Effects of preferential diffusion on soot modeling with the sectional method and FGM tabulated chemistry

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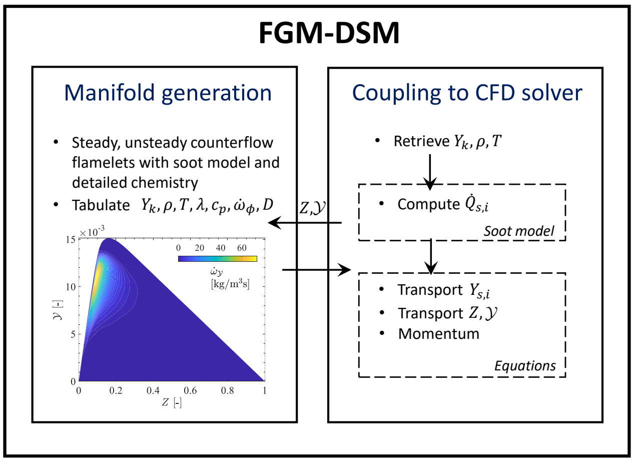
Objectives

- To couple a discrete sectional method[1] (DSM)-based soot model with Flamelet Generated Manifold[2] (FGM) tabulated chemistry for a computationally efficient chemistry modeling.
- To investigate the effects of preferential diffusion on the soot prediction in FGM-DSM simulations of laminar counterflow flames.
- To study the dynamic response of soot formation to the unsteady strain rate fluctuations under different transport models.

FGM-DSM coupling



FGM-DSM

Manifold generation

- Steady, unsteady counterflow flamelets with soot model and detailed chemistry
- Tabulate $Y_k, \rho, T, \lambda, c_p, \dot{\omega}_\phi, D$

$Z, \mathcal{Y}$

Coupling to CFD solver

- Retrieve Y_k, ρ, T

- Compute $\dot{Q}_{s,i}$

Soot model

- Transport $Y_{s,i}$
- Transport $Z, \mathcal{Y}$
- Momentum

Equations

Fig. 1 Schematic of FGM-DSM coupling in CHEM1D

Diffusion transport modeling

The transport equation for a control variable ($\phi = \sum \alpha_i Y_i$) in a general form:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial}{\partial x}(\rho u \phi) - \frac{\partial}{\partial x}\left(\frac{\lambda}{c_p}\frac{\partial \phi}{\partial x}\right) = \underbrace{\frac{\partial}{\partial x}\left(\mathscr{D}\frac{\partial \Phi}{\partial x}\right)}_{\text{Pref. diff. flux}} + \sum_{i=1}^{N_s} \alpha_i \dot{\omega}_i \qquad (1)$$

Model	Computation of Le_i in 1D flamelets	Computation of $\mathscr{D}$ from 1D flamelets and stored in FGM
MIXAVG	$\frac{\lambda}{\rho c_p D_i}$	$\left[\left(-\sum \rho \alpha_i U_i Y_i\right) - \frac{\lambda}{c_p}\frac{\partial \phi}{\partial x}\right] / \frac{\partial \Phi}{\partial x}$
CONLEW	fixed constants	$\left[\sum \left(\frac{1}{Le_i} - 1\right)\frac{\lambda}{c_p}\frac{\partial \phi}{\partial x}\right] / \frac{\partial \Phi}{\partial x}$
UNILEW	1	0
MIXUNI	$\frac{\lambda}{\rho c_p D_i}$	0

Table 1 Features of diffusion transport models

Results

A counterflow ethylene flame of Wang et al.[3] (WRC15) consisted of a pure C_2H_4 fuel, and oxidizer composition of 75% N_2 and 25% O_2 (% vol.) at atmospheric pressure and 300 K temperature.

Steady-state simulations

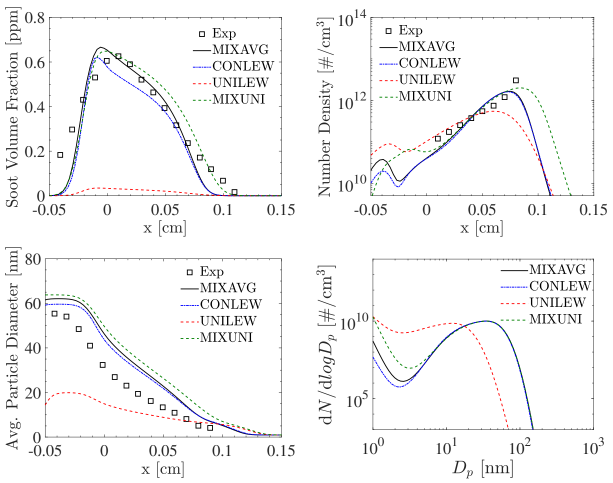


Fig. 2 Measured and computed (FGM) profiles of soot volume fraction, number density, particle diameter, and PSD for the WRC15 flame with various transport models.

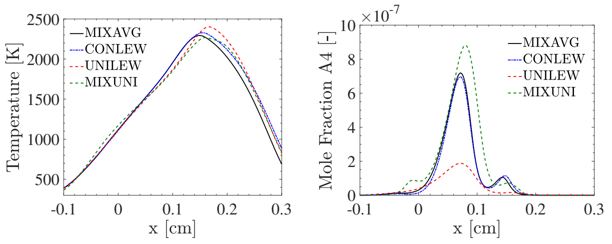


Fig. 3 Computed profiles (FGM) of temperature and mole fractions of A4 for the WRC15 flame with different transport models.

Unsteady simulations

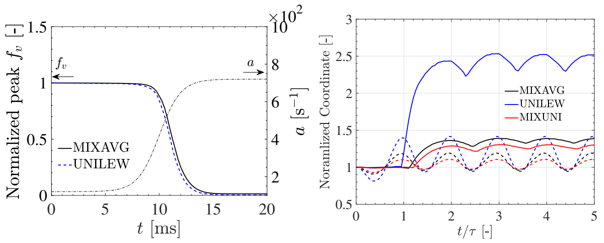


Fig. 4 Temporal evolution of normalized peak soot volume fractions under the time-dependent increasing strain rate (left), temporal evolution of normalized peak A4 mass fraction (dashed lines), peak soot volume fraction (solid lines) for different transport modeling approach under the oscillating strain rate in WRC15 flame (right).

Conclusions

- Neglecting preferential diffusion term can lead to significant underprediction of soot concentration.
- The formation of PAH, and thus the soot, are particularly sensitive to the diffusion of species such as H and H_2 from the reaction zone to the sooting zone.
- The dynamic response of soot formation to the unsteady strain rate fluctuations under different transport models is marginally affected under preferential diffusion.

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[1] *Hoerlle & Pereira, Combust. Flame 203, 2019*

[2] *Oijen & de Goey, Combust. Theo. Model. 4, 2004*

[3] *Wang et al., Combust. Flame 162, 2015*

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