NJFCP Area 2.5
Development and Validation of Reduced Kinetic Models

Objectives

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

Kinetic Model Reduction

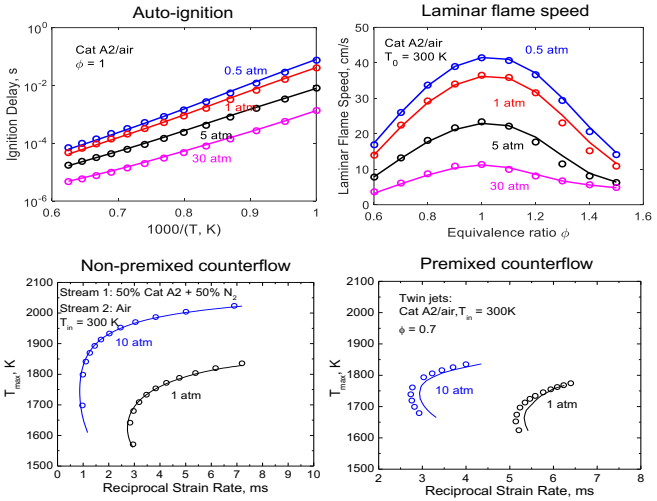
Major reduction methods

- Skeletal reduction using directed relation graph (DRG) (Lu and Law, PCI 2005), and DRG-aided sensitivity analysis (Zheng et al., PCI 2007)
- Timescale reduction based on analytically solved quasi steady state assumptions (QSSA) (Lu and Law, JPCA 2007)

Target fuels: Cat A2, C1, C5

Target systems: Auto-ignition for ignition chemistry and perfectly stirred reactors (PSR) for extinction and flame chemistry

Parameter range: p = 0.5-30 atm, ϕ= 0.5-1.5, T_0 = 1000-1600 K for ignition and T_{in} = 300 K for PSR.



Solid: detailed; Symbols: reduced

Summary

1. Developed fuel-specific reduced models for Cat A2, C1 and C5 based on the HyChem models (Ver. 2)

Models	A2	C1	C5
Detailed	119	119	119
Skeletal	41	34	41
Reduced	31	26	31

2. Developed 48/35-species universal skeletal/reduced models for A2, C1, C5.
3. Developed a reduced NO sub-model (15 species skeletal, 10 species reduced)
4. Reduced molecular diffusion models to 15 diffusive groups and a reduced molecular diffusion model developed to further improve the computational efficiency
5. Developed analytic Jacobian and advanced chemistry solvers that can improve computational efficiency by an order of magnitude
6. Implemented DAC into LES simulations and tested in premixed non-premixed flames

Next Steps

- Reduced fuel-x model, and PAH/soot sub-model for emission
- Implementation of the reduced models and advanced chemistry solvers into LES

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Reduced NO and Transport models

NO sub-chemistry (Luo et al. CNF 2011)

- Skeletal: 15 species, 77 reactions; Reduced: 10 species
- Includes both thermal and prompt NO

Reduced molecular transport model

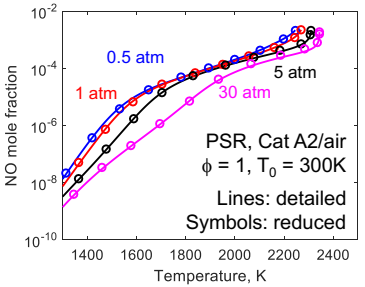
- Species with similar diffusivities bundled into groups

  For species i in group n: $\overline{D_i} \approx \frac{1-Y_i}{Q_n - \frac{X_i}{D'_{n,n}}}$, $Q_n = \sum_{m=1,K'} \frac{X'_m}{D'_{n,m}}$

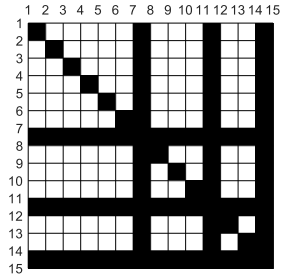
  Unimportant terms in the summation Q_n can be dropped

- Only 3 × 15 entries need to be evaluated with 10% error tolerance (black pixels) for different jet fuels

Validation of NO concentration in PSR



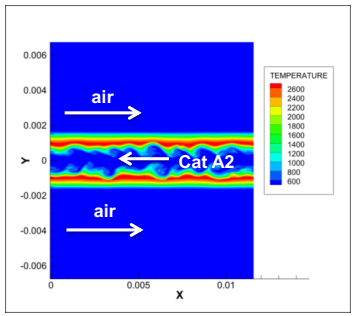
Bundled binary diffusion coefficient matrix



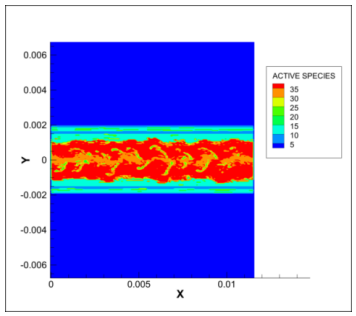
Dynamic Adaptive Chemistry

- OAK for DAC implemented into LES code (from S. Menon)
- Tested for premixed and non-premixed Cat A2 flames.
- Negligible difference between simulation w/o OAK
- Overall 3 times acceleration

Temperature field



Number of local active species



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