Combustion Data for Jet-A, its Constituent Components, and Surrogate Mixtures

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Multi-Agency Coordination Committee for Combustion Research – 2009 Fuels Summit

Generation of Comprehensive Surrogate Kinetic Models and Validation Databases for Simulating Large Molecular WeightHydrocarbon Fuels

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Key Tasks

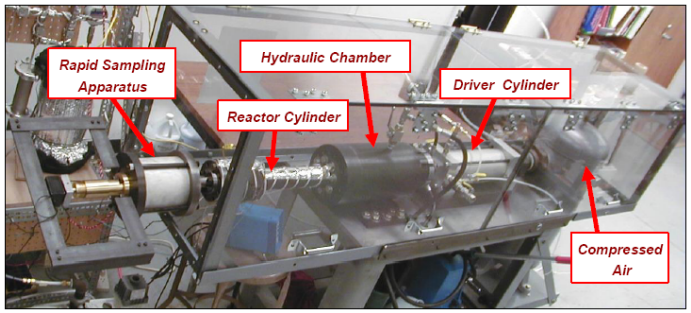
- Acquire comprehensive experimental validation database for jet fuels, their constituents, and surrogate mixtures.
  - Autoignition delays and pre-ignition species evolutions at elevated pressures and low-to-intermediate temperatures
  - Fundamental flame properties, including laminar flame speeds and extinction stretch rates
- Establish the pattern of ignition response for the neat components vis-à-vis fully blended jet fuels.
- Explore the feasibility of reproducing combustion trends of Jet-A using simple binary/ternary surrogates.

Progress to Date

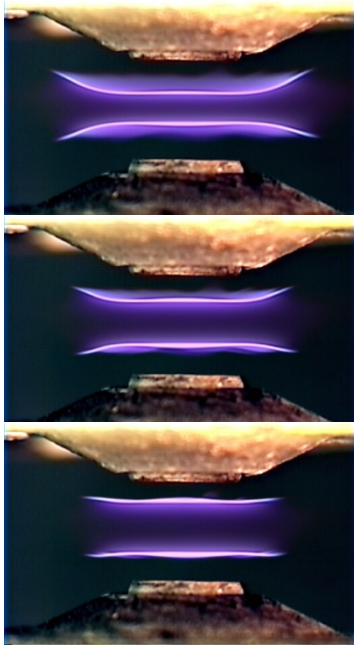
- Autoignition of real jet fuels, including *Jet-A*, *JP-8*, and *S-8*.
- Autoignition of neat hydrocarbon components under high pressure conditions: *n-decane*, *iso-octane*, *toluene*, *benzene*, *DME*, *DIB-1*, *MCH*, *1,2,4-TMB*, and *xylenes*.
- Chemical kinetic interactions in binary fuel blends: *toluene+iso-octane*, *toluene+DIB-1*, *n-decane+iso-octane*.
- Autoignition of Aachen surrogate and MURI mixture model.
- Laminar flame speeds of preheated fuel/air mixtures: *MCH*, *toluene*, *iso-octane*, *n-heptane*, *n-decane*, *n-dodecane*, *Jet-A*, and *S-8*.
- Extinction limits of preheated fuel/O_2/N_2 mixtures: *n-decane*, *n-dodecane*, *Jet-A*, and *S-8*.

Outline of Presentation

- **Autoignition Response**
  - Comprehensive ignition response for a key paraffin component: *n*-decane
  - Real jet fuels: Jet-A, JP-8, and S-8
  - Jet-A constituents: aromatics, cycloalkanes, branched alkanes
  - Binary blends and surrogates



- **Flame Response**
  - Laminar flame speeds and extinction stretch rates
  - Neat surrogate components and real jet fuels



- **Future Work**

Autoignition Response under High Pressure Conditions

Test Matrix: *n*-Decane

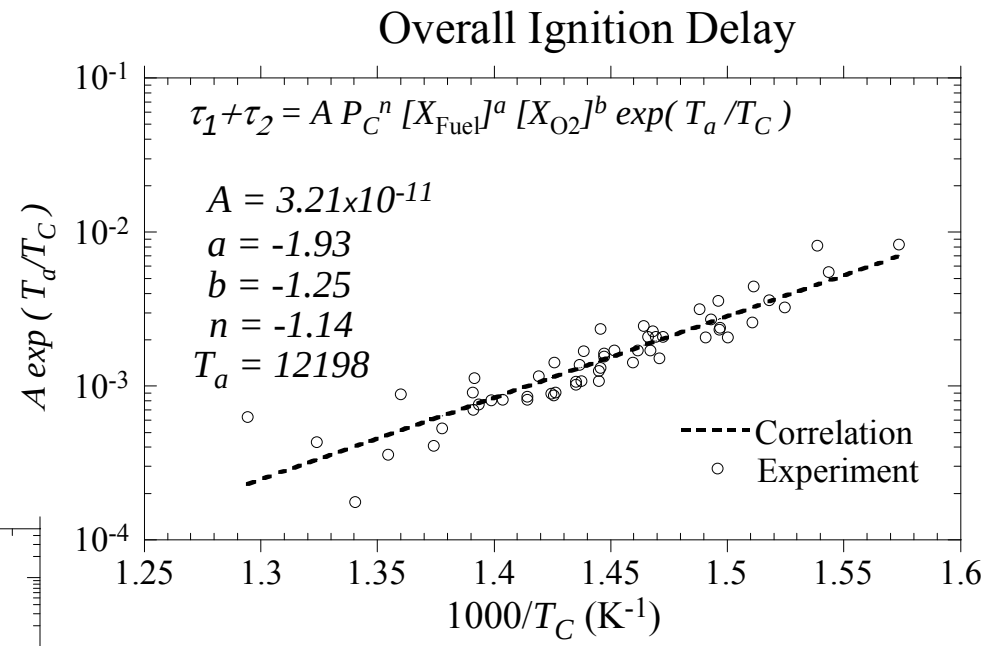
Molar Ratio			Molar composition (%)		
n-$C_{10}H_{22}$	O_2	N_2	X_{Fuel}	X_{O2}	X_{N2}
0.500	**15.5**	**58.28**	**0.673**	**20.87**	**78.46**
0.800	**15.5**	**58.28**	**1.073**	**20.78**	**78.14**
0.800	**15.5**	**88.03**	**0.767**	**14.86**	**84.38**
1.200	**15.5**	**140.00**	**0.766**	**9.89**	**89.34**
1.687	**15.5**	**140.00**	**1.073**	**9.86**	**89.07**
2.218	**15.5**	**189.00**	**1.073**	**7.50**	**91.43**
2.090	**15.5**	**292.80**	**0.673**	**4.99**	**94.33**

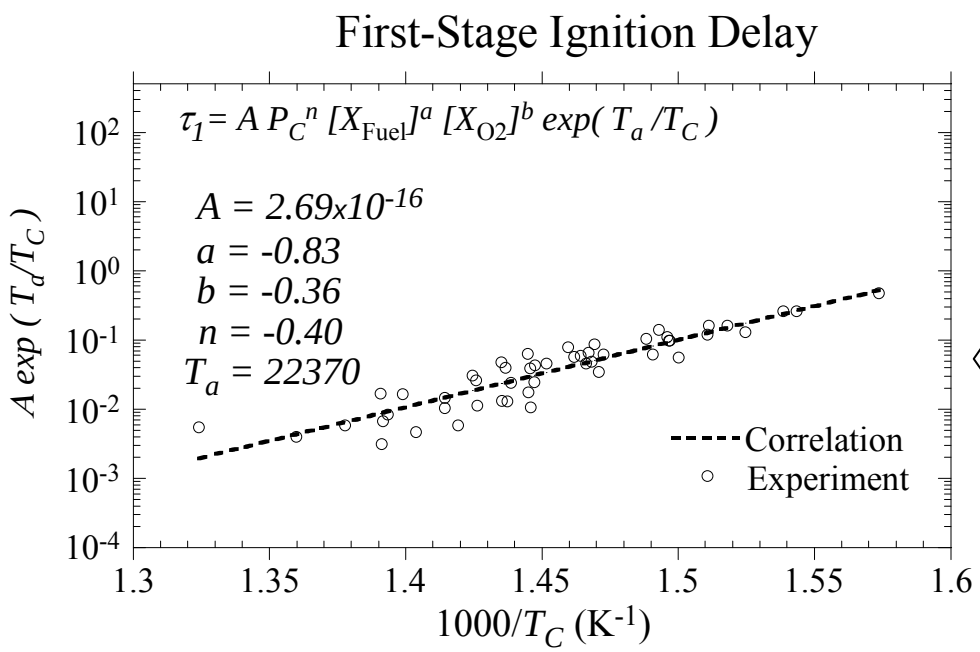
ϕ

- Compressed Temperature: $T_C = 630 - 770$ K
- Compressed Pressure: $P_C = 7 - 30$ bar

n-Decane Autoignition

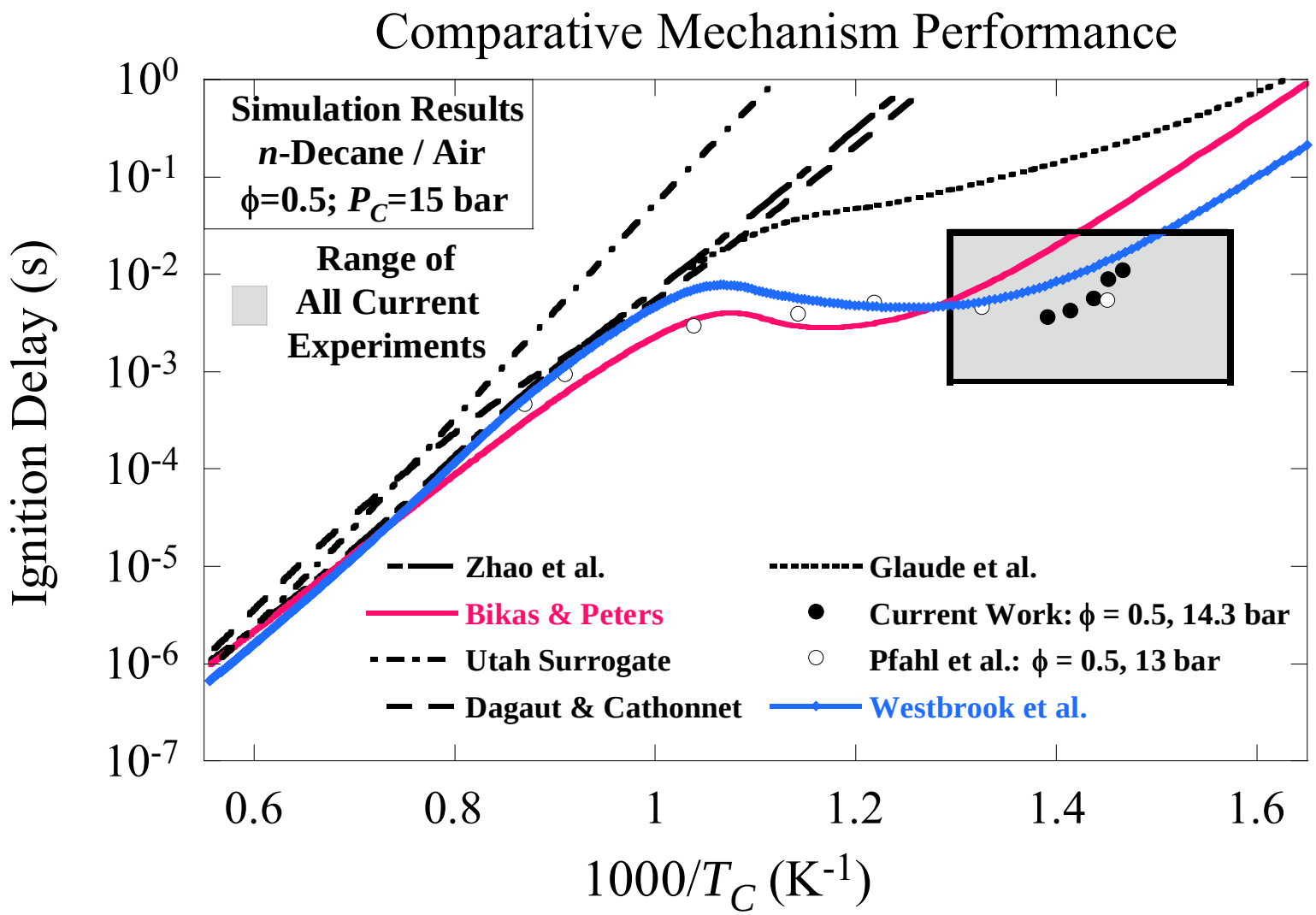
Data limited to two-stage activity region



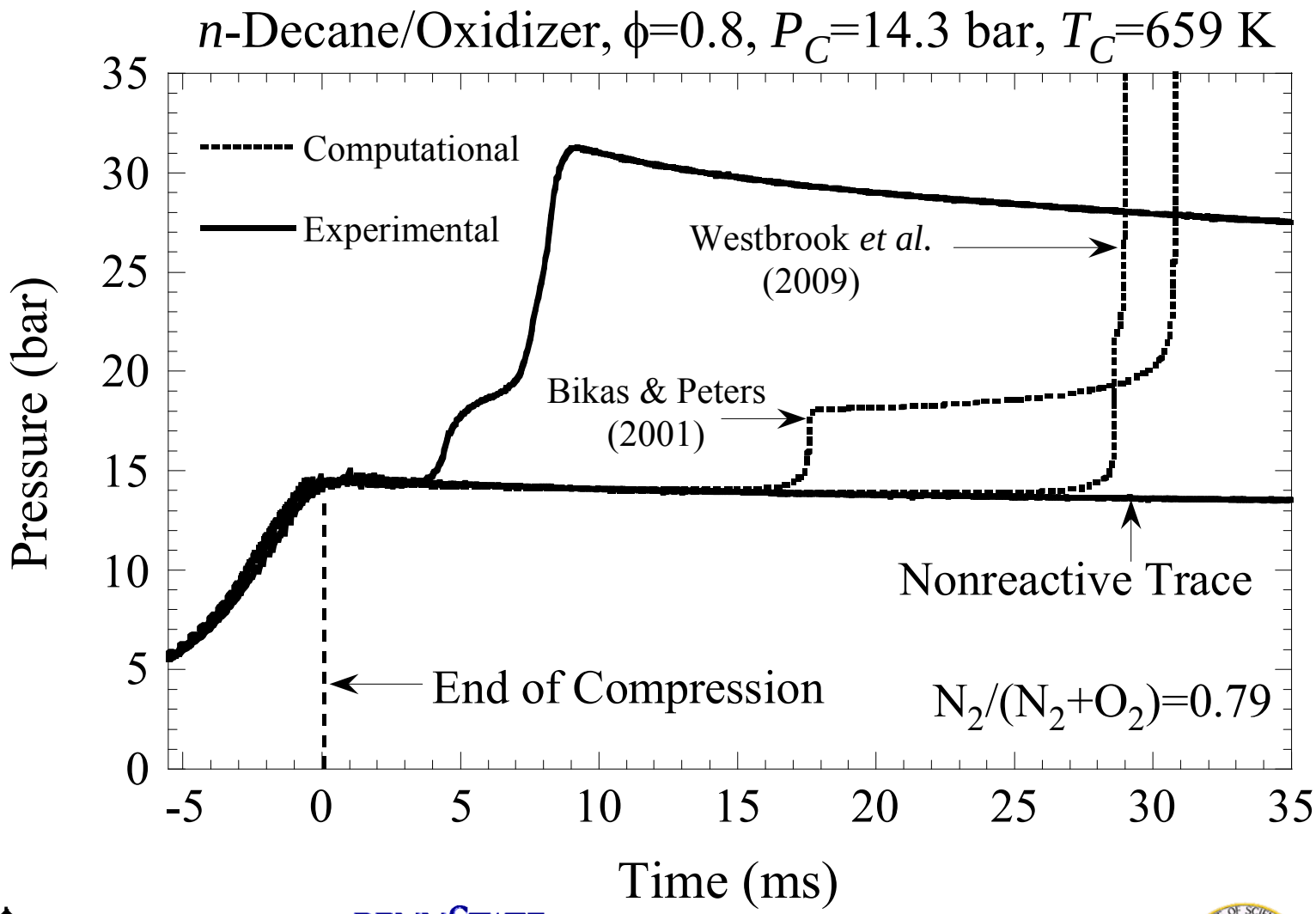


First stage delay has higher T sensitivity

Autoignition Comparison (1)



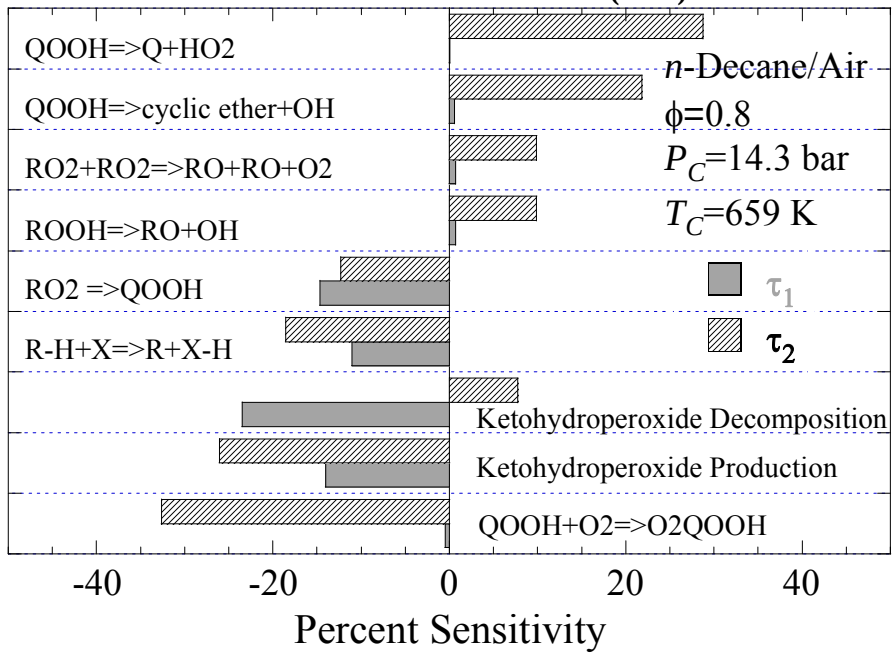
Autoignition Comparison (2)



Ignition Delay Sensitivity

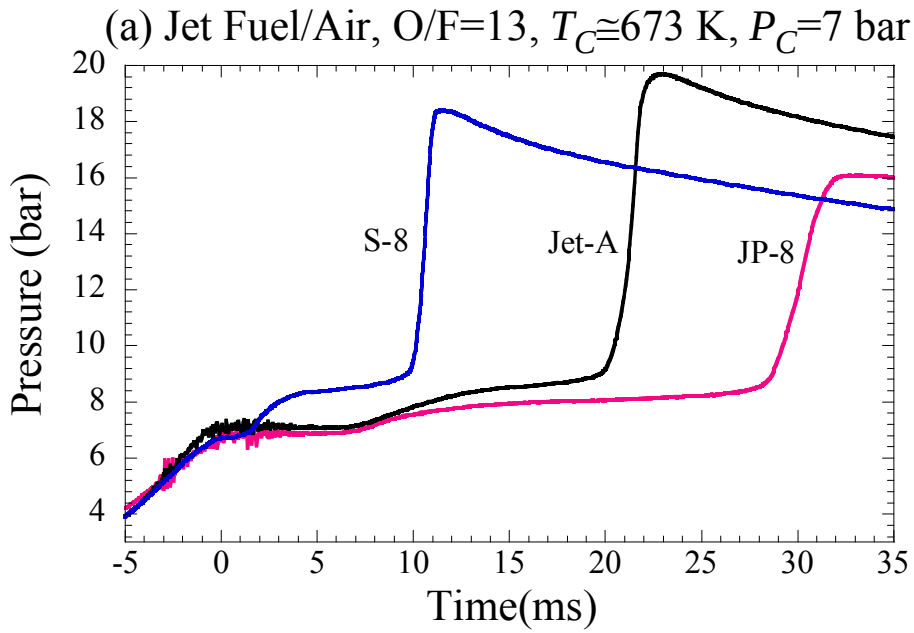
Sensitivity of Ignition Delay to Different Reaction Classes

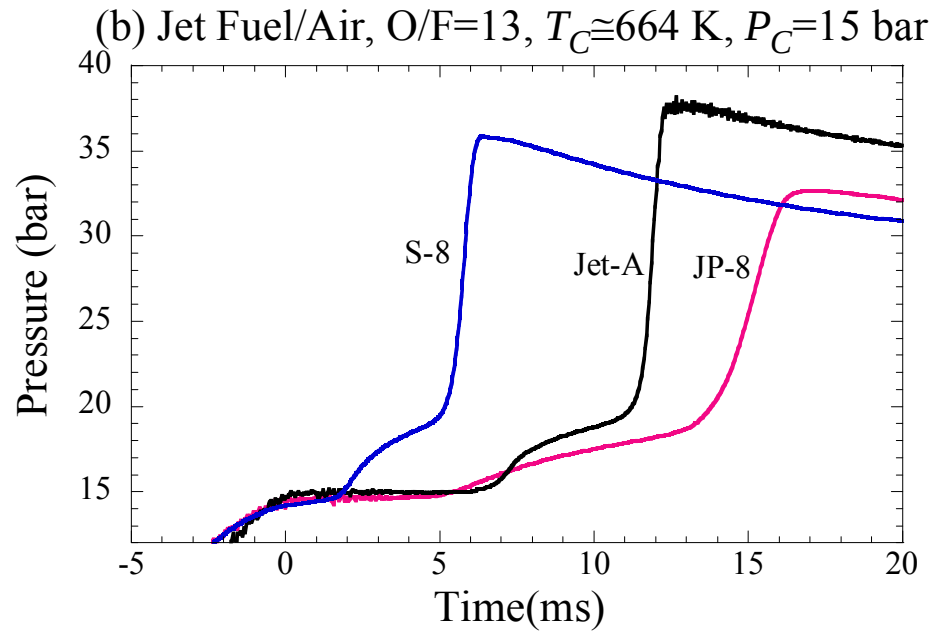
Mechanism of Westbrook *et al.* (2008)



- In general, the sensitivity of a particular class of reactions tends be in the same direction, for both τ_1 and τ_2.
- A noticeable exception is the ketohydroperoxide decomposition step, which is also the most endothermic of all the reactions pertinent to the low temperature chemistry.
- Increasing rate constants for the ketohydroperoxide decomposition class would decrease τ_1 and increase τ_2, while minimally affect the total ignition delay.

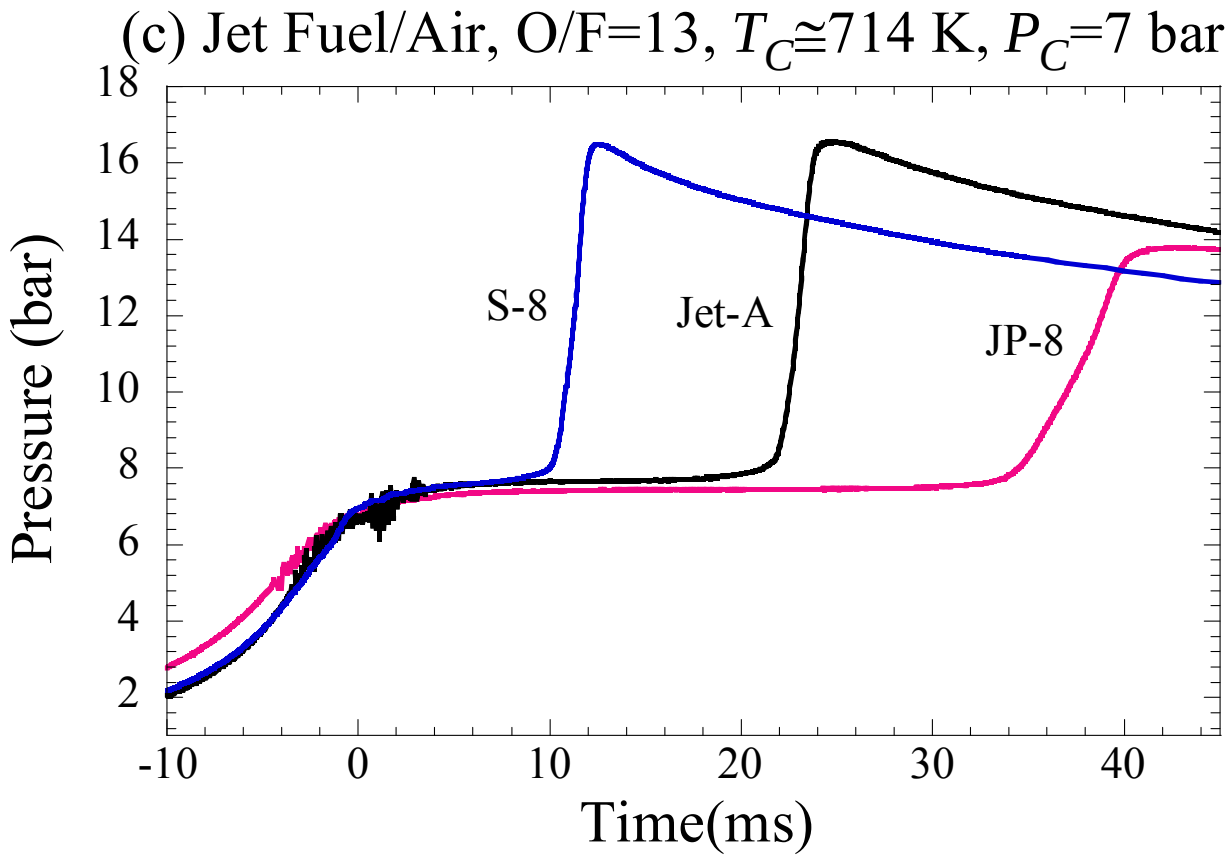
Jet Fuels Comparison (1)





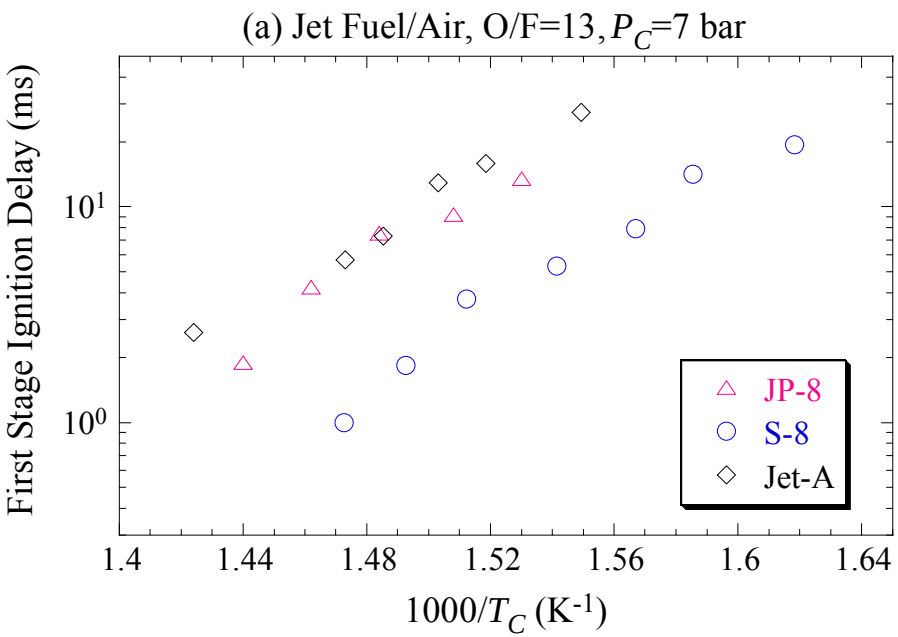
- Two-stage activity for all three fuels with similar first-stage ΔP.
- Nearly similar first stage ignition delay for conventional jet fuels.
  - Longer second stage ignition delay for JP-8.
- Shortest ignition delay for S-8.

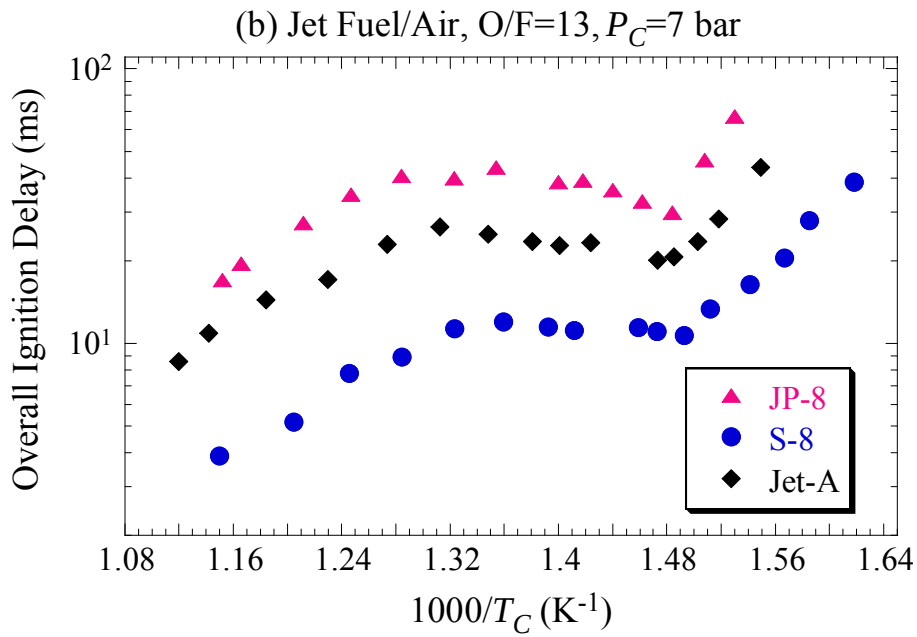
Jet Fuels Comparison (2)



- Two-stage activity suppressed at this higher temperature.
- Shortest ignition delay for S-8, followed by Jet-A and JP-8.

Jet Fuels Comparison (3)

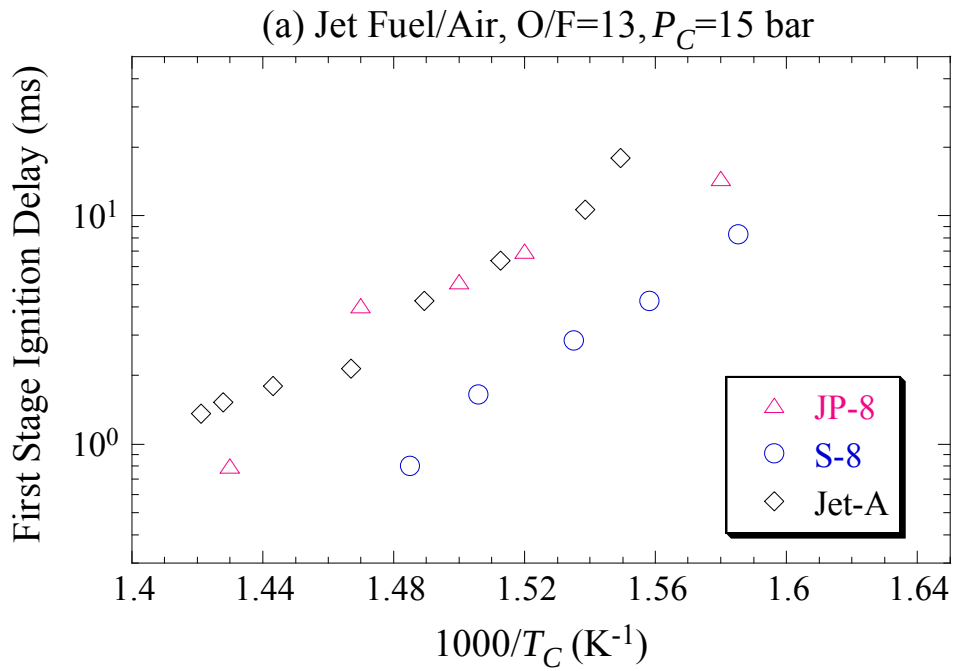


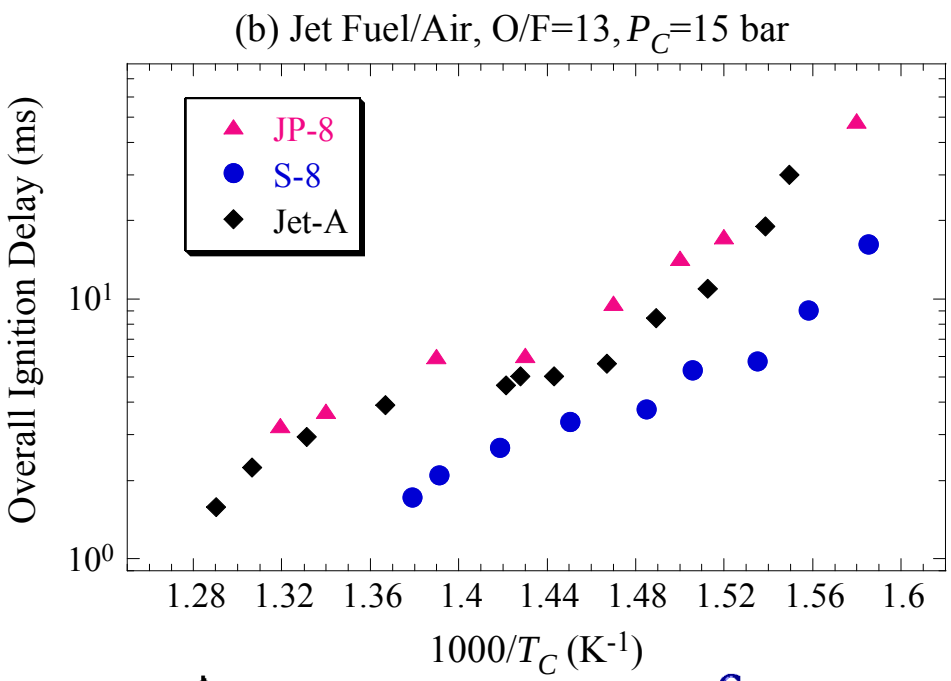


- First stage ignition delays for conventional jet fuels are similar.
- The alternative jet fuel has a shorter first stage ignition delay.
- Overall ignition delays for all three jet fuels differ: S-8<Jet-A<JP-8.

Jet Fuels Comparison (4)

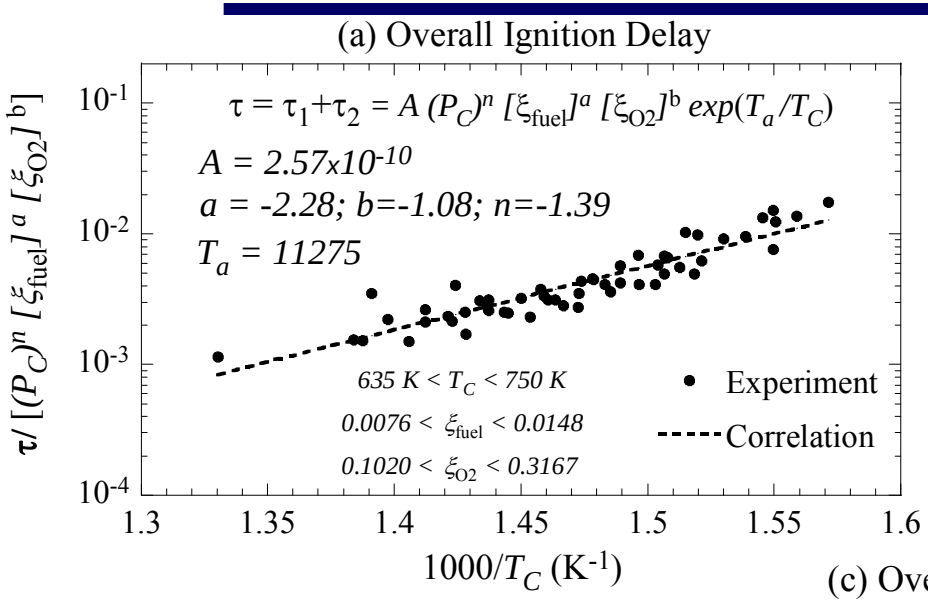
- Similar first stage delay for Jet-A and JP-8.

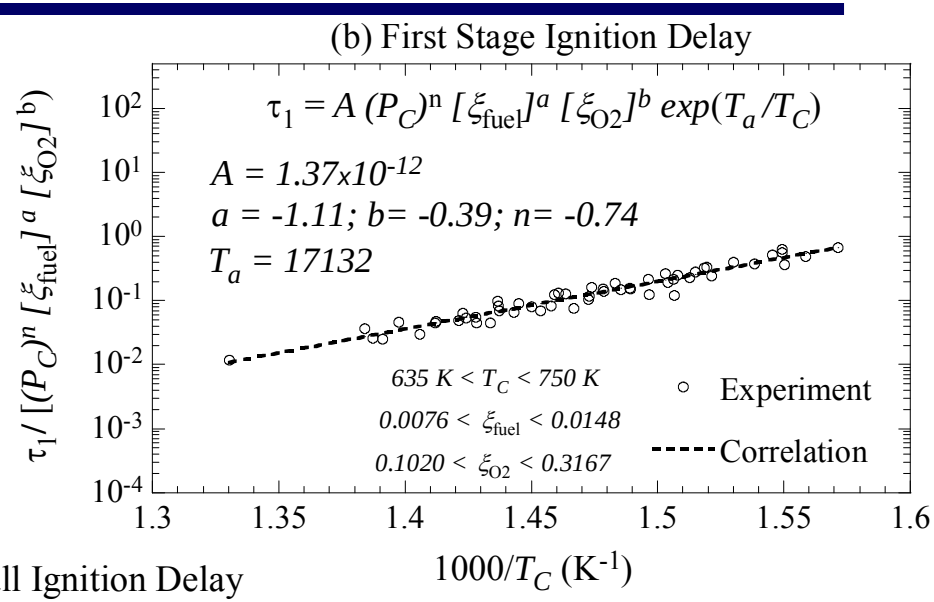


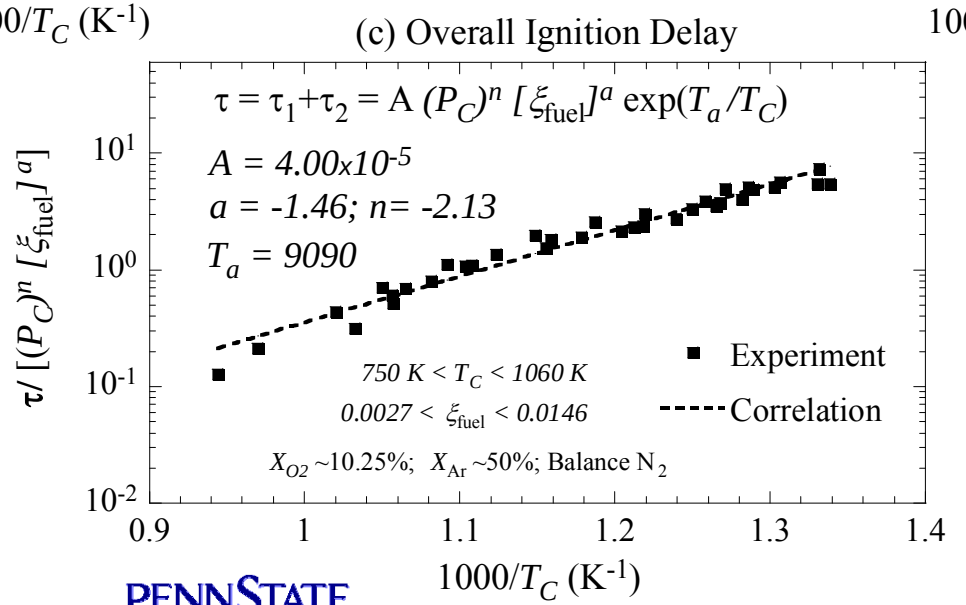


- S-8 shows highest reactivity.

Ignition Delay Correlations: Jet-A





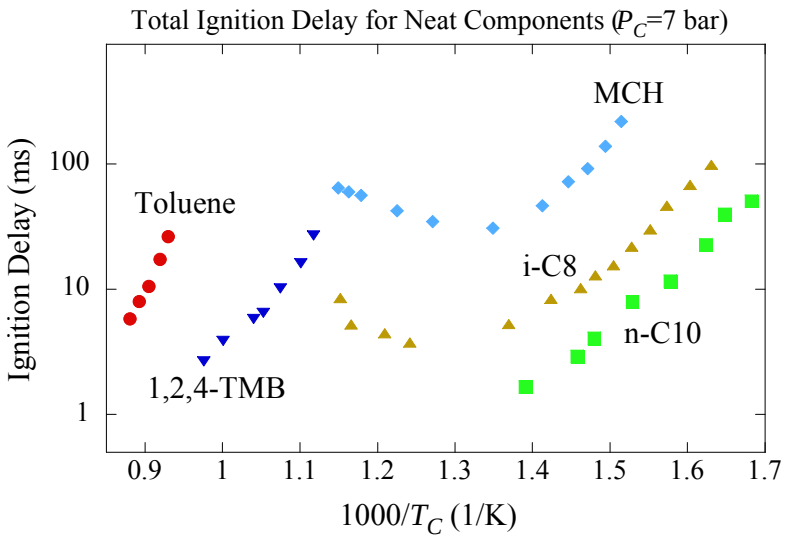


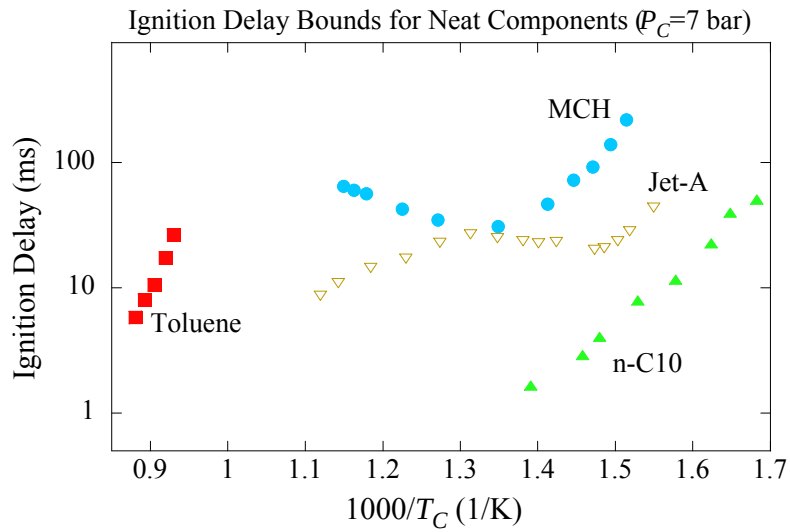
Autoignition Comparison: Jet-A vs. Neat Components (1)

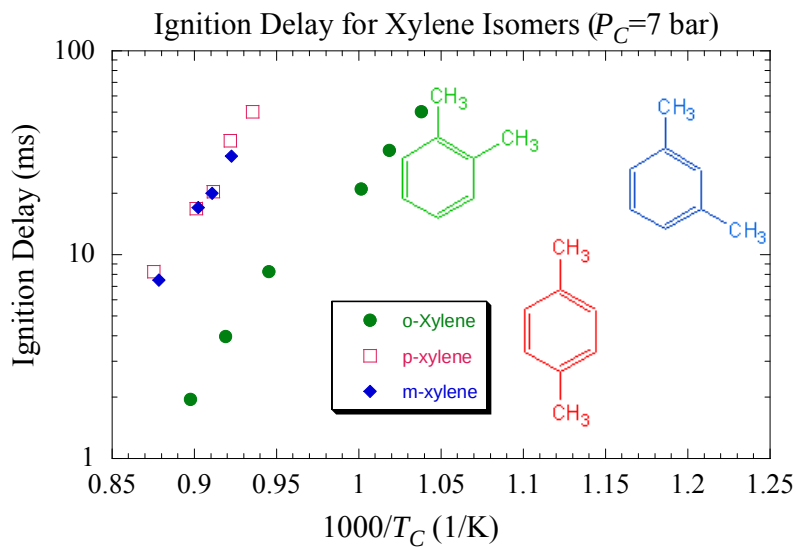
Test Conditions

Fuel	A/F Mass Ratio	ϕ	Diluent
iso-Octane	*13.0*	*1.16*	N_2
n-Decane	*13.0*	*1.15*	N_2
Methylcyclohexane	*12.7*	*1.16*	N_2
Toluene	*15.4*	*1.16*	*Ar*
1,2,4-Trimethyl Benzene	*15.8*	*1.16*	*Ar*
m-, o-, p-Xylene	*15.6*	*1.16*	*Ar*
MURI Mixture Model (49.5/28.2/22.3 liq. vol% n-decane/iso-octane/toluene)	*13.0*	*1.12*	N_2
Aachen Surrogate(20/80 mass% 1,2,4-TMB/n-decane)	*13.0*	*1.13*	N_2
Jet-A (04POSF4658)	*13.0*	*1.12*	N_2
Diluent : Oxygen = 3.76 : 1			

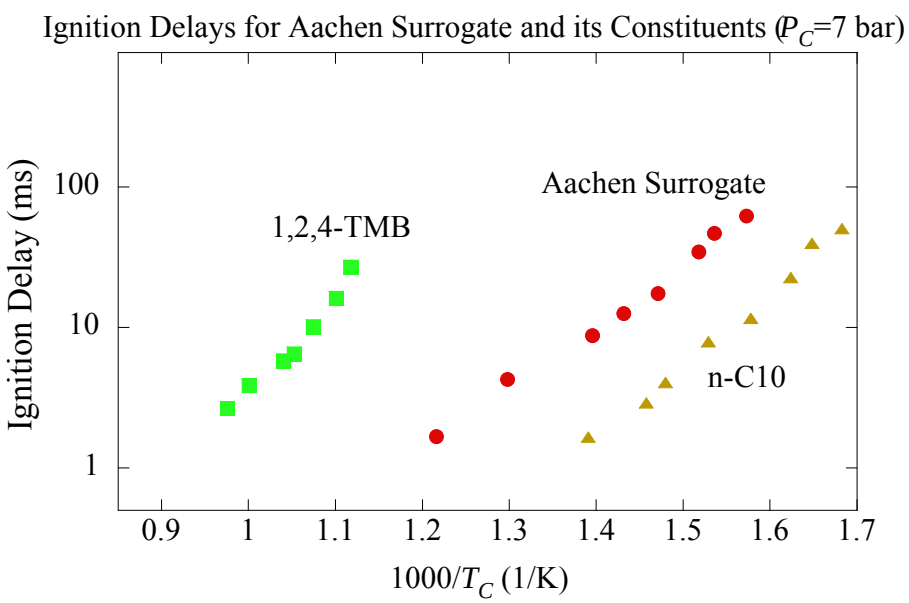
Autoignition Comparison: Jet-A vs. Neat Components (2)

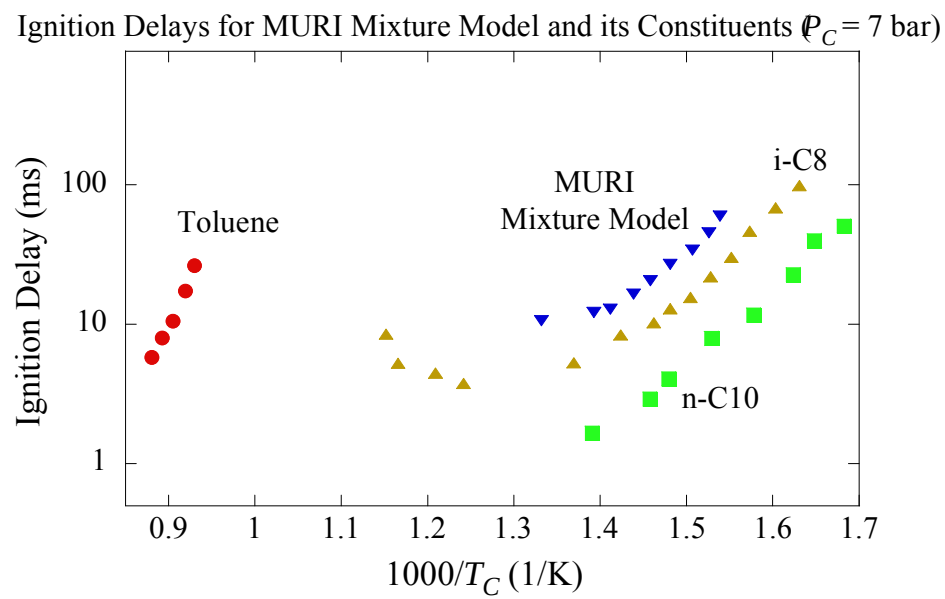






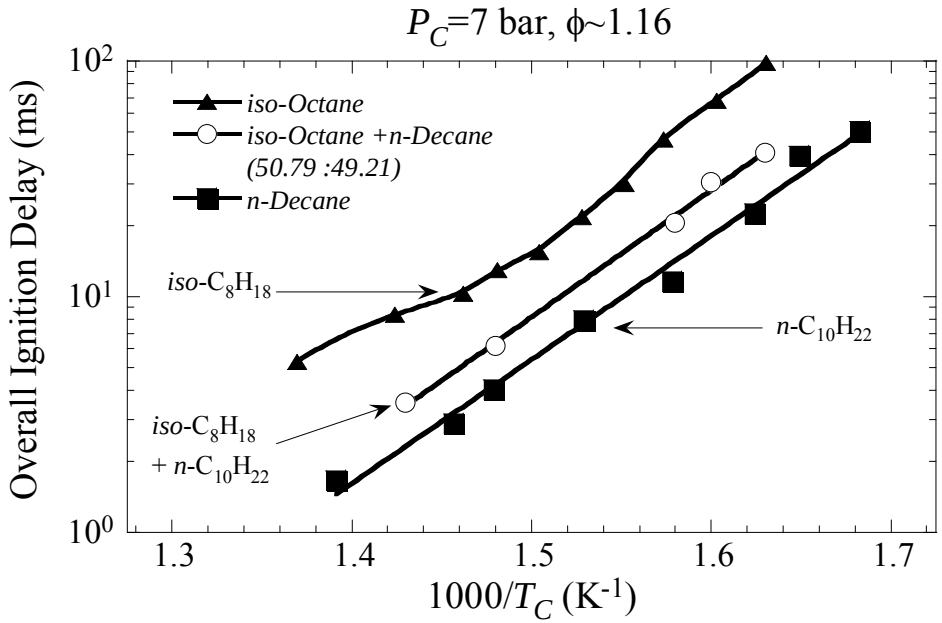
Autoignition Comparison: Surrogate Mixtures vs. Neat Components

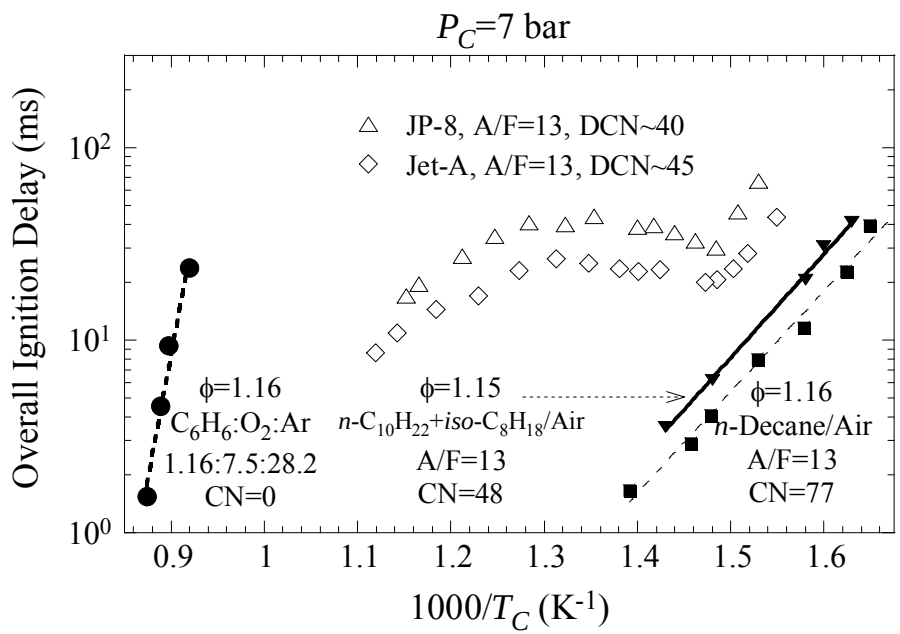




- Surrogate mixtures inherit the traits of the neat constituents
  - NTC trend from i-C_8 in the current range for MURI mixture model

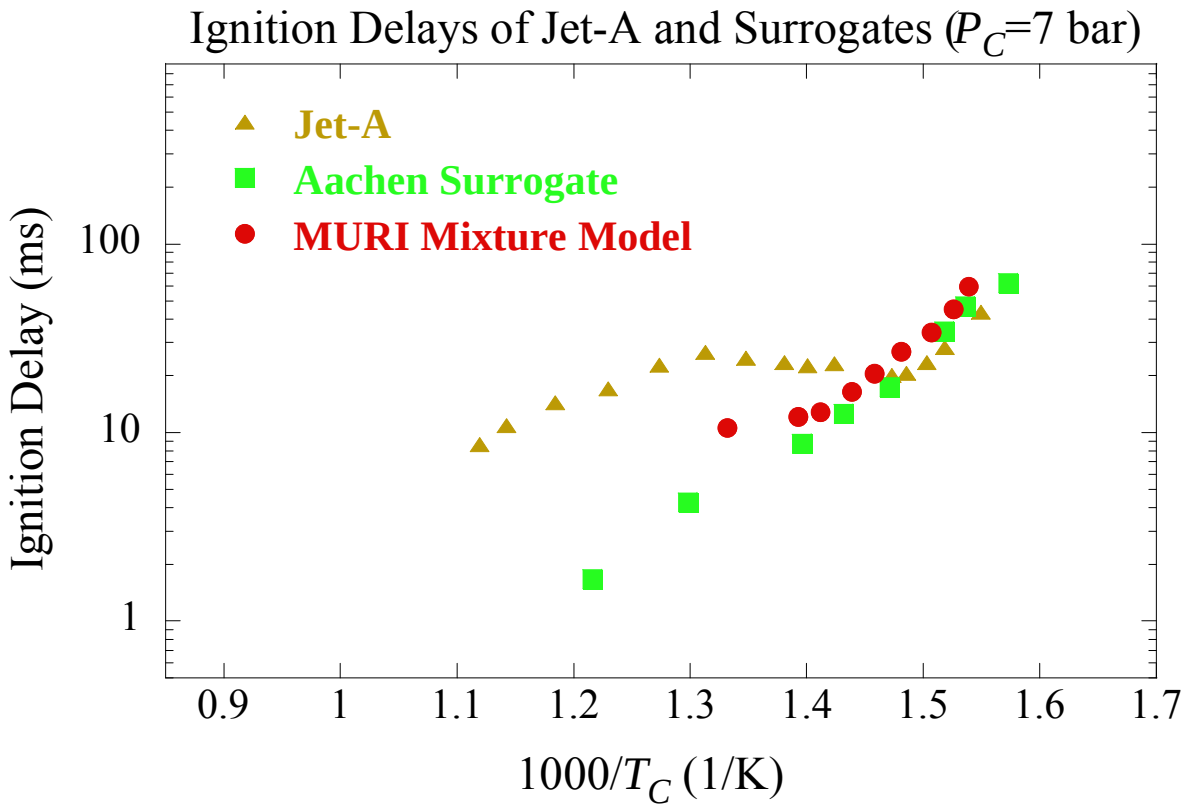
Autoignition Comparison: Jet-A vs. Binary Mixtures





- Fuel mixtures with similar CN, but different constituents, can display markedly different ignition delay times in the low-to-intermediate temperature range.
- While CN is a parameter, further refinement is required to reproduce the ignition characteristics of fully blended fuels.

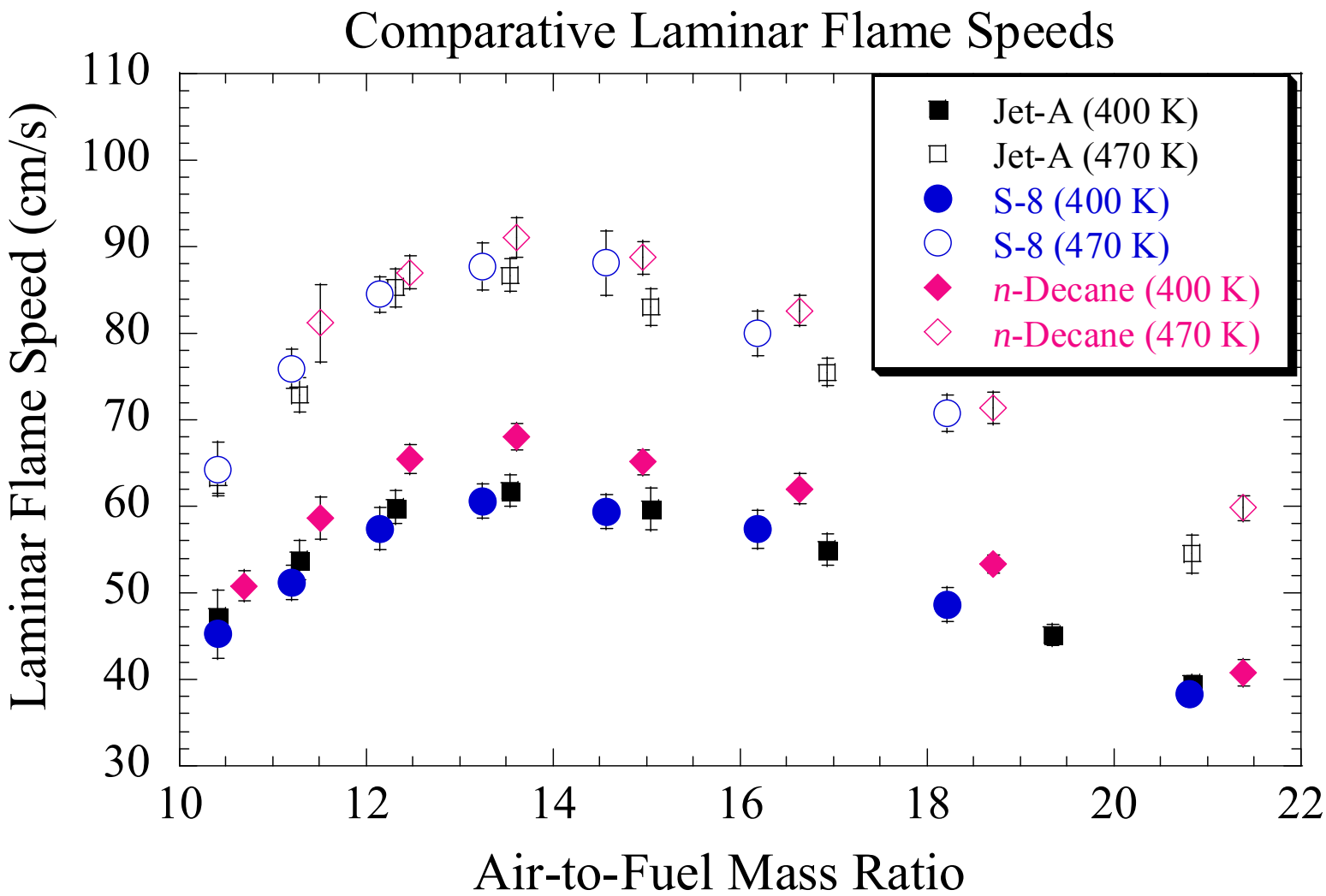
Autoignition Comparison: Jet-A vs. Surrogate Mixtures



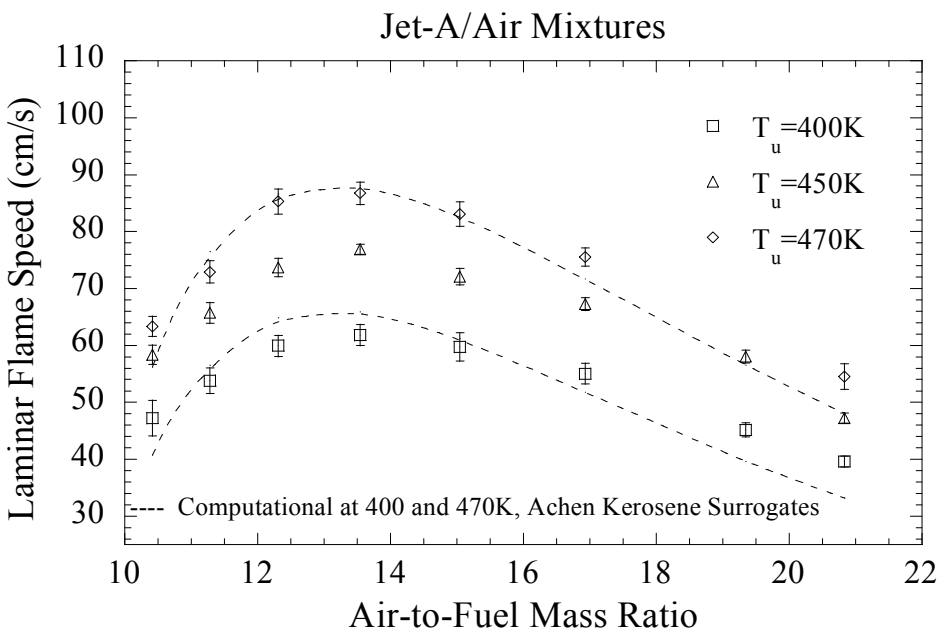
- Both surrogates perform well in the pre-NTC low-T range
- MURI mixture model appears to capture NTC, while the Aachen surrogate does not.

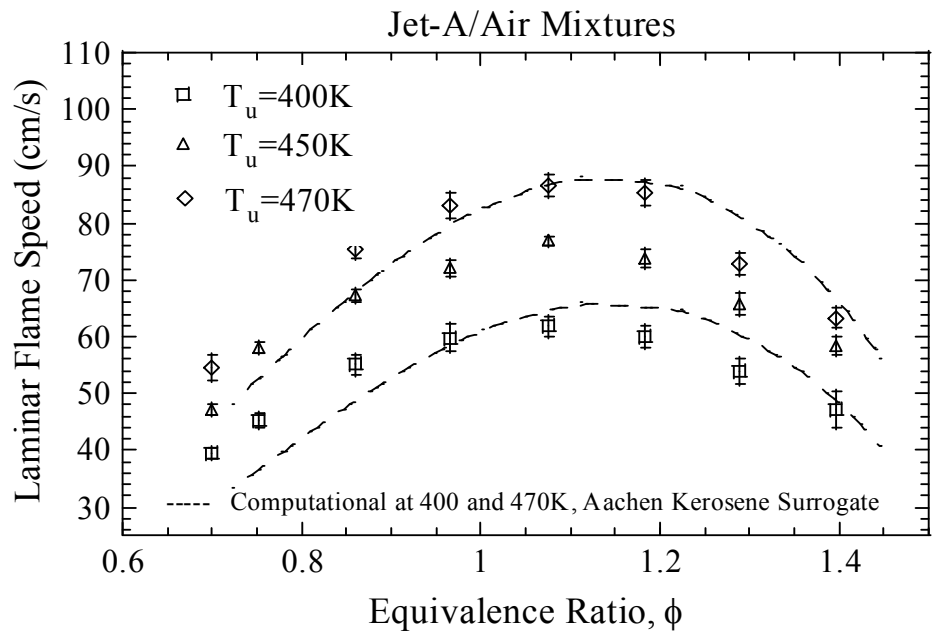
Laminar Flame Speeds and Extinction Limits of Preheated Fuel/Air Mixtures

Laminar Flame Speed Comparison



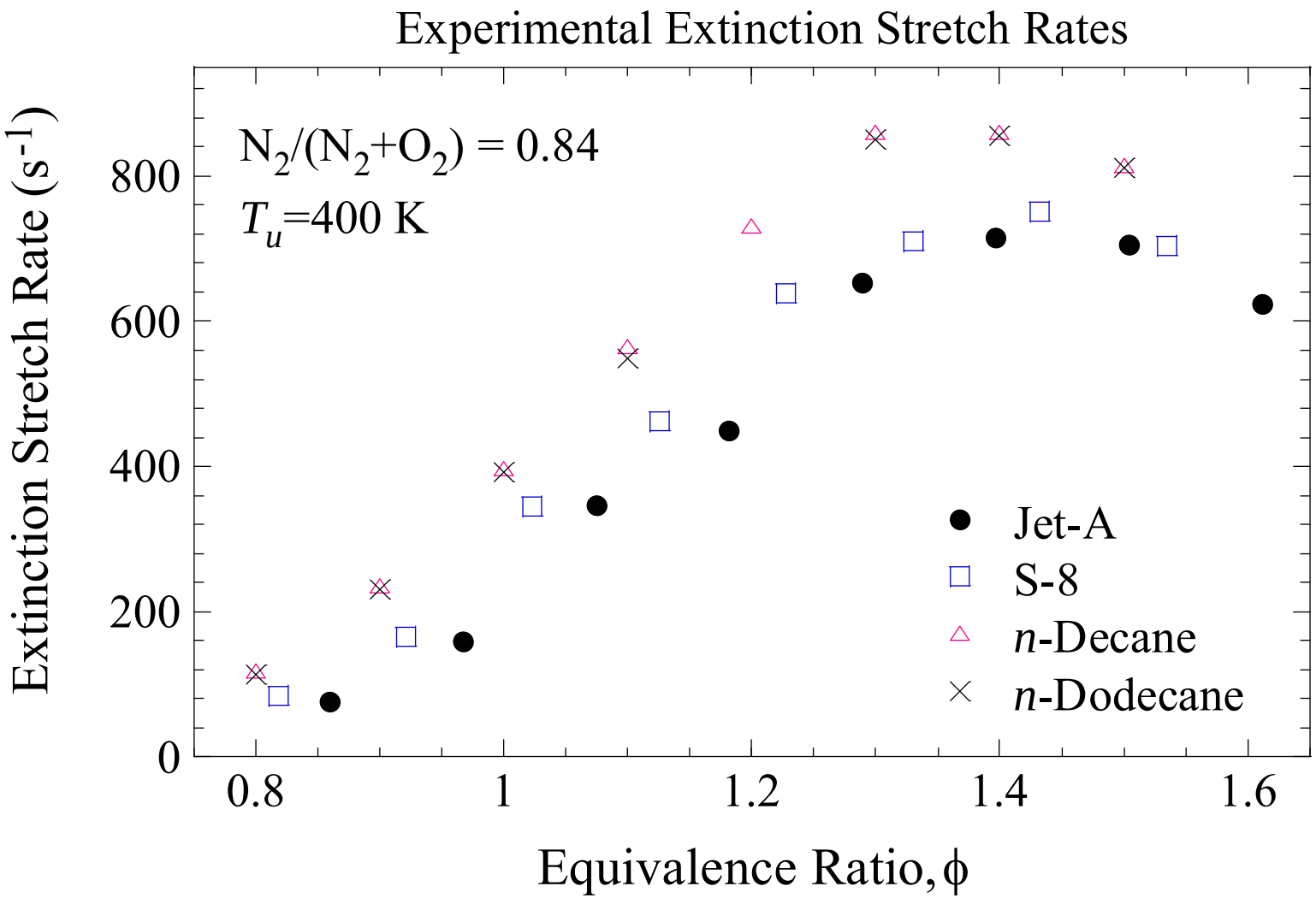
Laminar Flame Speeds: Jet-A vs. Aachen Surrogate



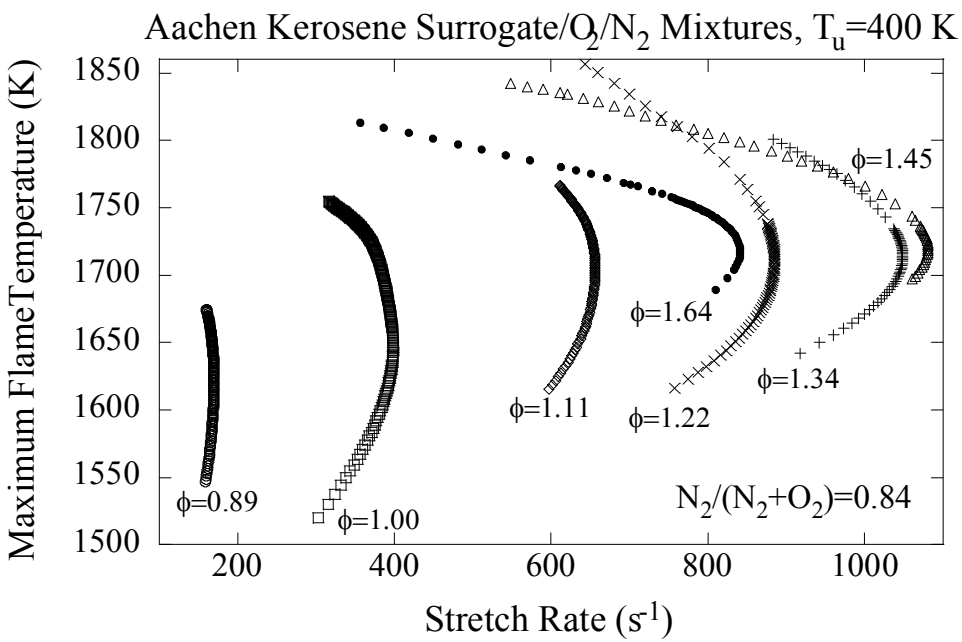


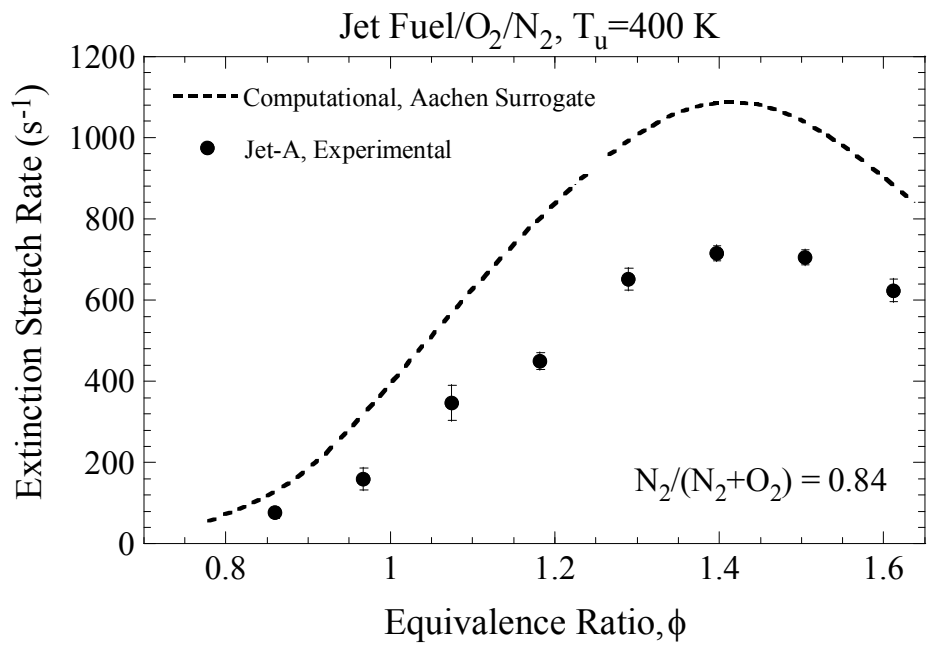
- Aachen kerosene surrogate performs well at stoichiometric conditions.

Extinction Limit Comparison



Extinction Stretch Rates: Jet-A vs. Aachen Surrogate

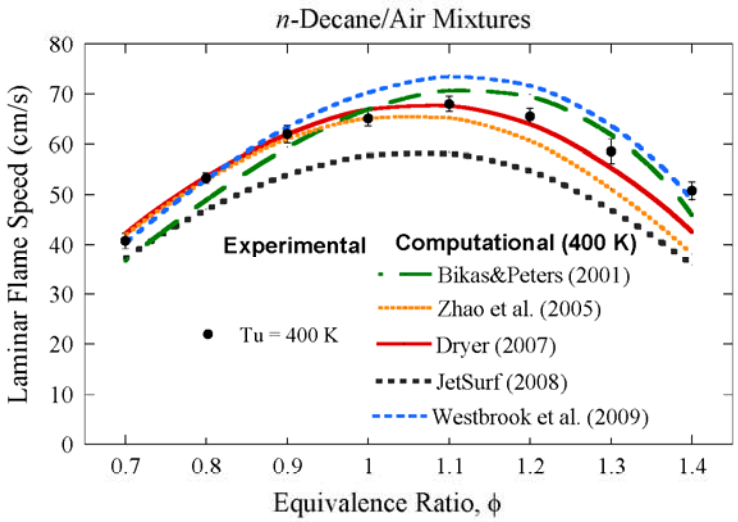


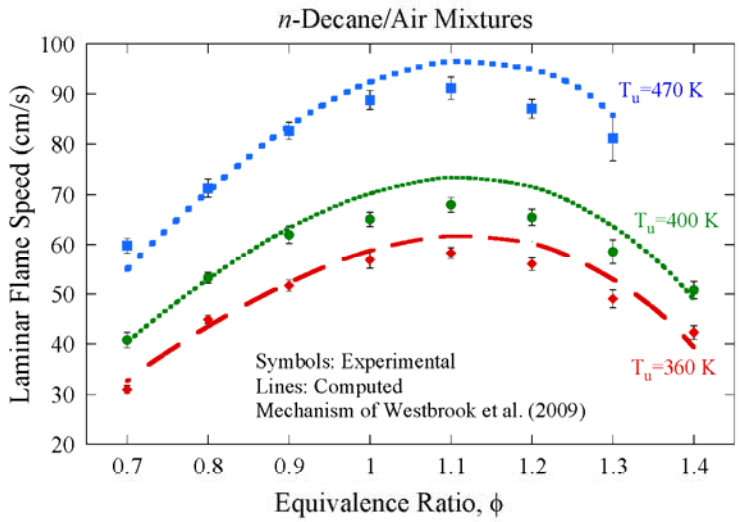


- Qualitative trend is well captured
- Significantly higher extinction stretch rates predicted
  - Fair agreement at lowest equivalence ratio

Laminar Flame Speed: Neat Component (1)

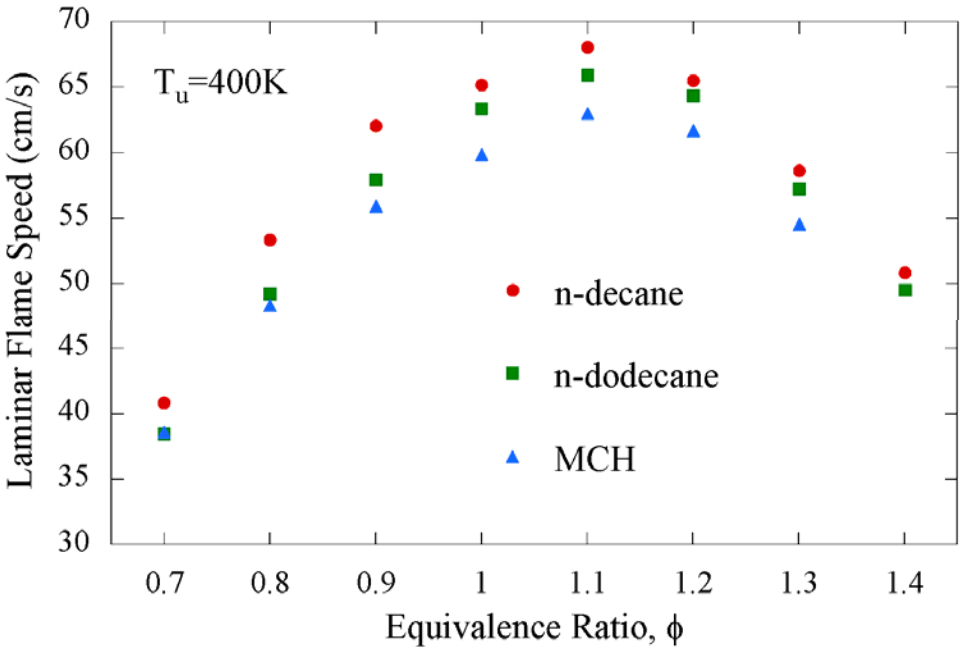
Kerosene Surrogate Component: *n*-decane.

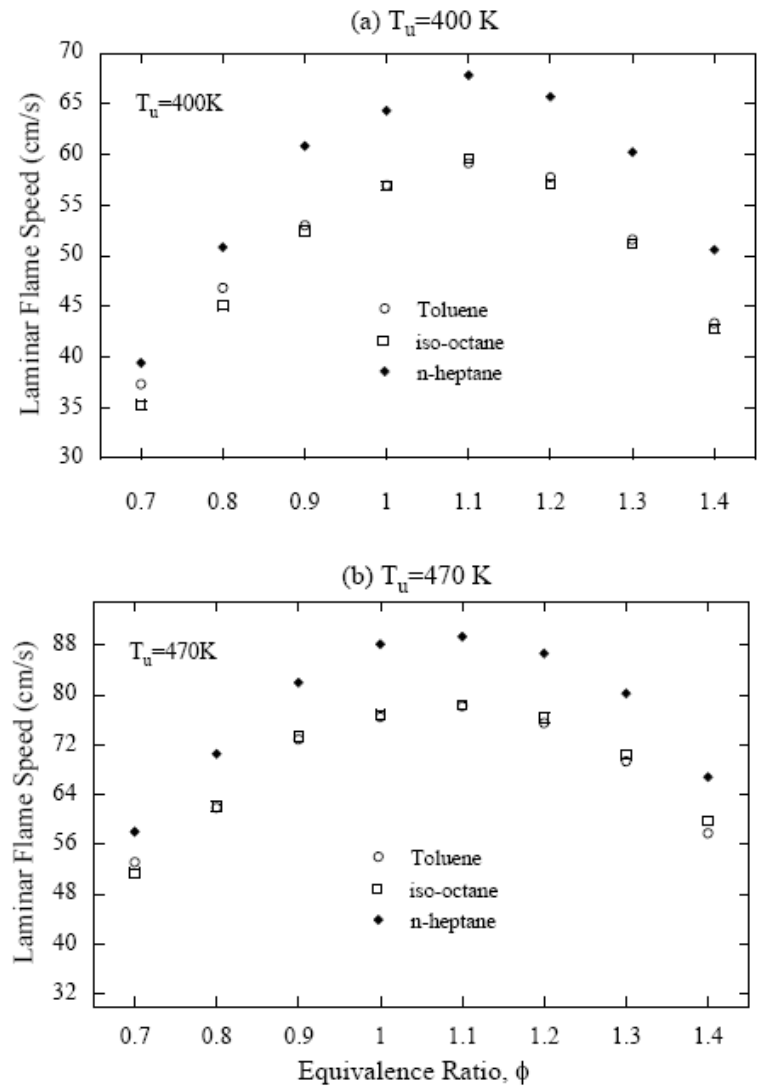




- Detailed mechanism of Westbrook et al.(2009) is in fair agreement.
  - Good agreement on lean side($\phi = 0.7 - 0.9$)
  - Overpredicts close to the stoichiometric region
- Performance of semi-detailed mechanisms vary considerably.
  - Mechanism of Bikas&Peters (2001) and Dryer (2008) show best agreement.

Laminar Flame Speed: Neat Component (2)



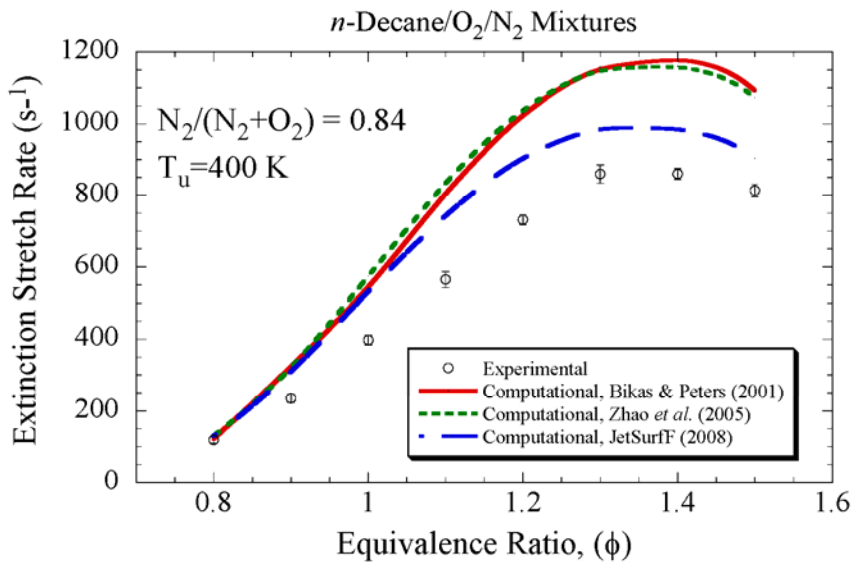


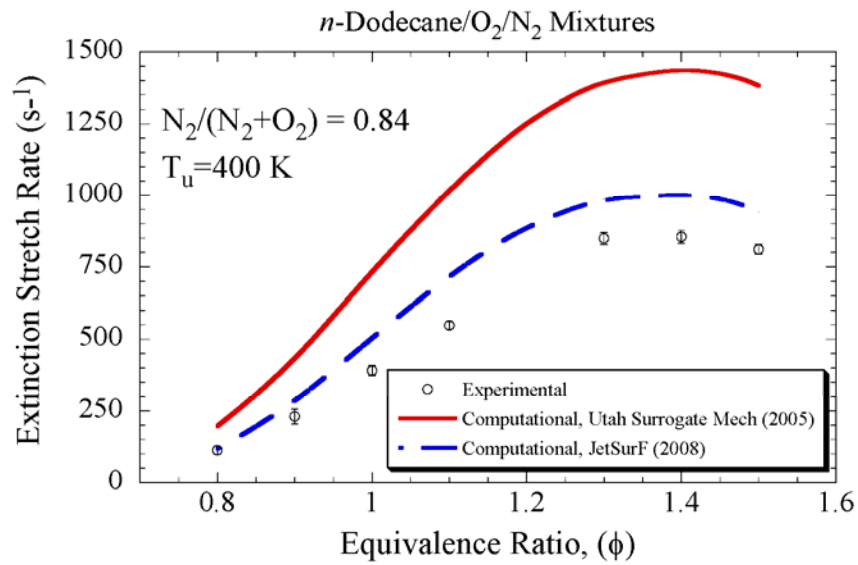
Flame Speed Comparison:

Linear Alkane > Cycloalkane > Branched Alkane ≈ Aromatic

Extinction Stretch Rate: Neat Component

Comparative Extinction Response for Kerosene Surrogate Components





- JetSurF provides the best match with the experimental data for extinction of both (n-$C_{10}H_{22}$) and (n-$C_{12}H_{26}$).

Future Work

- Acquire autoignition data of neat surrogate components.
  - *n*-dodecane, *n*-propylbenzene, 1,3,5-TMB, xylenes, etc.
  - Coordinated with Fred Dryer and Ken Brezinsky.
- Acquire autoignition data of surrogate mixtures and MURI mixture models.
  - Comparison with Jet-A.
  - Coordinated with Fred Dryer.
- Conduct high-pressure flame measurements for neat surrogate components, binary fuel blends, and real jet fuels.
  - Coordinated with Yiguang Ju.

Acknowledgements

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- Graduate Students: Xin Hui and Bryan Weber.