Modeling of Conserved Scalars under Supercritical Pressure Conditions

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Computations performed on the Jet Propulsion Laboratory/NASA and NERSC supercomputers

Outline

- Background
  - Difference between the equations solved for supercritical-pressure flows using Direct Numerical Simulation (DNS) and those for atmospheric-pressure using DNS
  - How does it affect the characteristics of the flow?
  - How does it affect Large Eddy Simulation (LES) modeling?

- The Subgrid-Scale (SGS) scalar variance under supercritical-pressure conditions (*Phys. Fluids,* 23(8), doi:085101 (22 pages), 2011)
  - Why are we interested in this subject prior to conducting DNS of supercritical-pressure reactive flows?
  - Results

- Summary and conclusions

Background

- Motivation → Modeling of very high pressure flows with special emphasis on diesel, HCCI and future engines

- Distinctive features of supercritical flows
  - experiments: ‘Fingers’ of fluid emerging from jets (e.g. Chehroudi et al. 1999, 2002; Mayer et al. 1996, 1998; Oschwald and Schik 1999)
  - DNS of mixing layers: High density-gradient magnitude regions ↔ ‘fingers’, arising from initial density stratification and from mixing (e.g. Miller et al. 2001; Okong'o et al. 2002)

- Want to develop models for LES of high-p turbulent reactive flows
  - Check whether atmospheric-p models apply → use DNS as a tool
  - When atmospheric-p models do not apply → develop appropriate models

- Goal of LES → duplicate on a local basis the DNS features

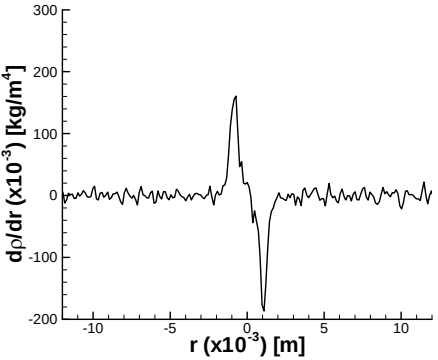
Some experimental data, 1 of 2

Pch=4.14 MPa
Reynolds=66,609
Mass flow=350 mg/s
Inj. Velocity=14.1 m/s

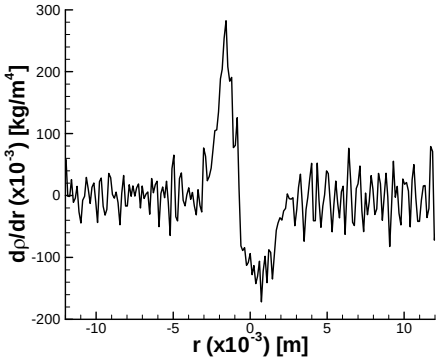
Pch=9.19 MPa
Reynolds=42,830
Mass flow=350 mg/s
Inj. Velocity=11.7 m/s

N_2 into N_2 injection
p_c = 3.4 MPa, T_c =126.2 K

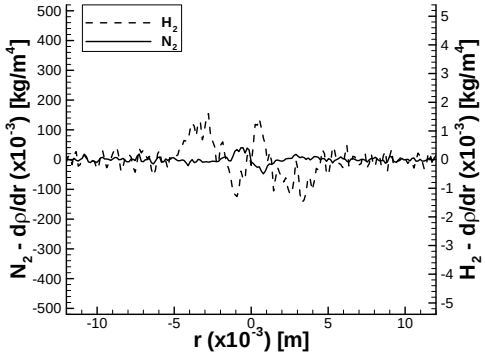
Some experimental data, 2 of 2



$Re=1.15\times10^5$

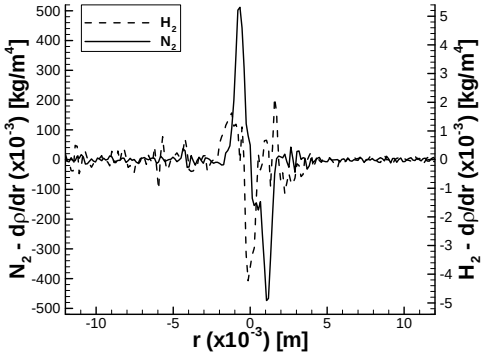


$Re=1.26\times10^5$



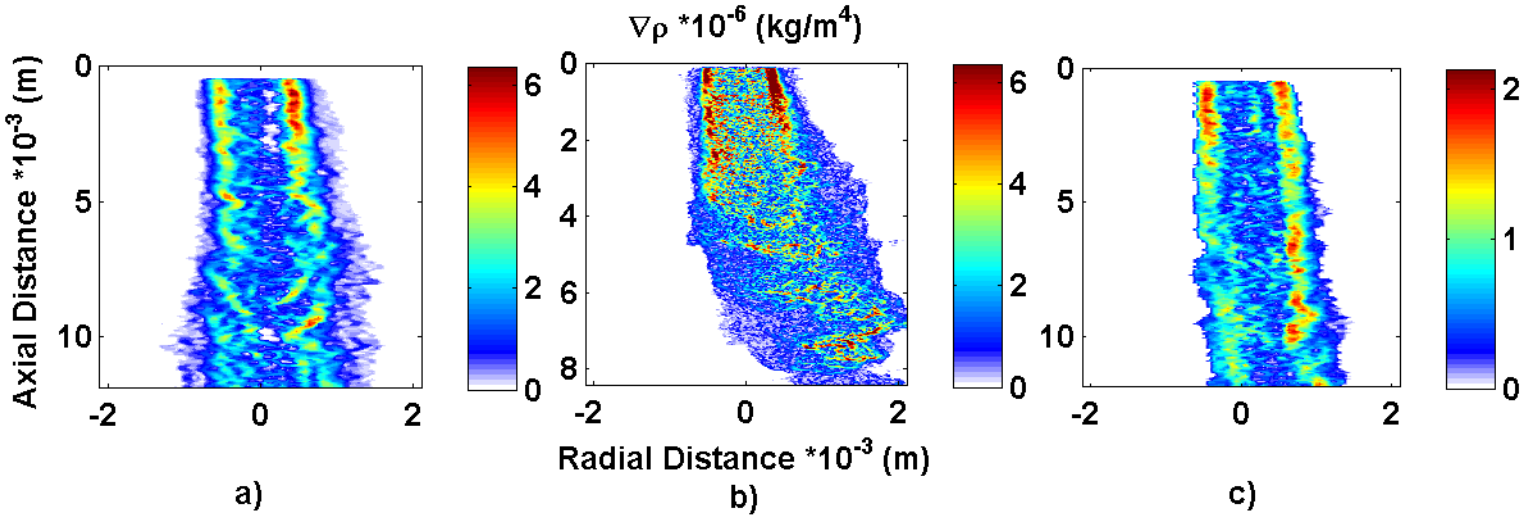
$Re_{N2}=3.14\times10^4$

$Re_{H2}=1.01\times10^4$



$Re_{N2}=1.22\times10^5$

$Re_{H2}=2.02\times10^4$



$Re_{jet} = 29{,}200$

$Re_{jet} = 58{,}600$

$Re_{jet} = 57{,}500$

Difference between supercritical-p and atmospheric-p formulations, 1 of 3

- Real-gas equations of state (here Peng-Robinson) for mixtures

$$p = R_u T/(v_{PR} - b_m) - a_m/(v_{PR}^2 + 2b_m v_{PR} - b_m^2)$$

$$v_S = v - v_{PR} \quad , \quad v = m/\rho$$

$$a_m = \sum_{i,j} X_i X_j a_{ij}(T)$$

$$b_m = \sum_i X_i b_i$$

where v_s is the volume shift (Okong'o et al., 2002)

$$v_S = \sum X_\alpha \frac{\partial G_\alpha^0}{\partial p}$$

and $G^0{}_\alpha$ is a curve-fitted reference Gibbs function (Harstad et al., 1997)

Difference between supercritical-p and atmospheric-p formulations, 2 of 3

- Species-mass and heat fluxes from fluctuation-dissipation theory (Keizer , 1987)

$$\mathbf{J}_\alpha = -\sum_{\beta=1}^{N} \frac{m_\alpha m_\beta}{m} (\rho D_{m,\alpha\beta} Y_\alpha Y_\beta) \mathbf{\Lambda}'_{\alpha\beta},$$

$$\mathbf{q} = -\lambda \nabla T - \frac{1}{2} R_u T \sum_{\beta=1}^{N} \sum_{\alpha=1}^{N} \alpha_{IK,\alpha\beta} (\rho D_{m,\alpha\beta} Y_\alpha Y_\beta) \mathbf{\Lambda}'_{\alpha\beta}$$

$$\mathbf{\Lambda}'_{\alpha\beta} = \frac{m}{m_\beta m_\alpha} \alpha_{IK,\alpha\beta} \frac{\nabla T}{T} + \frac{1}{R_u} \left[\frac{\nabla(\chi_\alpha/T)}{m_\alpha} - \frac{\nabla(\chi_\beta/T)}{m_\beta} \right]$$

$$\nabla\left(\frac{\chi_\alpha}{T}\right) = -\frac{h_\alpha}{T^2} \nabla T + \frac{v_\alpha}{T} \nabla p + R_u \sum_{\substack{\beta=1 \\ \beta\neq\alpha}}^{N} \frac{\alpha_{D\alpha\beta}}{X_\alpha} \nabla X_\beta$$

Binary-species case

$$\mathbf{j}_2(\psi) = B_Y(\psi) \nabla Y_2(\phi) + B_T(\psi) \nabla T(\phi) + B_P(\psi) \nabla p(\phi)$$

$$\mathbf{q}_{IK}(\psi) = C_Y(\psi) \nabla Y_2(\phi) + C_T(\psi) \nabla T(\phi) + C_P(\psi) \nabla p(\phi)$$

B's and C's are functions of ψ, m_α's, R_u, α_{IK}, α_D, Sc, Pr, μ, v, h.

Difference between supercritical-p and atmospheric-p formulations, 3 of 3

- Calculation of the mass diffusion factors

$$\alpha_{D\alpha\beta} = \partial X_\alpha / \partial X_\beta + X_\alpha \partial \ln \gamma_\alpha / \partial X_\beta$$

where

$$\gamma_\alpha \equiv \varphi_\alpha / \varphi_\alpha^o$$

and φ is the fugacity with superscript 0 denoting the pure species.

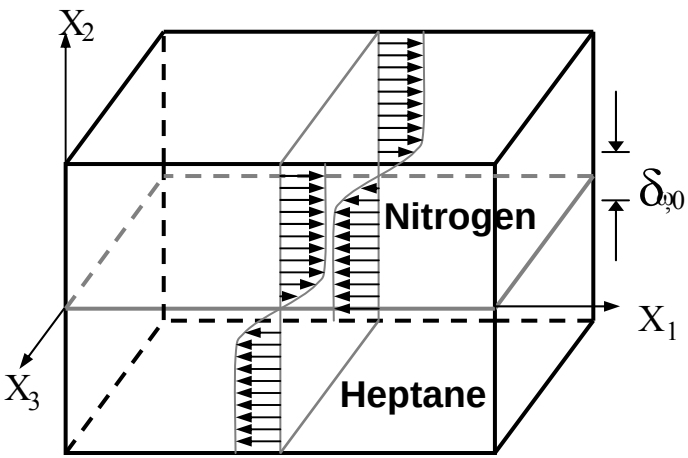
- Measures of departure from
  - Perfect gas: Compression factor $Z = p/(\rho T R_u / m)$
  - Mixture ideality: Mass diffusion factors $\alpha_D = 1 + X_\alpha \frac{\partial \ln(\varphi_\alpha)}{\partial X_\alpha}$

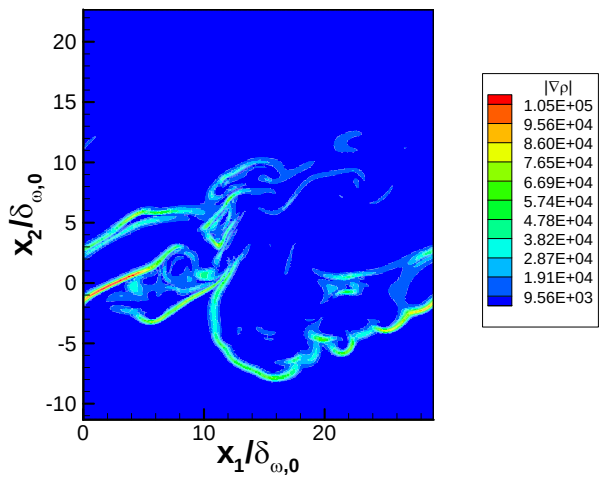
    for a binary-species system

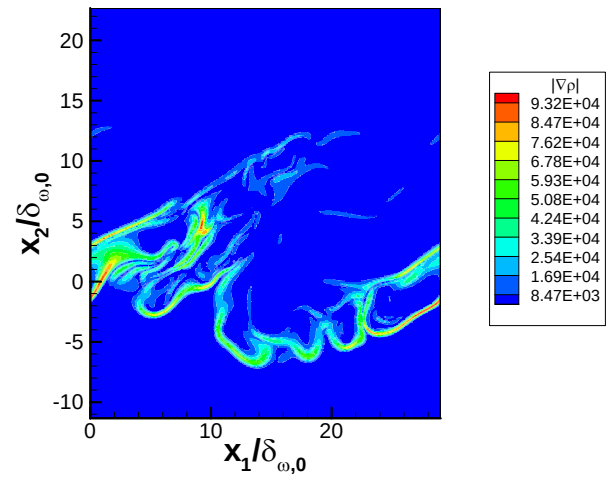
→ DNS is particularly well suited for
- understanding the flow features
- extracting information utilizable for LES

Are SGS-flux models sufficient when the small-scales are anisotropic?

- Small scales anisotropy ⇔ there are gradients at the small scales
- Can be checked using DNS
- Example: mixing of heptane/nitrogen at p=60 atm (Okong'o and Bellan, *JFM*, 2002)







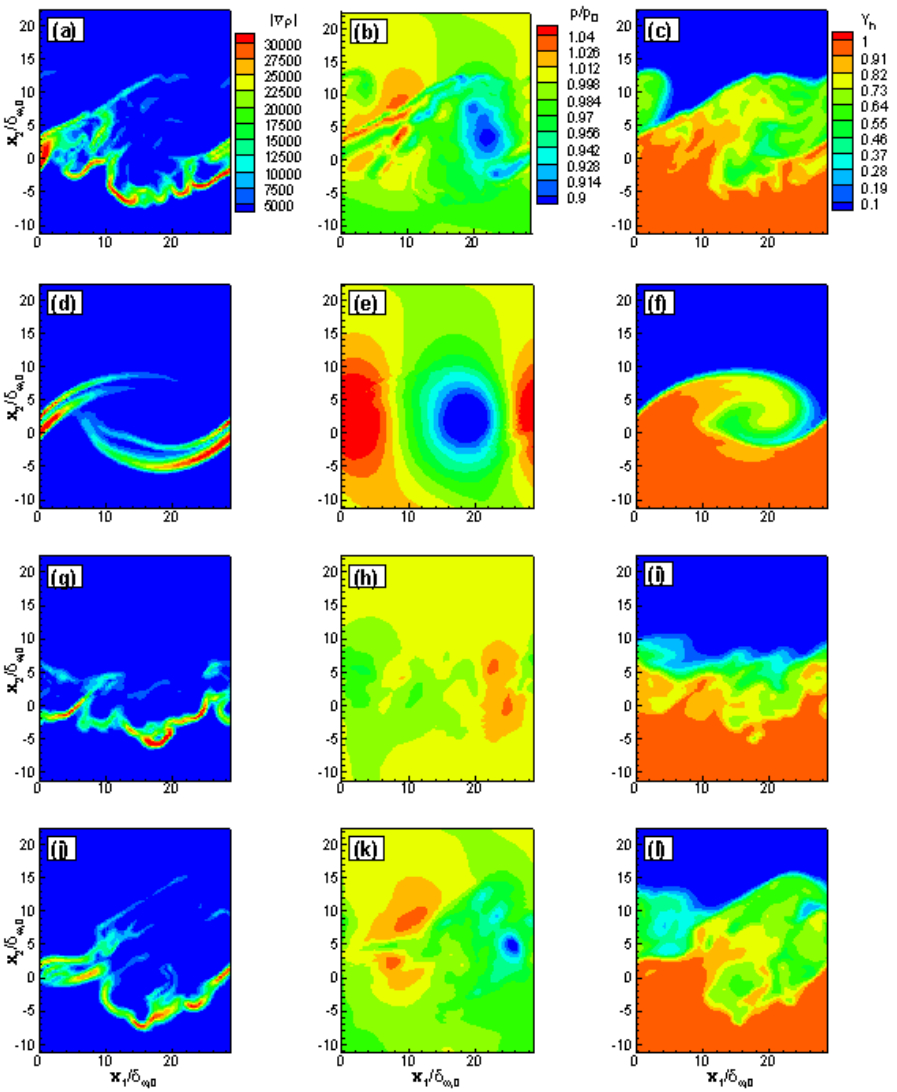
$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial p\left(\overline{\phi}\right)}{\partial x_i} + \frac{\partial \sigma_{ij}\left(\overline{\phi}\right)}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\bar{\rho}\tau_{ij}\right) - \frac{\partial}{\partial x_i}\left[\overline{p(\phi)} - p\left(\overline{\phi}\right)\right]$$

$$\tau_{ij} = \vartheta(\tilde{u}_i, \tilde{u}_j) \qquad \vartheta(\varphi,\theta) = \widetilde{\varphi\theta} - \tilde{\varphi}\tilde{\theta}$$

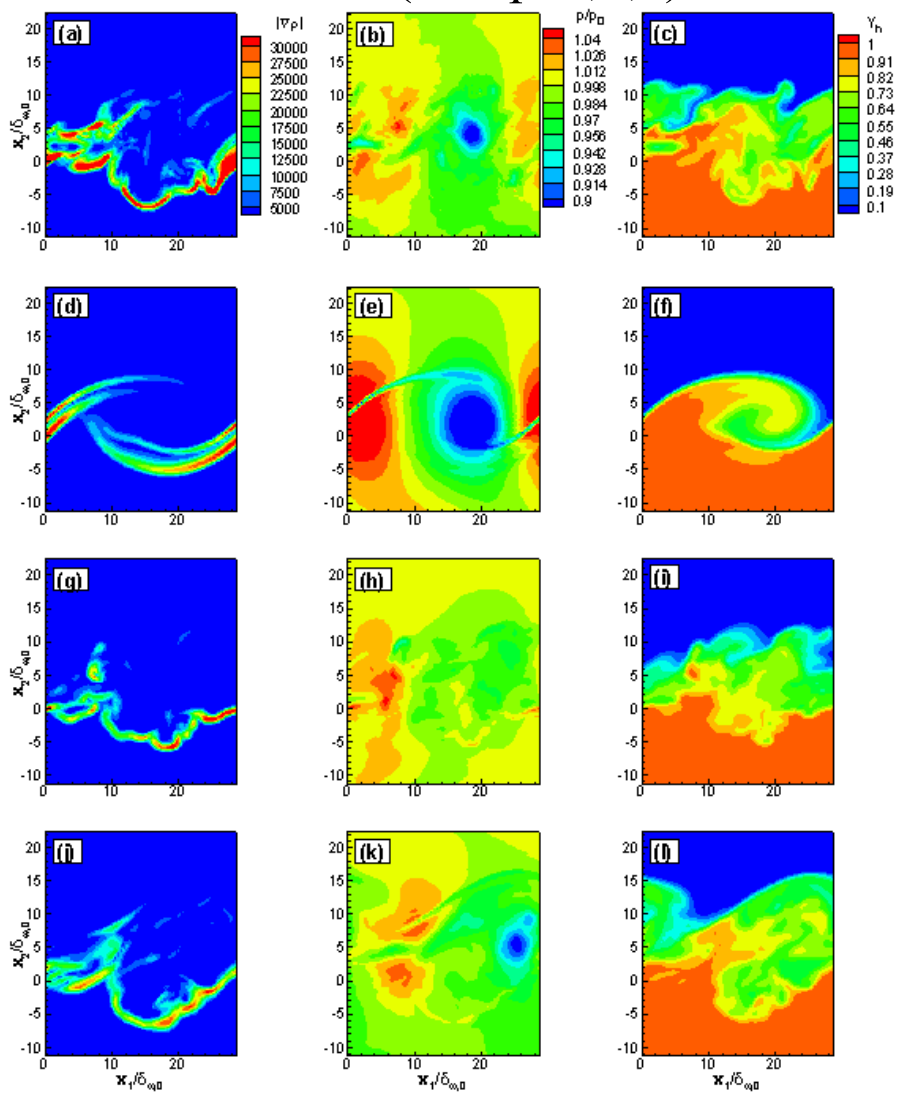
Example of LES without or with the extra SGS model (cst. coeff. SGS-flux models)

(*JFM*, **645**, 211-254, 2010)

without



with (except a,b,c)

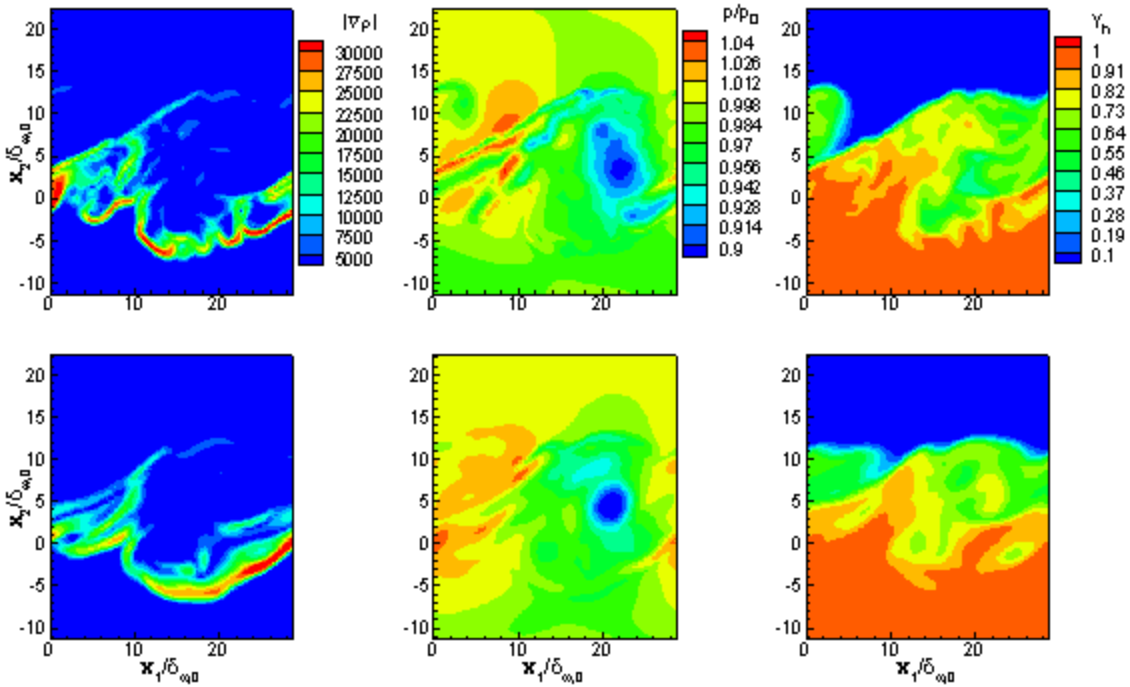


Example of LES with the extra SGS model: mixed dynamic model

(*JFM*, **645**, 211-254, 2010)

FCDNS

MSSD
with
p-correction



A factor of 15 reduction in computational time!

Why are we interested in the SGS scalar variance under supercritical-p conditions?

- Often made argument: flames are thinner as p increases → have flamelets (Williams) and may use the flamelet approach (Peters)
- Results from binary-species mixing
  - Seem to support the existence of flamelets
  - Flamelet approach, if a conserved scalar can be defined
  - Unclear though if a conserved scalar can be defined (to be determined in the future for reactive flows)
- Assuming that a conserved scalar can be defined
  - Is the SGS PDF of the conserved scalar of the form usually assumed so that can be determined with at most 2 moments?
  - If so, can the SGS scalar variance equation terms be modeled and the equation solved?
  - If the terms cannot be modeled, then can the SGS scalar variance be directly modeled?

Scalar variance and dissipation definition

Scalar variance

$$\sigma_Z = \{Z^2\} - \{Z\}^2$$

$$\{Z\} = \frac{\overline{\rho Z}}{\bar{\rho}},$$

$$\bar{g}(\mathbf{x}) = \int_\Omega g(\mathbf{x}')\overline{G}(\mathbf{x} - \mathbf{x}')d\mathbf{x}'$$

Scalar dissipation, i.e. irreversible entropy production

$$\chi_T = \frac{1}{\rho D \alpha_D}\mathbf{J}_\alpha \cdot \mathbf{J}_\alpha$$

$$\mathbf{j}_2(\psi) = B_Y(\psi)\nabla Y_2(\phi) + B_T(\psi)\nabla T(\phi) + B_P(\psi)\nabla p(\phi)$$

$$\chi_F = \rho D \alpha_D \nabla Z \cdot \nabla Z$$

The SGS scalar variance equation: form 1

$$
\begin{aligned}
\overline{\rho}\frac{D\sigma_Z}{Dt} = & \underbrace{\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\right\}\nabla\sigma_Z\right]}_{term\ 1} + \underbrace{2\overline{\rho}\left\{D\alpha_D\right\}\nabla\left\{Z\right\}\cdot\nabla\left\{Z\right\}}_{term\ 2} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{term\ 3} - \underbrace{\nabla\cdot\left(\overline{\rho}\omega\right)}_{term\ 4} + \underbrace{2\left\{Z\right\}\nabla\cdot\left(\overline{\rho}\eta\right)}_{term\ 5} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\nabla Z\cdot\nabla Z\right\} - \left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{term\ 6} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D Z\ \nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{Z\ \nabla Z\right\}\right]}_{term\ 7} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{\nabla Z\right\}\right]}_{term\ 8} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{\alpha_{BK}(1-Z)Z^2\frac{D}{T}\ \nabla T\right\}\right]}_{term\ 9} - \underbrace{2\overline{\rho}\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\cdot\nabla Z\right\}}_{term\ 10} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\frac{(1-Z)Z^2}{R_uT}\frac{m_1m_2}{m}\Lambda\ \nabla p\right\}\right]}_{term\ 11} \\
& - \underbrace{2\overline{\rho}\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\cdot\nabla Z\right\}}_{term\ 12} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\ \nabla T\right\}\right]}_{term\ 13} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\ \nabla p\right\}\right]}_{term\ 14}
\end{aligned}
$$

Common terms with the atmospheric pressure condition equation (e.g. *Jiménez et al. POF 2001*)

New terms due to the product of the diffusivity and the mass diffusion factor $D\alpha_D$ variation

$$\sigma_Z = \left\{Z^2\right\} - \left\{Z\right\}^2$$

$$\boldsymbol{\omega} = \left\{Z^2\mathbf{u}\right\} - \left\{Z^2\right\}\left\{\mathbf{u}\right\}$$

$$\boldsymbol{\eta} = \left\{Z\mathbf{u}\right\} - \left\{Z\right\}\left\{\mathbf{u}\right\}$$

New terms due to the temperature and pressure gradients

The SGS scalar variance equation: form 2

$$
\begin{aligned}
\overline{\rho}\frac{D\sigma_Z}{Dt} = & \underbrace{\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\right\}\nabla\sigma_Z\right]}_{\textit{Resolved Molecular Diffusion}} - \underbrace{\nabla\cdot\left[\overline{\rho}\left(\omega - 2\left\{Z\right\}\eta\right)\right]}_{\textit{SGS Turbulent Fluxes}} \\
& - \underbrace{2\overline{\rho}\left\{D\alpha_D\right\}\left[\left\{\nabla Z\cdot\nabla Z\right\} - \nabla\left\{Z\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{Fick-issued SGS Dissipation}} - \underbrace{2\overline{\rho}\eta\cdot\nabla\left\{Z\right\}}_{\textit{SGS Production}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D Z\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{Z\nabla Z\right\}\right]}_{\textit{SGS Diffusivity 1}} \\
& - \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{Z\right\}\left(\left\{D\alpha_D\nabla Z\right\} - \left\{D\alpha_D\right\}\nabla\left\{Z\right\}\right)\right]}_{\textit{SGS Diffusivity 2}} \\
& + \underbrace{2\left[\overline{\rho}\left\{D\alpha_D\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\nabla\left\{Z\right\}\right]\cdot\nabla\left\{Z\right\}}_{\textit{SGS Diffusivity 3}} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\nabla Z\cdot\nabla Z\right\} - \left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{\textit{SGS Diffusivity 4}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left(\left\{\alpha_{BK}(1-Z)Z^2\frac{D}{T}\nabla T\right\} - \left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\right\}\left\{Z\right\}\right)\right]}_{\textit{SGS Soret 1}} \\
& - \underbrace{2\overline{\rho}\left[\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\cdot\nabla Z\right\} - \left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{SGS Soret 2}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left(\left\{D\frac{(1-Z)Z^2}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\} - \left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\}\left\{Z\right\}\right)\right]}_{\textit{SGS Pressure 1}} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\cdot\nabla Z\right\} - \left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{SGS Pressure 2}}
\end{aligned}
$$

Common terms with the atmospheric pressure condition equation (e.g. *Pera et al., Combust. Flame 2006*)

New SGS terms due to the product of the diffusivity and the mass diffusion factor $D\alpha_D$ variation

$$\sigma_Z = \left\{Z^2\right\} - \left\{Z\right\}^2$$

$$\boldsymbol{\omega} = \left\{Z^2\mathbf{u}\right\} - \left\{Z^2\right\}\left\{\mathbf{u}\right\}$$

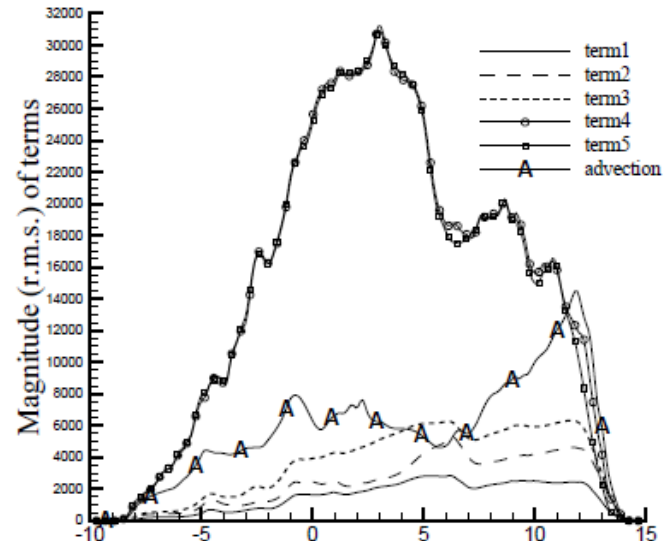
$$\boldsymbol{\eta} = \left\{Z\mathbf{u}\right\} - \left\{Z\right\}\left\{\mathbf{u}\right\}$$

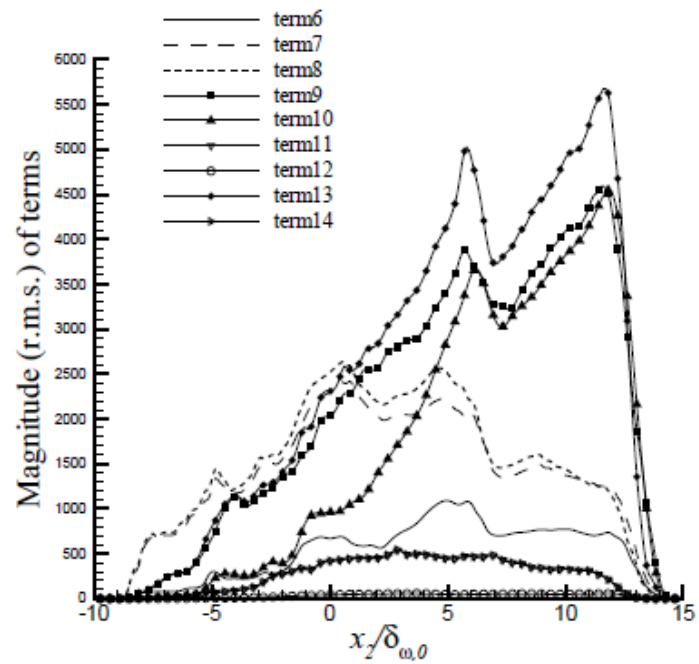
New SGS terms due to the temperature and pressure gradients

SGS scalar variance equation assessment: form 1: database HN600

$$
\begin{aligned}
\overline{\rho}\frac{D\sigma_Z}{Dt} = & \underbrace{\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\right\}\nabla\sigma_Z\right]}_{term\ 1} + \underbrace{2\overline{\rho}\left\{D\alpha_D\right\}\nabla\left\{Z\right\}\cdot\nabla\left\{Z\right\}}_{term\ 2} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{term\ 3} - \underbrace{\nabla\cdot\left(\overline{\rho}\omega\right)}_{term\ 4} + \underbrace{2\left\{Z\right\}\nabla\cdot\left(\overline{\rho}\eta\right)}_{term\ 5} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\nabla Z\cdot\nabla Z\right\} - \left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{term\ 6} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D Z\ \nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{Z\ \nabla Z\right\}\right]}_{term\ 7} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{\nabla Z\right\}\right]}_{term\ 8} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{\alpha_{BK}(1-Z)Z^2\frac{D}{T}\ \nabla T\right\}\right]}_{term\ 9} - \underbrace{2\overline{\rho}\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\cdot\nabla Z\right\}}_{term\ 10} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\frac{(1-Z)Z^2}{R_uT}\frac{m_1m_2}{m}\Lambda\ \nabla p\right\}\right]}_{term\ 11} \\
& - \underbrace{2\overline{\rho}\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\cdot\nabla Z\right\}}_{term\ 12} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\ \nabla T\right\}\right]}_{term\ 13} \\
& - \underbrace{2\left\{Z\right\}\nabla\cdot\left[\overline{\rho}\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\ \nabla p\right\}\right]}_{term\ 14}
\end{aligned}
$$

C_7H_{16} / N_2

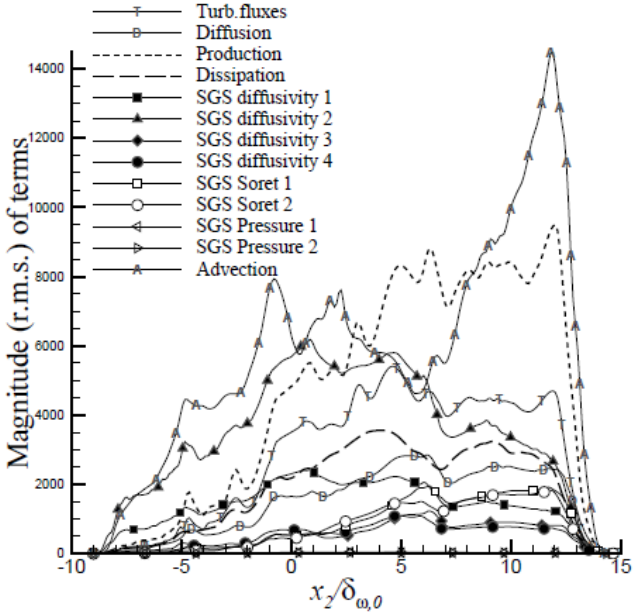


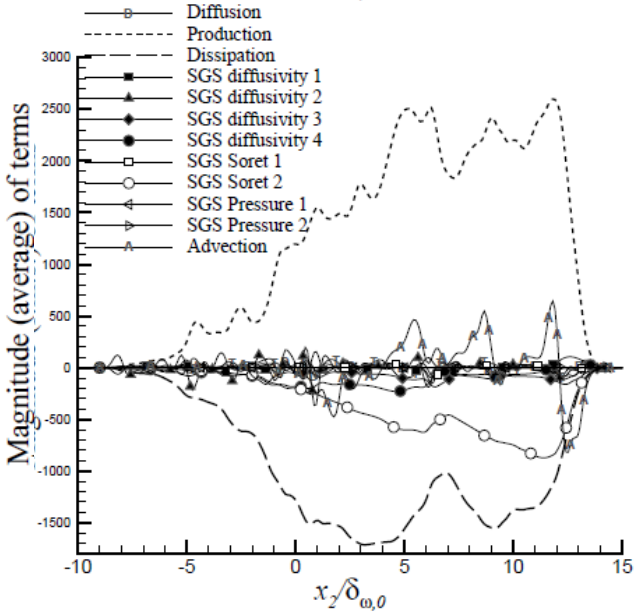


SGS scalar variance equation assessment: form 2: database HN600

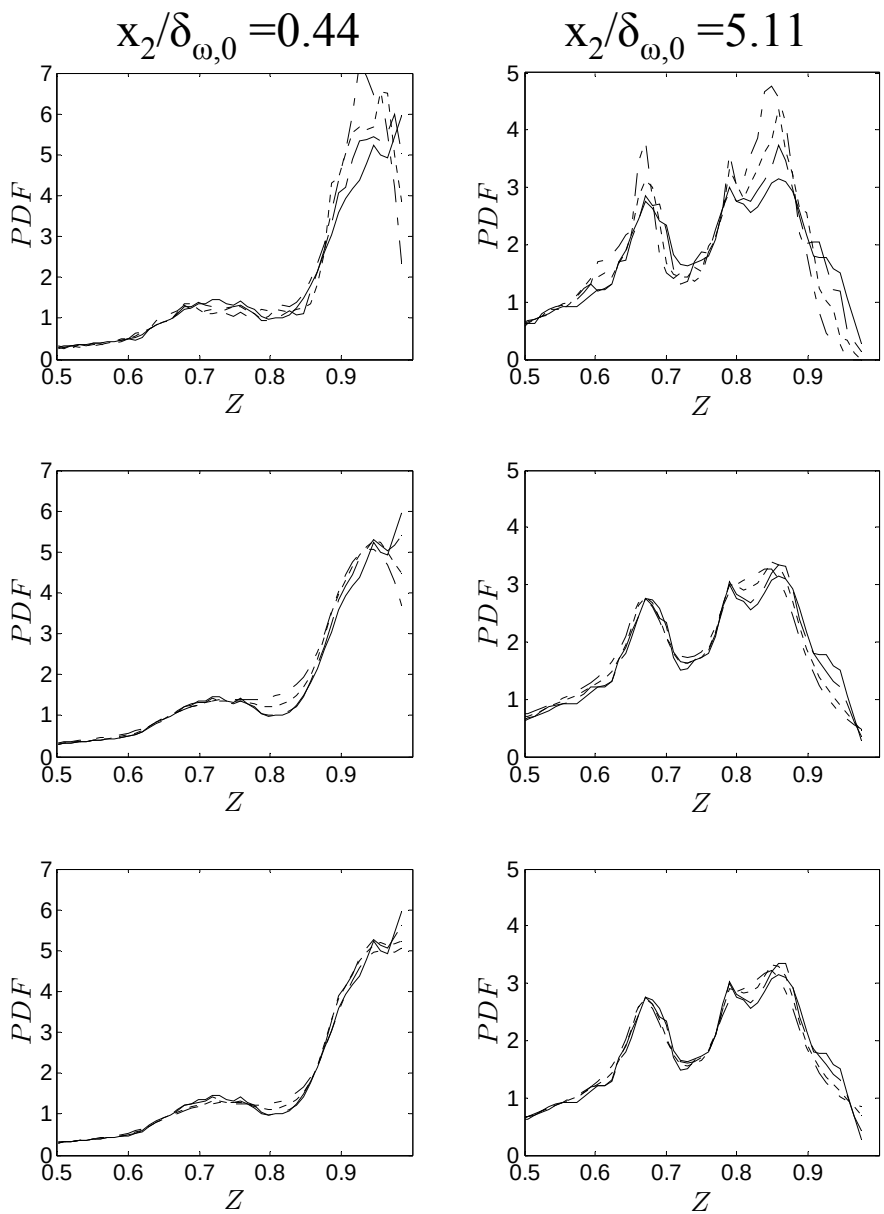
$$
\begin{aligned}
\overline{\rho}\frac{D\sigma_Z}{Dt} = {} & \underbrace{\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D\right\}\nabla\sigma_Z\right]}_{\textit{Resolved Molecular Diffusion}} - \underbrace{\nabla\cdot\left[\overline{\rho}\left(\omega - 2\left\{Z\right\}\eta\right)\right]}_{\textit{SGS Turbulent Fluxes}} \\
& - \underbrace{2\overline{\rho}\left\{D\alpha_D\right\}\left[\left\{\nabla Z\cdot\nabla Z\right\} - \nabla\left\{Z\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{Fick-issued SGS Dissipation}} - \underbrace{2\overline{\rho}\eta\cdot\nabla\left\{Z\right\}}_{\textit{SGS Production}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{D\alpha_D Z\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\left\{Z\nabla Z\right\}\right]}_{\textit{SGS Diffusivity 1}} \\
& - \underbrace{2\nabla\cdot\left[\overline{\rho}\left\{Z\right\}\left(\left\{D\alpha_D\nabla Z\right\} - \left\{D\alpha_D\right\}\nabla\left\{Z\right\}\right)\right]}_{\textit{SGS Diffusivity 2}} \\
& + \underbrace{2\left[\overline{\rho}\left\{D\alpha_D\nabla Z\right\} - \overline{\rho}\left\{D\alpha_D\right\}\nabla\left\{Z\right\}\right]\cdot\nabla\left\{Z\right\}}_{\textit{SGS Diffusivity 3}} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\alpha_D\nabla Z\cdot\nabla Z\right\} - \left\{D\alpha_D\right\}\left\{\nabla Z\cdot\nabla Z\right\}\right]}_{\textit{SGS Diffusivity 4}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left(\left\{\alpha_{BK}(1-Z)Z^2\frac{D}{T}\nabla T\right\} - \left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\right\}\left\{Z\right\}\right)\right]}_{\textit{SGS Soret 1}} \\
& - \underbrace{2\overline{\rho}\left[\left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\cdot\nabla Z\right\} - \left\{\alpha_{BK}(1-Z)Z\frac{D}{T}\nabla T\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{SGS Soret 2}} \\
& + \underbrace{2\nabla\cdot\left[\overline{\rho}\left(\left\{D\frac{(1-Z)Z^2}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\} - \left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\}\left\{Z\right\}\right)\right]}_{\textit{SGS Pressure 1}} \\
& - \underbrace{2\overline{\rho}\left[\left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\cdot\nabla Z\right\} - \left\{D\frac{(1-Z)Z}{R_uT}\frac{m_1m_2}{m}\Lambda\nabla p\right\}\cdot\nabla\left\{Z\right\}\right]}_{\textit{SGS Pressure 2}}
\end{aligned}
$$

C_7H_{16} / N_2





SGS PDF of the scalar : HN600



Dirac

Exact SGS PDF: evaluated by mass-averaging the Z PDF over coarsened-grid planes

Gaussian

Exact SGS PDF; solid

$\overline{\Delta}/\Delta x_{DNS} = 4$; dash

$\overline{\Delta}/\Delta x_{DNS} = 8$; dot

$\overline{\Delta}/\Delta x_{DNS} = 12$; dash-dot

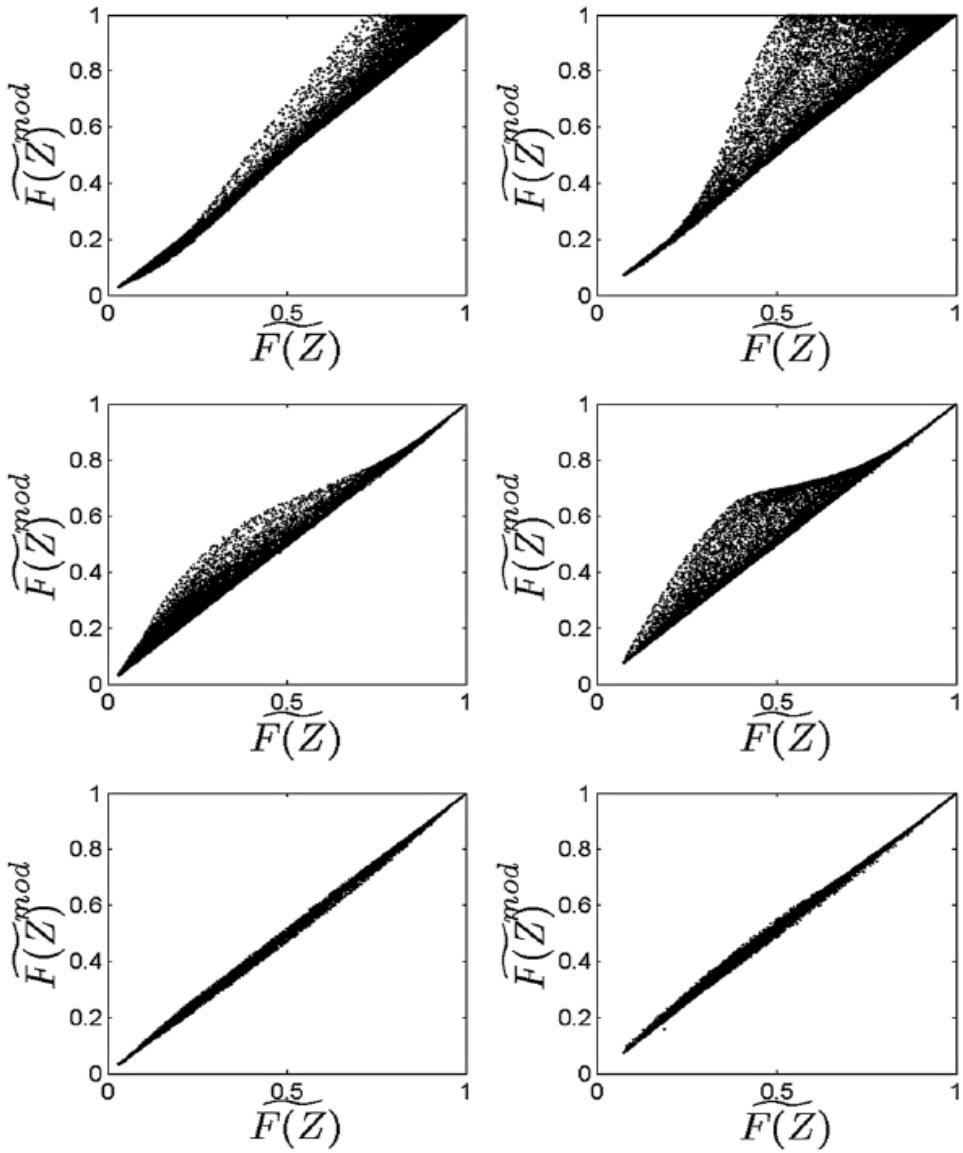
β-PDF

Assessment of point-wise modeling of a non-linear function

Dirac

Gaussian

β PDF



Subcritical dissipation for 1D unsteady mixing layer:

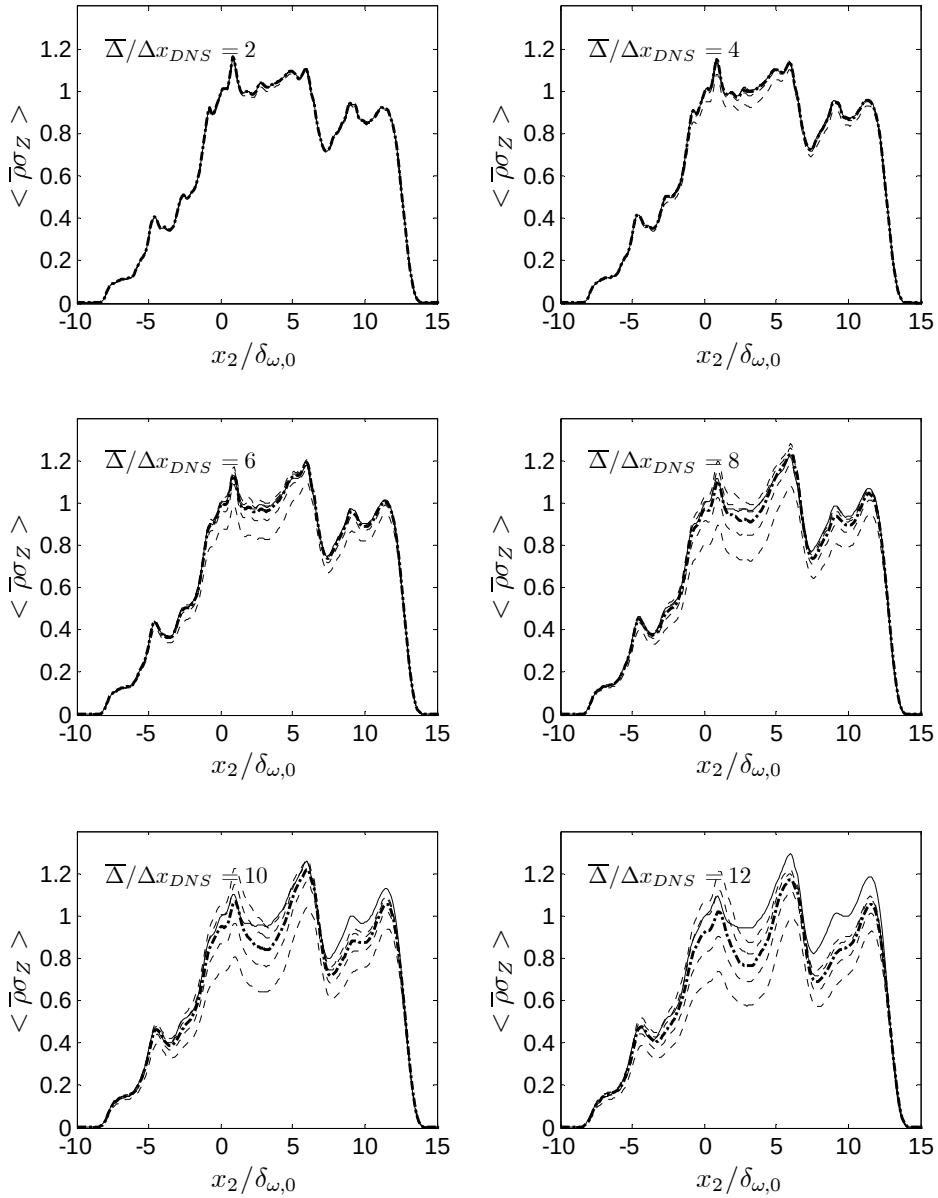
$$F(\xi) = \exp\left\{-2\left[erf^{-1}(2\xi - 1)\right]^2\right\}$$

$\widetilde{F(Z)}^{mod}$ Computed using the PDF with exact moments

$\widetilde{F(Z)}$ Computed using the database

ADM of the Favre SGS scalar variance

Approximate Deconvolution Model applied to conservative quantities



Exact SGS scalar variance: solid

1st ,2nd, 4th, 5th order approximations: dotted

3rd order approximation: dash-dotted

$$Z^* = \overline{Z} + \left(\overline{Z} - \overline{\overline{Z}}\right) + \left(\overline{Z} - 2\overline{\overline{Z}} + \overline{\overline{\overline{Z}}}\right) + \ldots..$$

$$\rho^* = \overline{\rho} + (\overline{\rho} - \overline{\overline{\rho}}) + \left(\overline{\rho} - 2\overline{\overline{\rho}} + \overline{\overline{\overline{\rho}}}\right) + \ldots..$$

$$(\rho Z)^* = \overline{\rho Z} + \left(\overline{\rho Z} - \overline{\overline{\rho Z}}\right) + \left(\overline{\rho Z} - 2\overline{\overline{\rho Z}} + \overline{\overline{\overline{\rho Z}}}\right) + \ldots..$$

$$Z^{**} = (\rho Z)^*/\rho^*$$

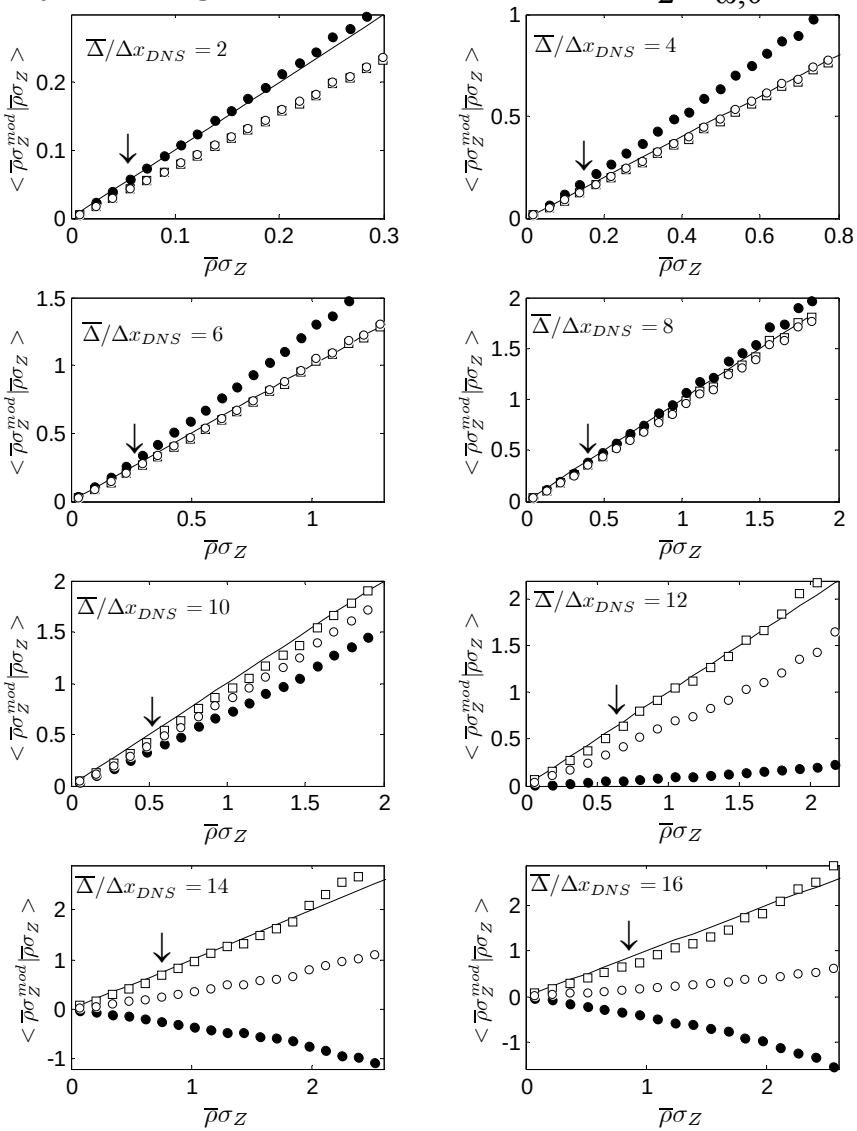
invoking the assumption

$$Z^{**} \simeq Z^*$$

$$\sigma_Z = \frac{\overline{\rho^* Z^{**} Z^{**}}}{\overline{\rho^*}} - \frac{\overline{\rho^* Z^{**}}}{\overline{\rho^*}} \frac{\overline{\rho^* Z^{**}}}{\overline{\rho^*}}$$

Dynamic gradient-based modeling of the SGS scalar variance, 1 of 4

Dynamic gradient-based model, $x_2/\delta_{\omega,0}$ =0.44



Planar averages

- 45 degrees line
- □ Our model
- ○ Classical model with

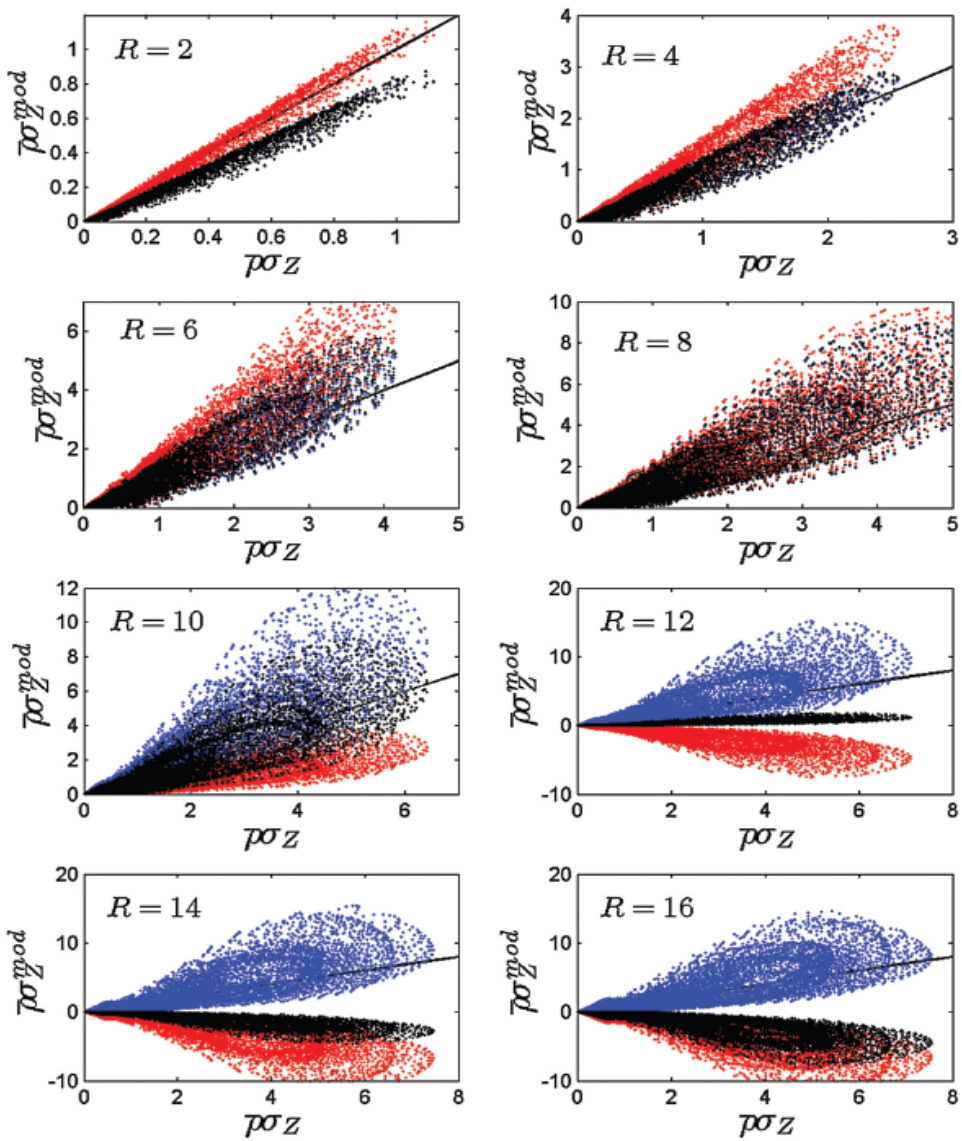
$$\widehat{\overline{\Delta}}^2 = \widehat{\Delta}^2 + \overline{\Delta}^2$$

- ● Classical model with

$$\widehat{\overline{\Delta}} = \widehat{\Delta}$$

Arrow indicates the planar mean

Dynamic gradient-based modeling of the SGS scalar variance, 2 of 4



Scatter plots in plane

$$x_2/\delta_{\omega,0} = 5.11$$

$$R \equiv \bar{\Delta}/\Delta x_{DNS}$$

blue: our model

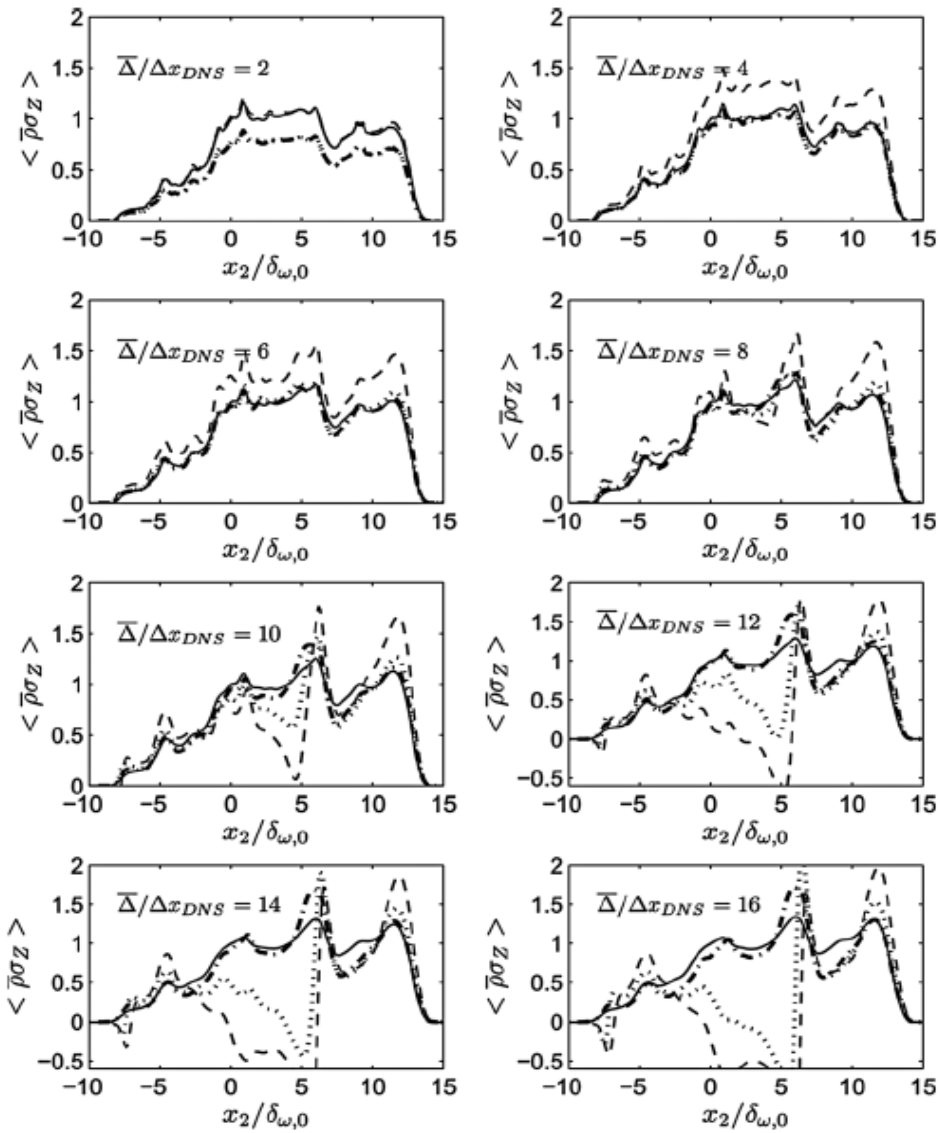
black: classical model

$$\widehat{\bar{\Delta}}^2 = \widehat{\Delta}^2 + \bar{\Delta}^2$$

red: classical model

$$\widehat{\bar{\Delta}} = \widehat{\Delta}$$

Dynamic gradient-based modeling of the SGS scalar variance, 3 of 4



Cross-stream profiles

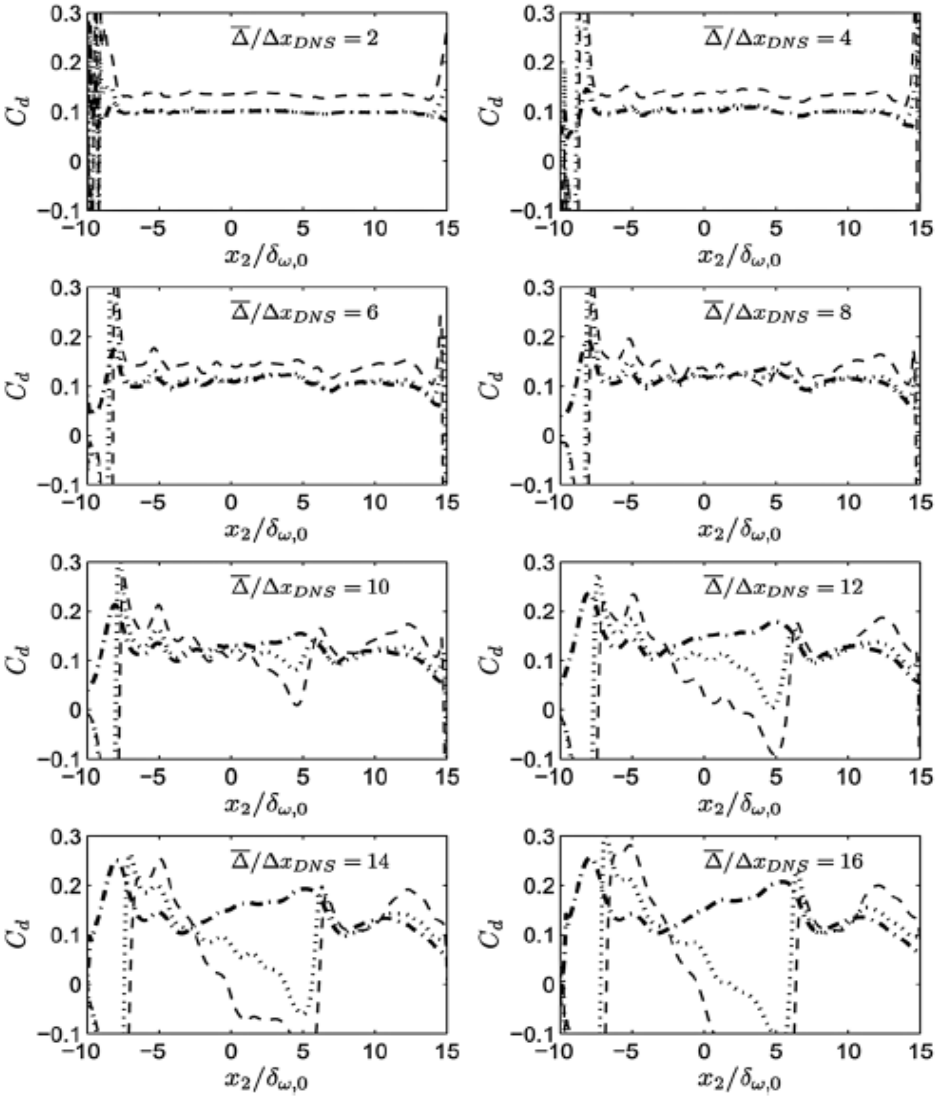
Exact: solid

New model: dash-dot

Classical model with correct filter $\widehat{\overline{\Delta}}^2 = \widehat{\Delta}^2 + \overline{\Delta}^2$: dotted

Classical model with incorrect filter $\widehat{\overline{\Delta}} = \widehat{\Delta}$: dashed

Dynamic gradient-based modeling of the SGS scalar variance, 4 of 4



Model coefficient

New model: dash-dot

Classical model with correct filter

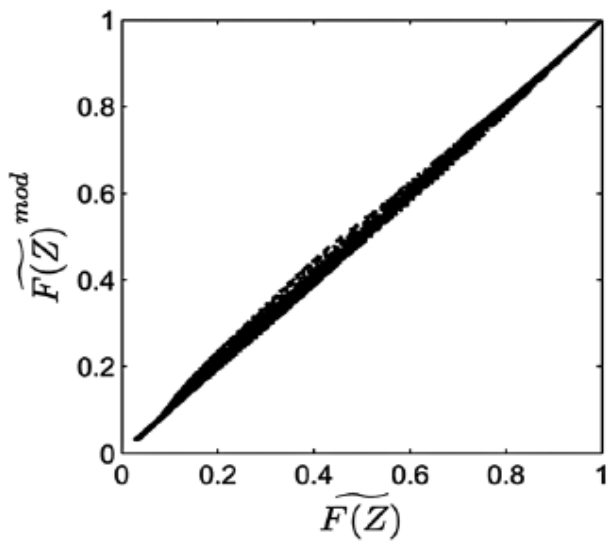
$\widehat{\overline{\Delta}}^2 = \widehat{\Delta}^2 + \overline{\Delta}^2$: dotted

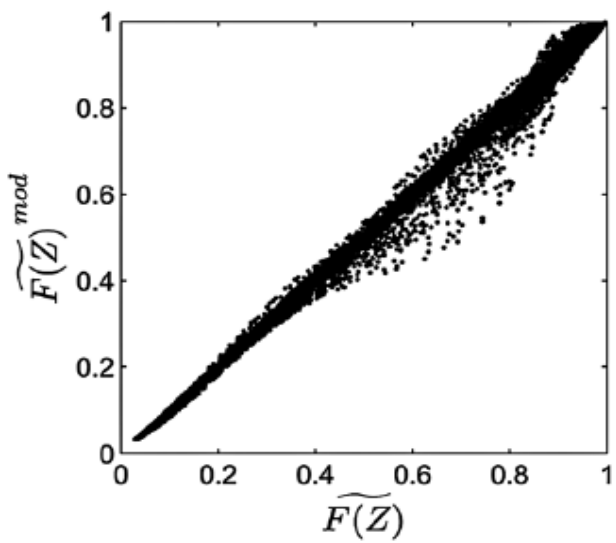
Classical model with incorrect filter $\widehat{\overline{\Delta}} = \widehat{\Delta}$: dashed

Reproducing a non-linear function with the models

Subcritical dissipation for 1D unsteady mixing layer:

$$F(\xi) = \exp\left\{-2\left[erf^{-1}(2\xi - 1)\right]^2\right\}$$





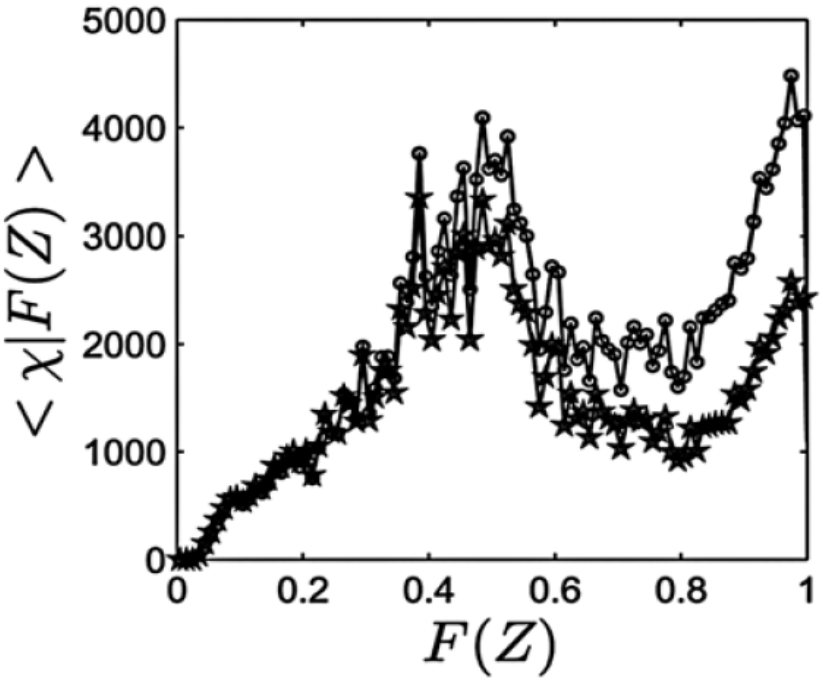
σ_Z model: 3rd order ADM Gradient model

$$x_2/\delta_{\omega,0} = 0.44$$

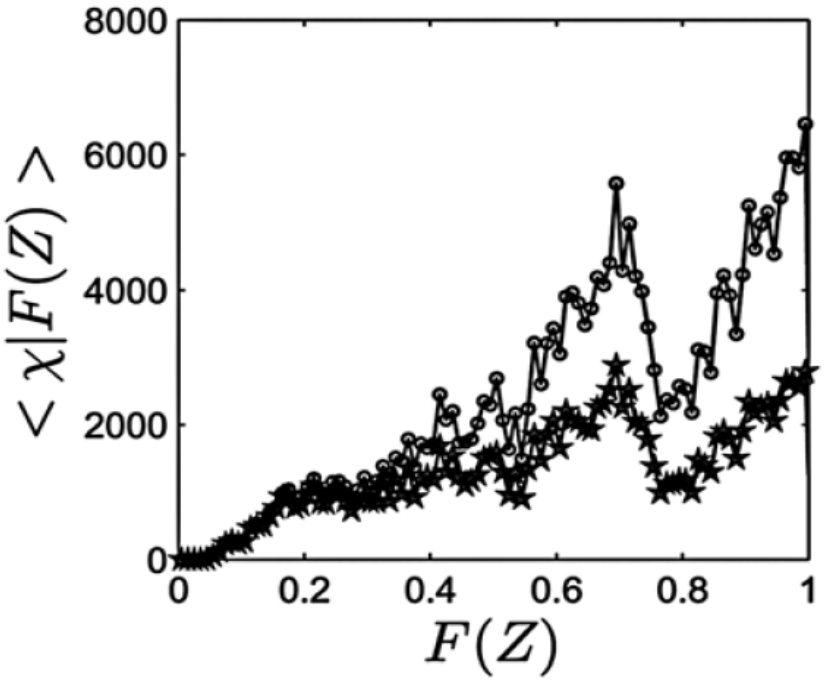
Total scalar dissipation versus Fick's scalar dissipation

Conditional averages on F(Z): χ_T (circles) and χ_F (stars).

$$F(\xi) = \exp\left\{-2\left[erf^{-1}(2\xi - 1)\right]^2\right\}$$



$x_2/\delta_{\omega,0} = 0.44$



$x_2/\delta_{\omega,0} = 5.11$

Summary and conclusions

- Studied the SGS PDF of the scalar and the scalar variance, σ_Z, under supercritical-pressure conditions
  - Showed that the pdf of the scalar can be well approximated by a β distribution
  - Equation for σ_Z contains significant terms due to non-uniform diffusion coefficients and Soret effects
  - Provided two models for σ_Z : Approximate Decomposition Model and a new Gradient Model
- Showed that
  - The ADM model is not necessarily convergent for compressible flows, although some of its approximations can be more accurate than the new Gradient Model
  - The new Gradient model is accurate for very large filter to DNS-grid ratios
  - The total scalar dissipation is not necessarily well modeled by the Fick's scalar dissipation