ASCENT Projects 25, 26, 28a
Chemical Kinetics Working Group: Experiments, Modeling, Model Reduction

Motivation and Objectives

➢ Motivations

- Next gen of jet engines will operate at higher pressures for fuel efficiency improvement.
- Quick and inexpensive fuel certification methods are needed for approval of new alternative fuels.
- Modeling methods are needed that describe accurately the behavior of real fuels in gas turbines.

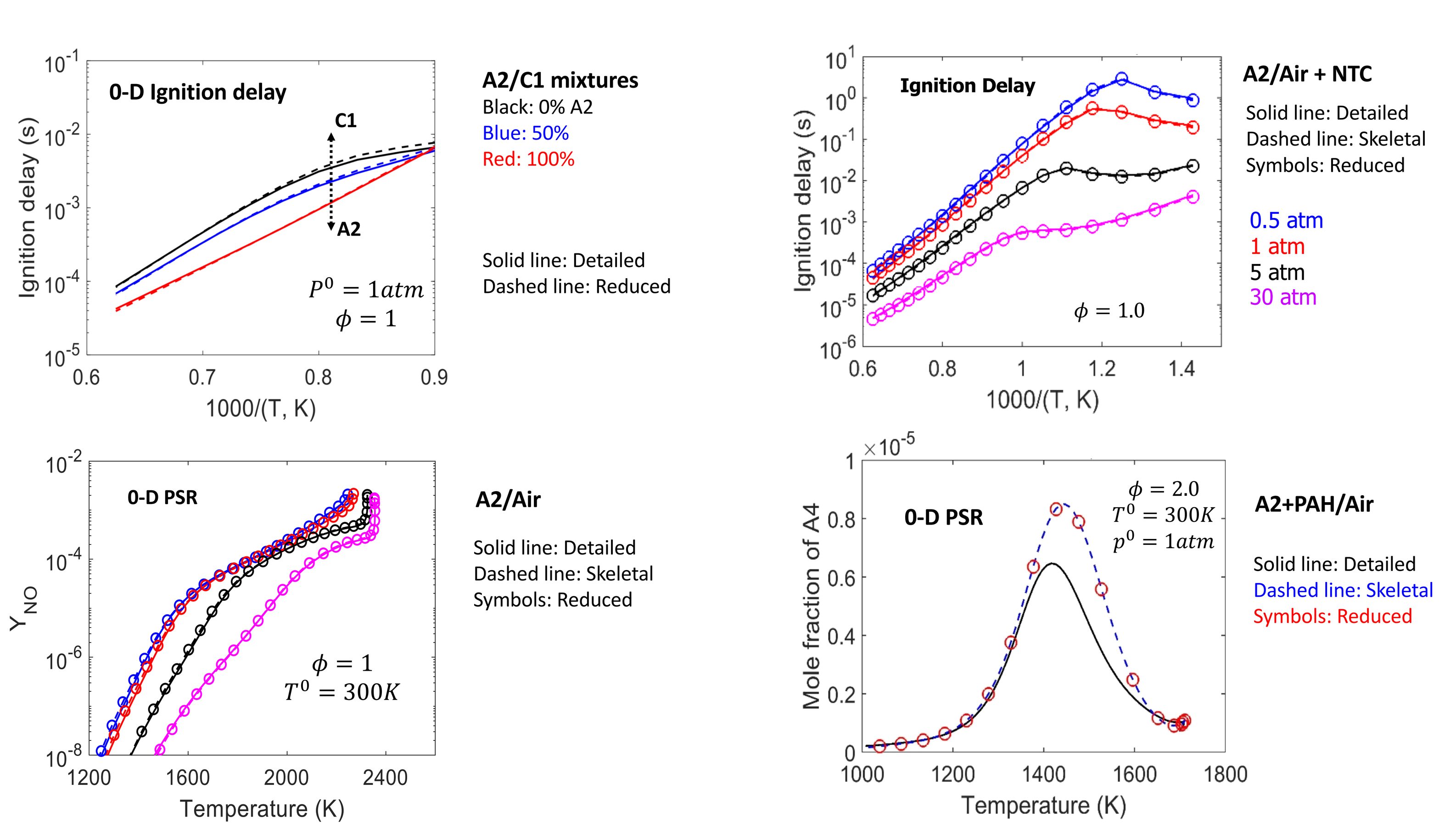
➢ Objectives

- Experiments: Apply optical methods to quantitatively measure multiple fuel pyrolysis products to: 1) constrain HyChem model, 2) achieve closure on mass balance, and 3) develop correlations between fuel spectroscopic, kinetics properties, and possibly combustor performance
- Model Reduction: Develop 1) reduced kinetic models for Cat A2/C1 mixtures, A2/A2a/A3 with NTC, and A2 with NOx and PAH sub-chemistry, 2) a new method for direct calculation of extinction and ignition in perfectly stirred reactors (PSR)

Results – Model Reduction (1/2)

➢ Reduced HyChem models and selected validations

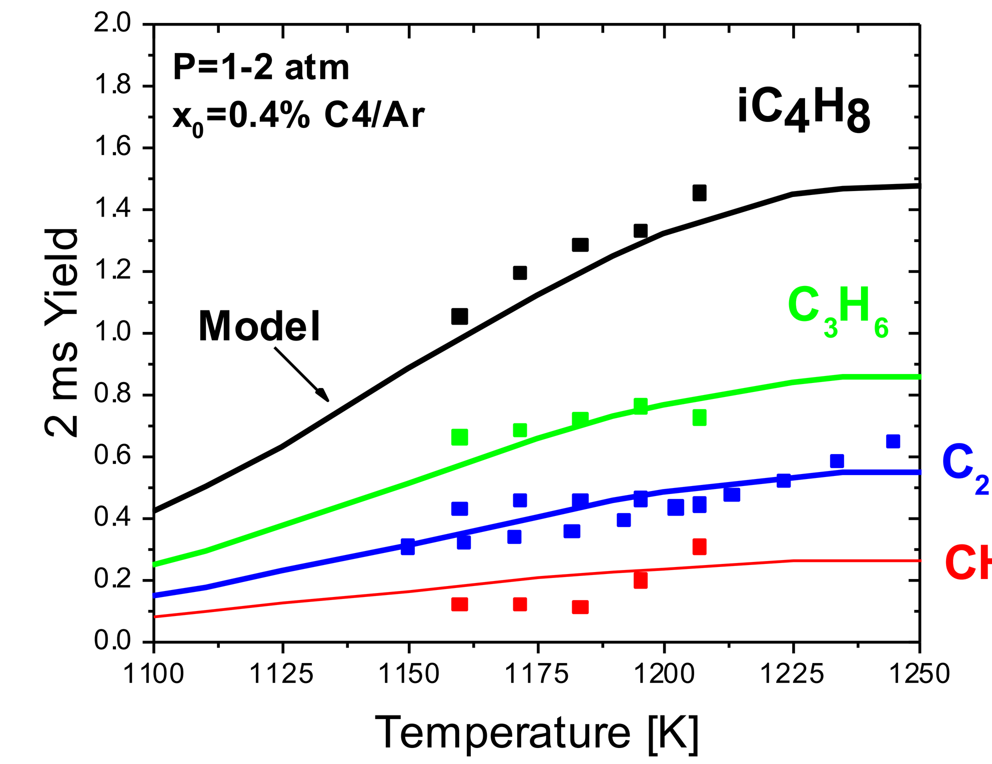
	Detailed	Skeletal	Reduced	Based models
A2/C1 Mixture	120	51	39	Detailed HyChem models
A2/A2a/A3 with NTC	125	48/47/50	34/35/36	HyChem+semi-global NTC steps
A2 with NOx	201	71	51	HyChem+NOx (Glarborg et al., 2018)
A2 with PAH	210	79	62	HyChem+KAUST-PAH (Wang et al., 2013)



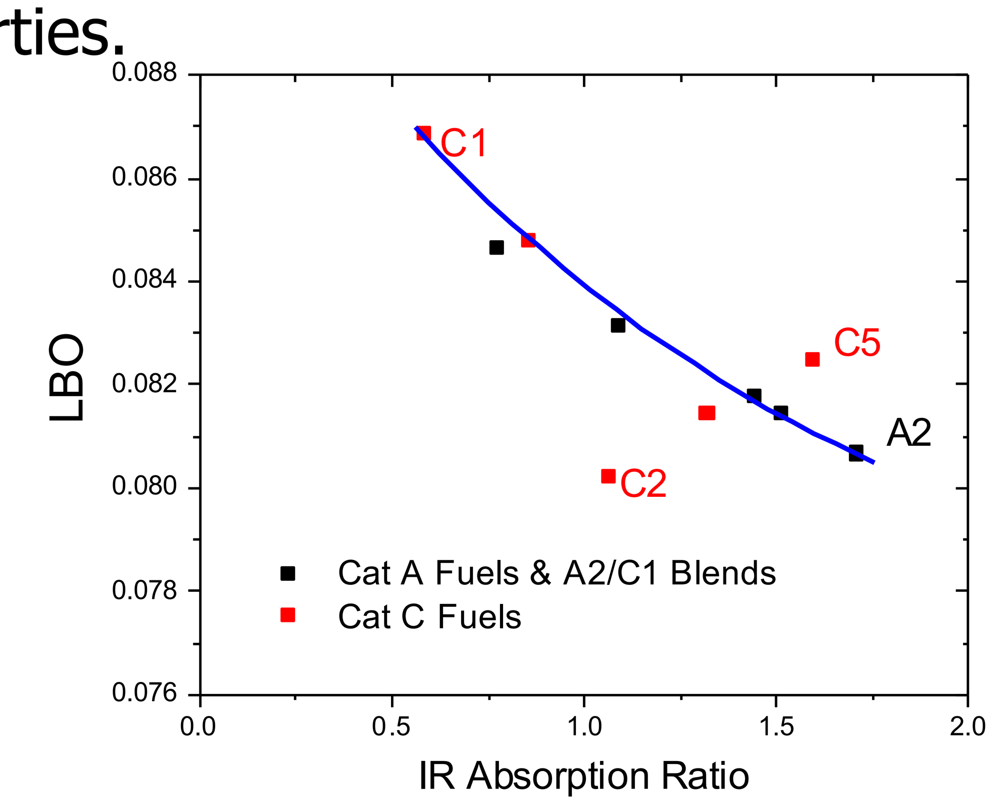
Results – Experiments

➢ Shock Tube and Spectroscopy

- Development of C4 HyChem model; model development based on multi-species database: CH4, C2H4, C3H6, iC4H8



- Development of IR Absorption Ratio Correlations with jet fuel LBO, IDT, DCN and C2H4 yields.
- IR ratio correlation provides simple link between FTIR fuel measurements and fuel kinetics properties.



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Results – Model Reduction (2/2)

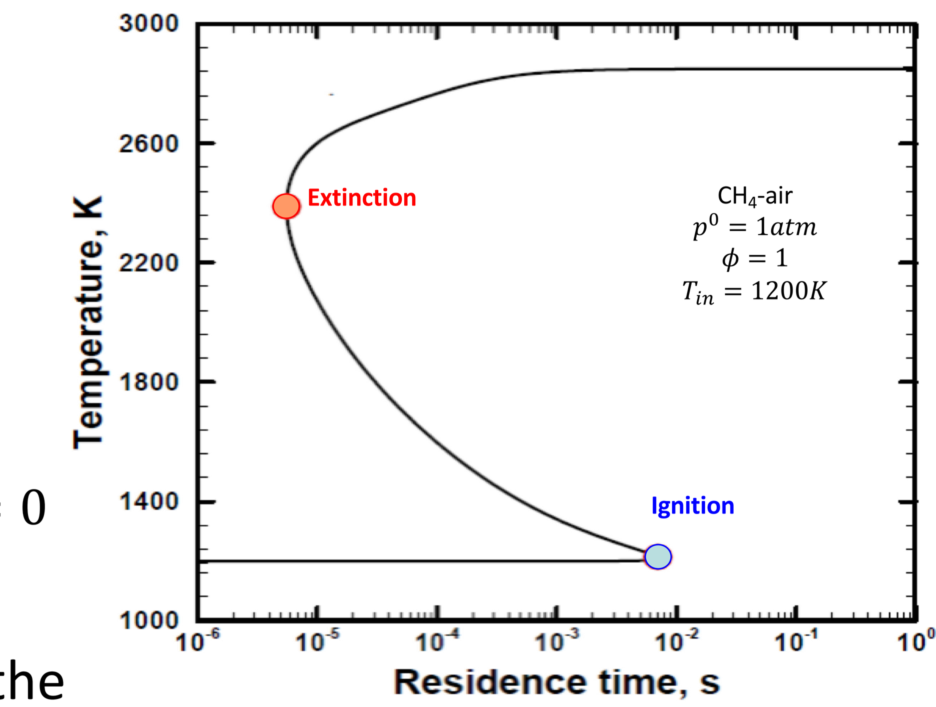
➢ Direct Computation of Ignition/Extinction states

- A novel numerical method is developed to predict PSR turning points using Lagrangian multiplier
- Methodology

minimize (or maximize): τ

Subject to

$$f(\mathbf{y},T,\tau) = \begin{cases} \dfrac{y_i - y_i^0}{\tau} - \dfrac{\sum_{i=1}^{K}\dot{\omega}_i W_i}{\rho} = 0 \\ \sum_{i=1}^{K} y_i h_i - \sum_{i=1}^{K} y_i^0 h_i^0 = 0 \end{cases}$$



Using Lagrangian multipliers, the optimization problem can be transformed to the following equations

$$\nabla\tau + \sum_{j}^{K+1} \lambda_j \nabla f_j = 0$$

The set of variables to be solved:

$$2K+3: \{y_1, \dots, y_K, T, \tau, \lambda_1, \dots, \lambda_{K+1}\}$$

K: number of species
τ: residence time
y_i: mass fraction
h: specific enthalpy
$\dot{\omega}_i$: production rate
W_i: molecular weight
ρ: mixture density
λ: Lagrangian multiplier
j: j^{th} governing equation
Subscript i: i^{th} species
Superscript o: inlet condition

- Marching is needed in the previous methods
- The new method captures ignition & extinction turning points directly with high efficiency and accuracy and can be applied on-the-fly in CFD

Conclusions and Next Steps

- Experiment: We have developed a correlation that relates IR absorption ratio to fuel combustion (LBO) properties.
- Next step: Relate FTIR spectra of jet fuel to fuel composition.
- Model Reduction: Reduced HyChem models for A2/C1 mixture, pure C1, A2/A2a/A3 with NTC, A2/NOx, and A2/PAH chemistry are developed and validated. A novel method for a direct computation of PSR turning points is developed and validated.
- Next step: Extend the present extinction study to investigate the controlling processes in LBO

Reference

Y. Wang, D. F. Davidson, R. K. Hanson, "A New Method of Predicting Derived Cetane Number for Hydrocarbon fuels, submitted to Fuel , September 2018.