NJFCP Area 2.5

Development and Validation of Reduced Kinetic Models

Objectives

- Develop reduced kinetic models for jet fuels with fuel sensitivity based on the detailed HyChem models.
- Develop reduced sub-models for emissions, including NO, PAH and soot.
- Develop advanced chemistry solvers and dynamic adaptive chemistry (DAC) for efficient large eddy (LES) simulations.

Kinetic Model Reduction

Detailed HyChem models version 2 are systematically reduced, resulting in compact models for computationally efficient large-scale flame simulations.

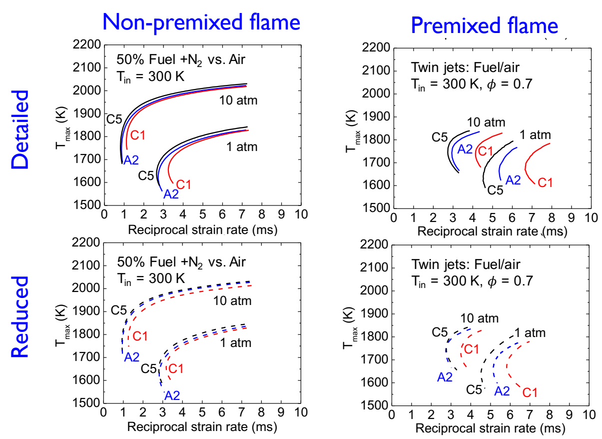
Target fuels: Cat A2, C1, and C5

Major reduction methods

Skeletal reduction	Timescale reduction
Directed relation graph (DRG) (Lu and Law, PCI 2005) DRG-aided sensitivity analysis (Zheng et al., PCI 2007)	Analytically solved quasi steady state approximations (QSSA) (Lu and Law, JPCA 2007)

Fuel sensitivity in Counterflow Extinction

- Trends in global flame behaviors are retained in reduced models.
- Extinction limits of A2 and C5 are close.
- C1 flames can survive higher strain rates than A2, C5.



Summary

1. Developed fuel-specific and universal skeletal/reduced models based on version 2 HyChem models.
2. Developed a reduced NO sub-model (Luo et al. CNF 2011) compatible with HyChem models.

# of species in kinetic models

Models	A2	C1	C5
Detailed	119	119	119
Skeletal	41	34	41
Reduced	31	26	31
Universal	48 skeletal, 35 reduced		
w/ NOx	63 skeletal, 45 reduced		

3. Fuel sensitivities in ignition-delay, PSR extinction, flame speed and counterflow extinction are well captured by the reduced models.
4. Developed and validated reduced diffusion models and obtained speedup factors up to ~55 and worst case error within 1cm/s in flame speed.

Next Steps

- Develop smaller reduced models specific to lean blow-out etc.
- Identification of kinetic processes controlling critical flame behaviors (e.g. ignition delay, LBO etc.)
- Develop reduced soot models

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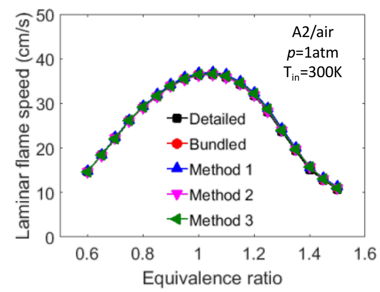
Reduced Mixture-Averaged Diffusion Models

Mixture-averaged diffusion (MAD) model is computationally expensive. As such, efficient and accurate reduced MAD models are developed in this work.

Detailed: Original MAD model.
Bundled: Species with similar diffusivities are bundled. (Lu and Law, CNF 2007)

Method 1: Only important binary coefficients are evaluated.
Method 2: For premixed fuel/air combustion, where N_2 is typically abundant, species MAD coefficient can be approximated with its binary diffusion coefficient with respect to N_2, i.e. $D_i = D_{i,N_2}$.
Method 3: Method 2 is further combined with species bundling, $D_i = DG_{g(i),g(N_2)}$. Compared with detailed MAD model, the computational cost is reduced from a quadratic function to a linear function.

Validation of reduced MAD models (w/ 35 species universal reduced)



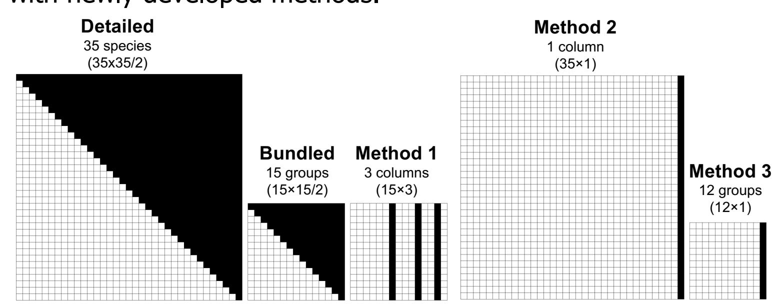
Worst-case error is under 1 cm/s in the flame calculation

Speed up factors for reduced MAD models (w/ 35 species universal reduced)

MAD models	Speedup factors
Bundled	4.0
Method 1	7.5
Method 2	44.9
Method 3	55.2

Binary coefficient matrix

The number of evaluation (black pixel) is significantly reduced with newly developed methods.



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