SAND2015-2894C

NC15
Avignon

An *a priori* DNS study of molecular mixing models in a planar stationary premixed flame

Xinyu Zhao
University of Connecticut, Storrs, CT 06269, USA
Hemanth Kolla
Jacqueline H. Chen
Sandia National Laboratories, Livermore, CA 94550, USA

Presented at the 15th International Conference on Numerical Combustion, Avignon, France

UCONN

Motivation

- The requirement of higher efficiency and lower pollutants from engines and combustors calls for the construction of regime-independent computational combustion models.
- Transported PDF methods have proven to be robust in many turbulent combustion scenarios. However, the level of the results largely depend on the choice of mixing model parameters. (For example, a range of 1.5 to 25 has been reported for the C_{Φ} value in premixed flames, compared to 1.5 to 4 for non-premixed flames. You might not need to write this out.)
- Why mixing is difficult to model in premixed flames than non-premixed flames?(Is this necessary? If yes, could we put some figures from Swami's paper to show the tight coupling between mixing and reaction?)

Mixing models on premixed flame

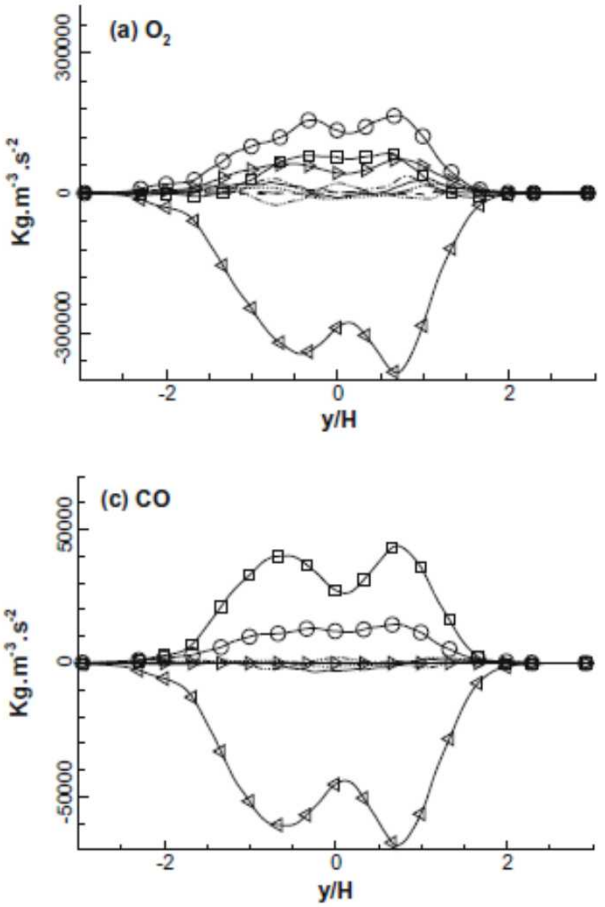
IEM model:

$$\frac{d\phi^*}{dt} = -\frac{C_\phi}{\tau}(\phi^* - \langle\phi^*\rangle)$$

Rates of mixing

Shapes of the composition space

Existing transported PDF studies on premixed flames employed a modified C_Φ parameter, which considers the scalar dissipation rate of progress variable.



E. S. Richardson et al. Combustion and Flame 157 (2010) 506-515.

The joint PDF of mass fraction, enthalpy, and mass fraction gradient.

$$\frac{D\phi_\beta}{Dt} = S_\beta - \rho^{-1}\frac{\partial J_i^\beta}{\partial x_i}$$

$$\frac{D\phi_\beta^l}{Dt} = \frac{\partial S_\beta}{\partial x_l} - \frac{\partial}{\partial x_l}\left(\rho^{-1}\frac{\partial J_i^\beta}{\partial x_i}\right) - \frac{\partial u_i}{\partial x_l}\frac{\partial \phi^\beta}{\partial x_i}$$

$$\phi_\gamma = \phi_\beta^l \equiv \frac{\partial \phi_\beta}{\partial x_l} \qquad \gamma = 3(\beta - 1) + l + Ns$$

$\beta = 1, 2, \ldots, N_s$

$\gamma = Ns + 1, \ldots, 4N_s$

$$\frac{\partial \mathcal{F}}{\partial t} + \frac{\partial}{\partial x_i}[\tilde{u}_i \mathcal{F}] + \frac{\partial}{\partial \psi_\alpha}[S_\alpha(\boldsymbol{\psi})\mathcal{F}] =$$

$$\boldsymbol{\phi} = (\phi_\beta, \phi_\gamma, h)$$

Composition variable $\boldsymbol{\phi}$

$$-\frac{\partial}{\partial x_i}[\langle u_i'' | \boldsymbol{\psi}\rangle \mathcal{F}] + \frac{\partial}{\partial \psi_\alpha}\left[\left\langle \rho^{-1}\frac{\partial J_i^\alpha}{\partial x_i} | \boldsymbol{\psi}\right\rangle \mathcal{F}\right] - \delta_{\alpha\gamma}\frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial}{\partial x_l}\left(\rho^{-1}\frac{\partial J_i^\alpha}{\partial x_i}\right) | \boldsymbol{\psi}\right\rangle \mathcal{F}\right]$$

$$+\delta_{\alpha\gamma}\frac{\partial}{\partial \psi_\alpha}\left[\frac{\partial S_\alpha(\boldsymbol{\psi})}{\partial x_l}\mathcal{F}\right] - \delta_{\alpha\gamma}\frac{\partial}{\partial \psi_\alpha}\left[\left\langle \frac{\partial u_i}{\partial x_l}\frac{\partial \phi^\beta}{\partial x_i} | \boldsymbol{\psi}\right\rangle \mathcal{F}\right]$$

Models to close mixing and additional terms.

$$\left\langle \rho^{-1} \frac{\partial J_i^{\alpha}}{\partial x_i} | \boldsymbol{\psi} \right\rangle$$

$$\left\langle \frac{\partial}{\partial x_l} (\rho^{-1} \frac{\partial J_i^{\alpha}}{\partial x_i}) | \boldsymbol{\psi} \right\rangle$$

$$\frac{\partial S_{\alpha}(\boldsymbol{\psi})}{\partial x_l}$$

$$\left\langle \frac{\partial u_i}{\partial x_l} \frac{\partial \phi^{\beta}}{\partial x_i} | \boldsymbol{\psi} \right\rangle$$

- Conventional mixing models (EMST, MC, IEC, etc..) can be used to close the molecular mixing term, with the scalar mixing rate calculated by its corresponding scalar gradient for each individual species.
- The molecular diffusion term can be modeled using similar model forms as the molecular mixing models. (What we are going to explore here)
- The reaction gradient term is closed. (you might want to show why)
- You know how =)

The cons and pros of the proposed joint PDF method

CONS

- The computational cost will be increased by transporting 3 *Ns* composition variables and by demanding higher grid resolution to capture the gradients properly.
- Introducing additional terms for modeling.

OBJECTIVE

A priori DNS evaluation of the mixing models and other unclosed Terms.

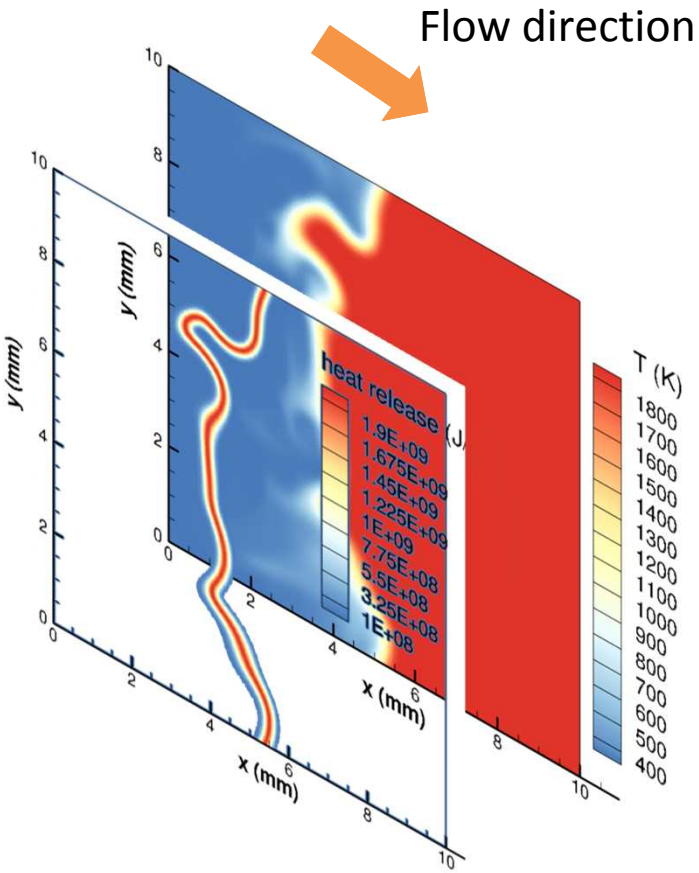
PROS

- The instantaneous scalar dissipation rates could be correctly captured, given that the scalar gradient for each individual species can be solved correctly.
- The coupled effect of chemistry on molecular mixing is automatically included by transporting the scalar gradients.

A lean (Φ=0.7) premixed methane flame is simulated using DNS (s3d).

Methodology

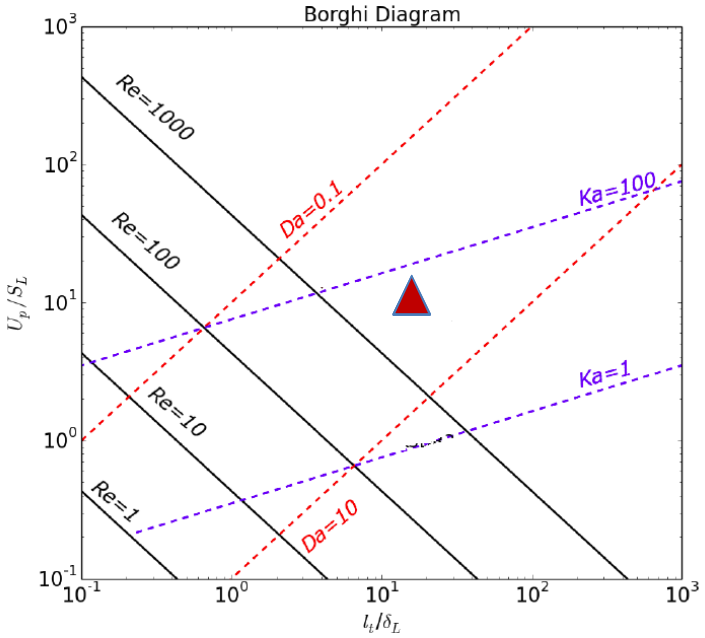
- The flame is designed to be homogeneous in y and z direction (statistically one dimensional).
- The turbulent flame is anchored around x = 4 mm by feeding back turbulent fluctuating velocity to the inlet (x = 0).
- The turbulent fluctuating velocity is calculated by volumetric integration of the velocity field.
- Passive tracer particles are launched at x = mm after the flame reaches statistically stationary state (~ 2 t_j).
- A six-species methane mechanism with unity Lewis number is used to isolate the effect of differential diffusion.



A lean (Φ=0.7) premixed methane flame is simulated using DNS (s3d).

The statistically 1-D premixed methane flame falls into the challenging category for mixing models to capture.

Numerical details	
Computational domain	10 mm × 10 mm × 10 mm
Grid resolution	500 × 500 × 500
Turbulent Re #	200
Da #	~ 2
Ka #	~ 6
Integral time scale	1.25 ms
Integral length scale l_T	2 mm
Turbulent flame speed u'	3.2 m/s
Laminar flame speed S_L	0.2 m/s

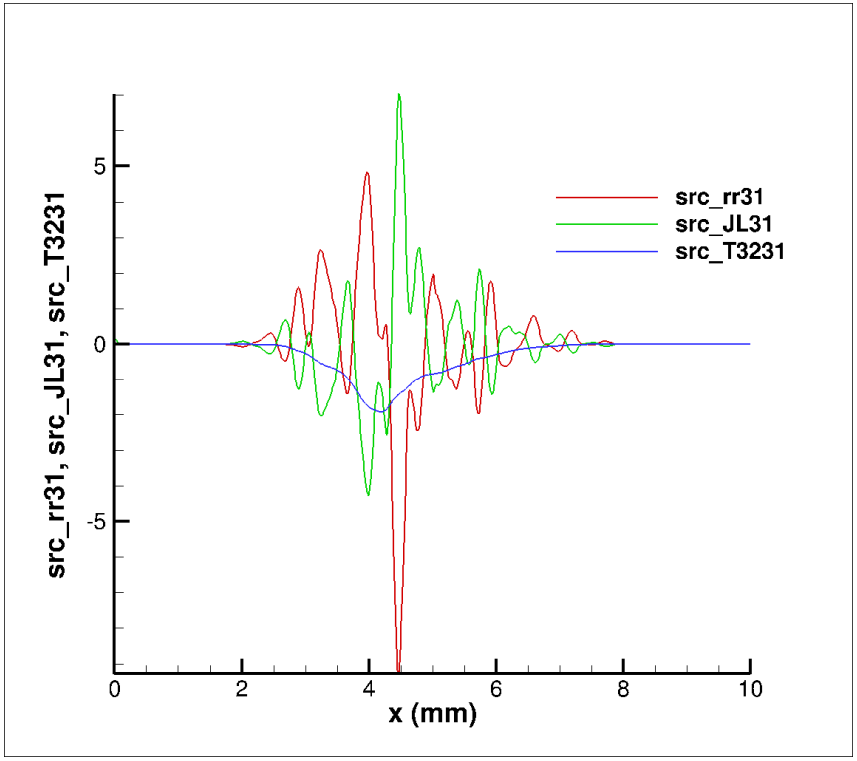


$$Ka = \left(\frac{S_L \delta_L}{\nu_0}\right)^{1/2} \left(\frac{u'}{S_L}\right)^{3/2} \left(\frac{l_T}{\delta_L}\right)^{-1/2}$$

$$\mathrm{Da} = \left(\frac{S_L}{u'}\right)\left(\frac{l_T}{\delta_L}\right)$$

The diffusion gradient balances the reaction source gradient, especially for minor species CO

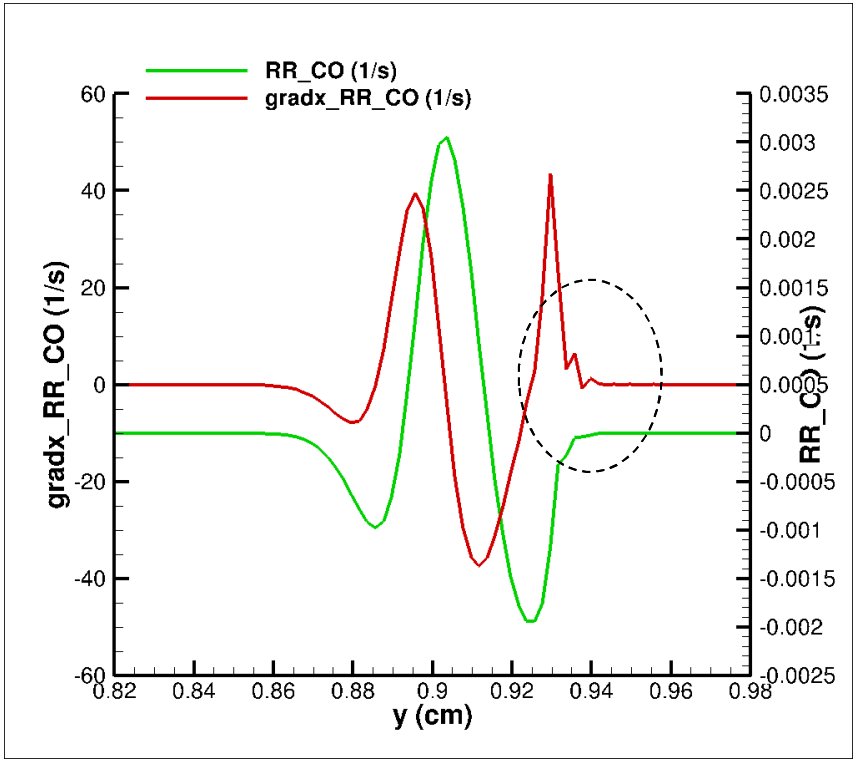
CO (time-averaged over 500 steps)



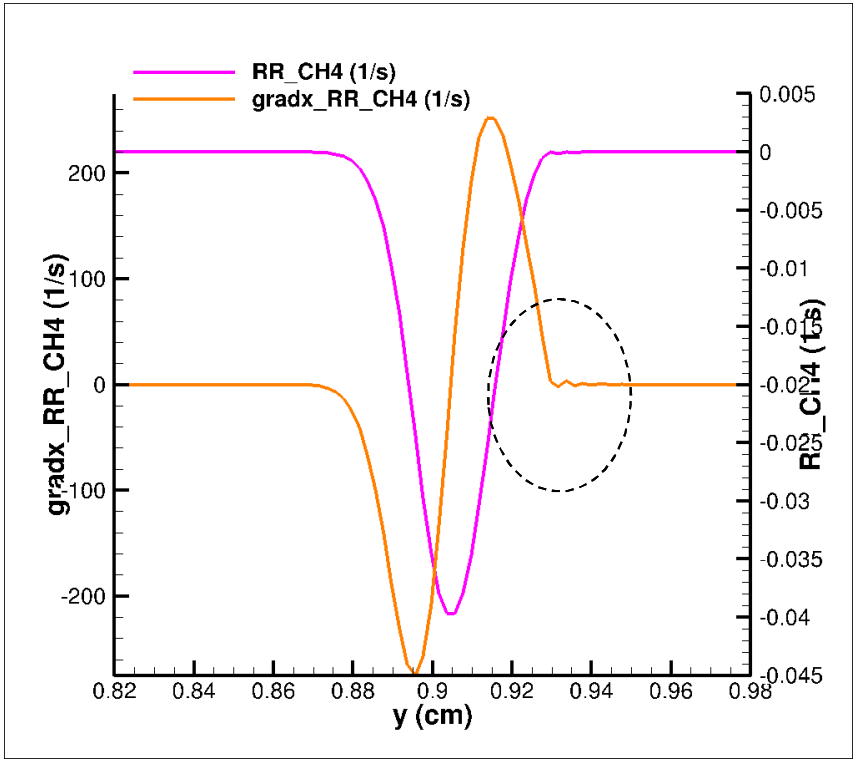
CO2 (time averaged over)

1D laminar flame study suggests the resolution might not be sufficient to capture the gradient.

CO



CH_4



Conclusions

- A joint transported probability density function method with scalar-gradient composition variable is proposed in this work.
- The DNS database of a statistically one-dimensional stationary lean premixed methane flame are generated to study the mixing models.
- Lagrangian statistics can be obtained using this database through the use of passive tracer particles launched during the DNS run.
- The additional terms generated by the addition of scalar gradients are evaluated using DNS for each species, and their closure is proposed.
- The reaction rates gradient balances the diffusion gradient term in this flame, especially for minor species CO.
- Future work includes evaluating mixing models by comparing Lagrangian statistics of mixing models with Eulerian statistics generated from DNS.

Thank you for your attention!

Questions?