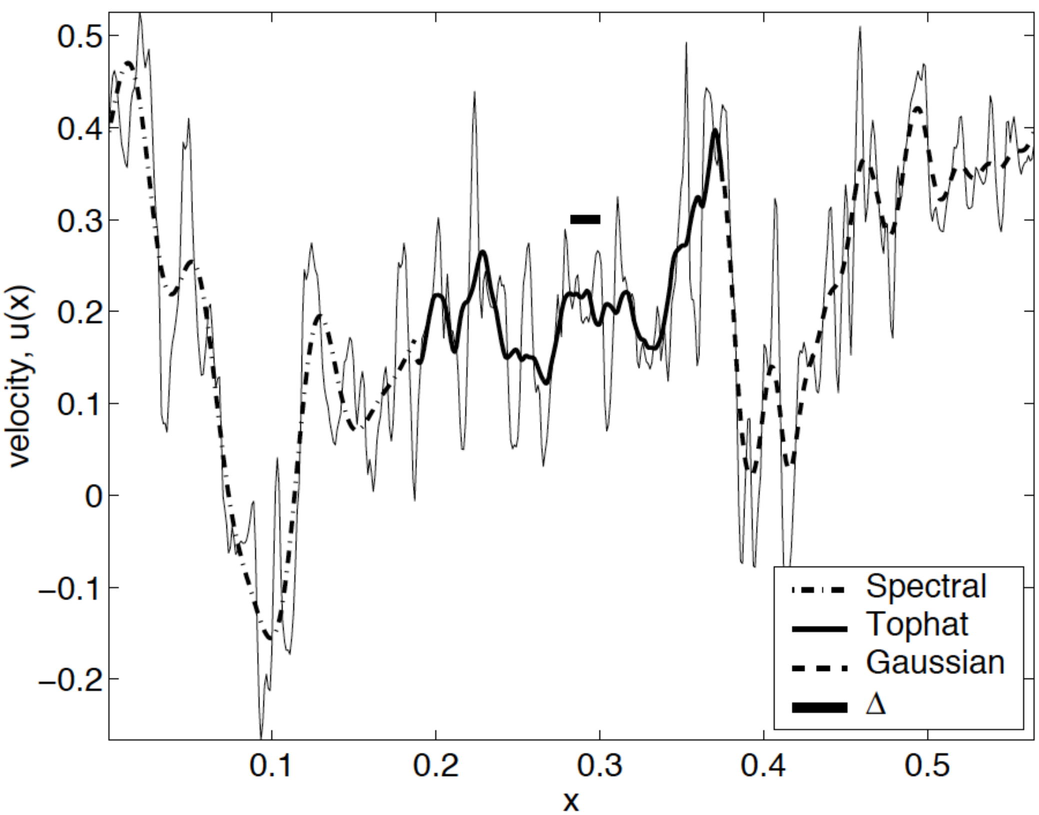


Courtesy R.J. McDermott

$$\bar{\bar{\phi}} \neq \bar{\phi}$$

$$\bar{\phi'} \neq = 0$$

$$\overline{\bar{\phi}\varphi'} \neq 0$$



Courtesy R. J. McDermott

- Filter governing equations. (similar procedure as for RANS, but a little more complicated).
- Write models for unclosed terms.
- Solve filtered equations (for filtered variables).
- Provides time-varying solutions at a "coarse" level.

Variable Density

$$\frac{\partial \rho \omega_i}{\partial t} = -\nabla \cdot \rho \omega_i \mathbf{v} - \nabla \cdot \mathbf{j}_i + s_i.$$

Favre-averaging (RANS)
Favre-filtering (LES)

$$\tilde{\phi} \equiv \frac{\overline{\rho \phi}}{\bar{\rho}} \longrightarrow \bar{\rho}\tilde{\phi} = \overline{\rho \phi}$$

$$\begin{aligned} \frac{\partial \bar{\rho}\tilde{\omega}_i}{\partial t} &= -\nabla \cdot \bar{\rho}\widetilde{\omega_i \mathbf{v}} - \nabla \cdot \bar{\mathbf{j}}_i + \bar{s}_i \\ &= -\nabla \cdot \bar{\rho}\tilde{\omega}_i \tilde{\mathbf{v}} - \nabla \cdot \left(\bar{\mathbf{j}}_i + \mathbf{j}_{i,\mathrm{turb}} \right) + \bar{s}_i \end{aligned}$$

Leads to many additional complications, most of which are typically ignored...

example:

$$\begin{aligned} \bar{\mathbf{j}}_i &= \sum_{k=1}^{n} \overline{\rho D_{ik}^{o} \nabla \omega_k} \\ &\stackrel{?}{\approx} \bar{\rho} \sum_{k=1}^{n} \bar{D}_{ik}^{o} \nabla \tilde{\omega}_k \end{aligned}$$

Δ = "filter width"

LES: if $\Delta \gg \ell_B, \ \Delta \gg \eta$ then $\mathbf{j}_{i,\mathrm{turb}} \gg \bar{\mathbf{j}}_i$

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