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

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MURI Objectives

- Compare fundamental combustion properties of real jet fuel and 1st / 2nd generation surrogate mixtures.
- Acquire extensive experimental database for validating surrogate chemical kinetic model.
  - Neat Surrogate Components
  - Fuel blends
- Generate comprehensive reduced chemistry for CFD simulations.

Autoignition Characterization

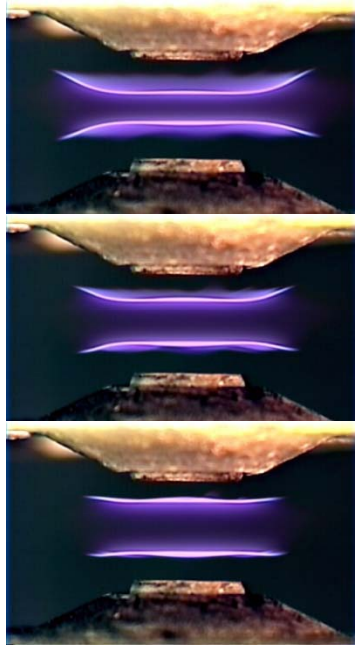
- Obtain experimental data for autoignition delays at elevated pressures and low-to-intermediate temperatures, using a heated rapid compression machine.

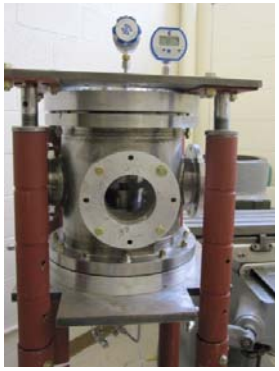
Real Jet Fuels	*Jet-A (with and w/o additive), JP-8, and S-8*
Neat Components	*n-decane, n-dodecane, iso-octane, toluene, benzene, DME, DIB-1, MCH, xylenes, 1,2,4-TMB, 1,3,5-TMB, and n-PB*
Fuel Blends	*toluene+iso-octane, toluene+DIB-1, n-decane+iso-octane, n-decane+1,2,4-TMB, n-decane+iso-octane+toluene, and n-dodecane+iso-octane+1,3,5-TMB+n-PB*

Fundamental Flame Properties

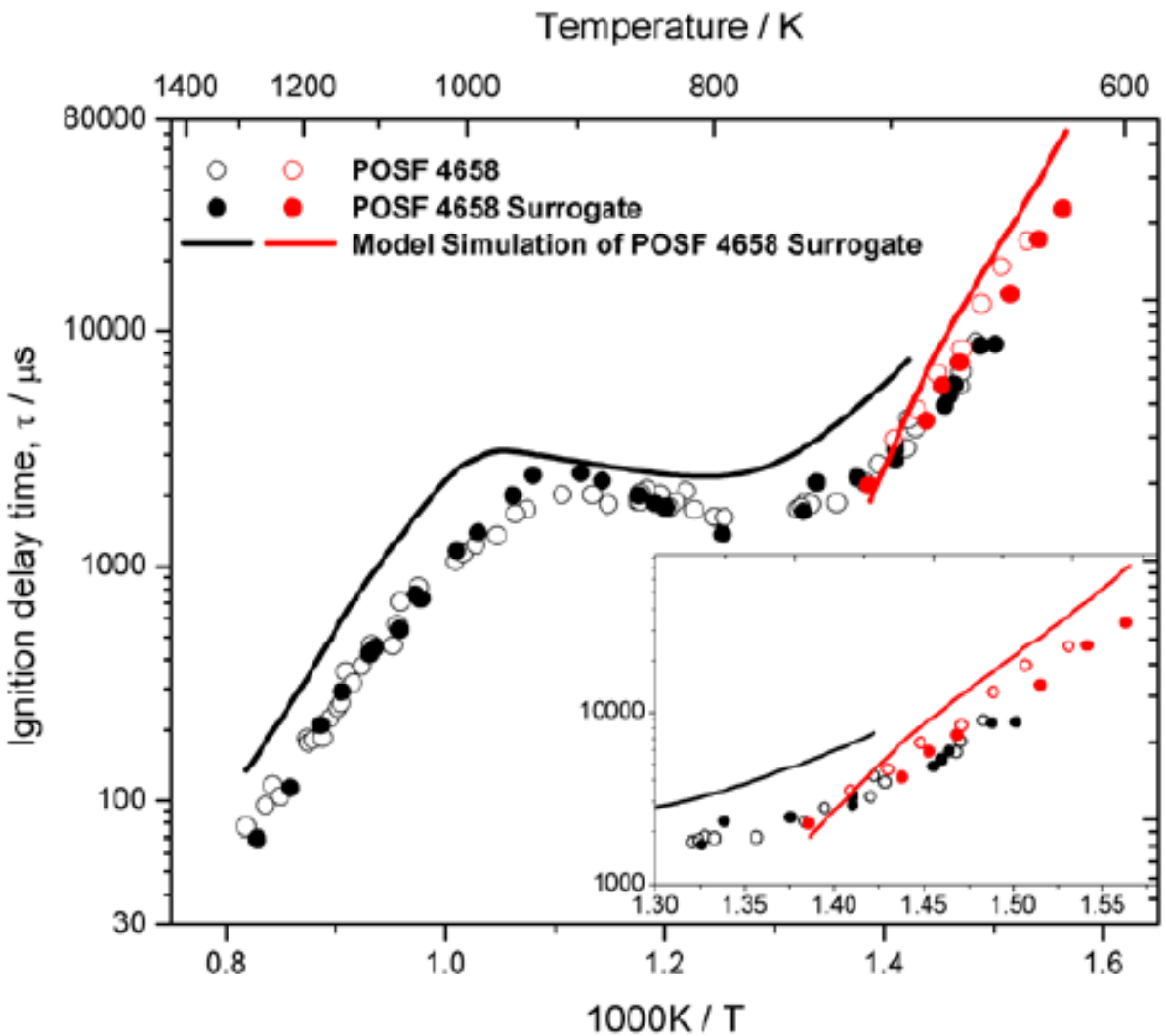
- Determine laminar flame speeds and extinction stretch rates of preheated fuel/oxidizer mixtures over a range of equivalence ratios, using counterflow flame experiments.

Real Jet Fuels	*Jet-A and S-8*
Neat Components	*n-heptane, n-decane, n-dodecane, iso-octane, toluene, MCH, 1,2,4-TMB, 1,3,5-TMB, and n-PB*
Fuel Blends	*n-decane+iso-octane+toluene*





First Generation POSF-4658 Surrogate



Solid Symbols: POSF-4658

Open Symbols: surrogate

Lines: model simulations

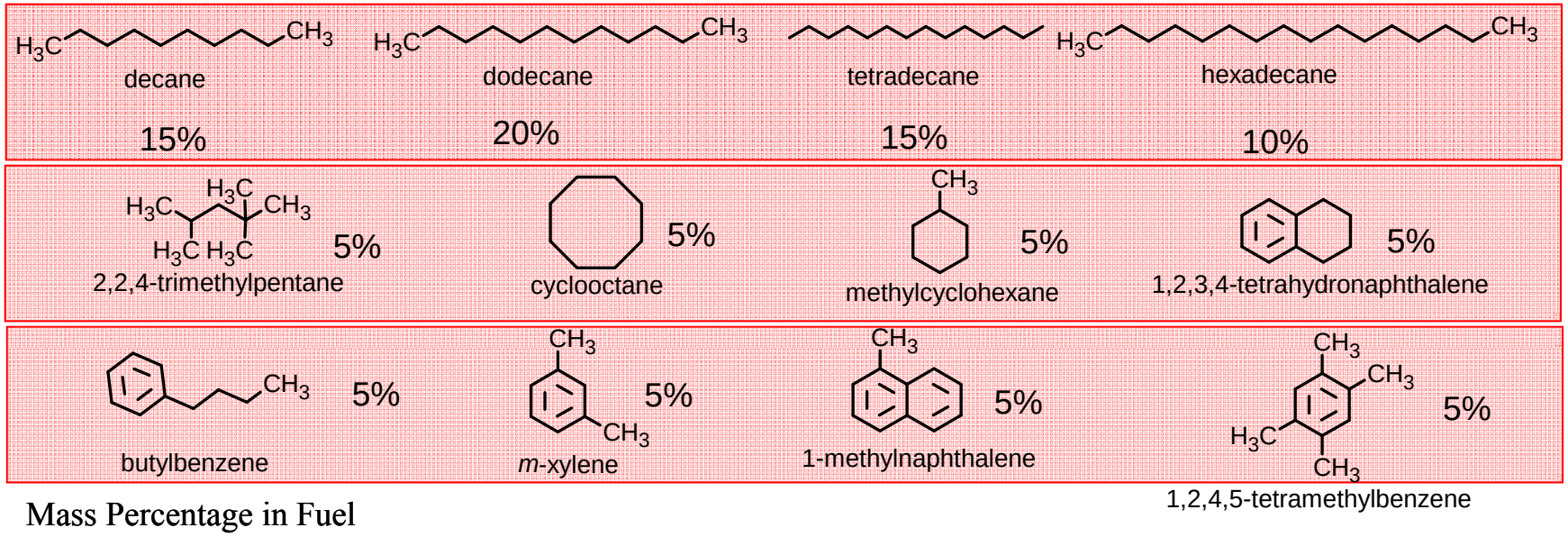
Mole Fraction:

1st Generation surrogate	*n*-decane	*iso*-octane	Toluene
	0.427	0.33	0.243

Uncertainty of Jet-A Thermodynamic Properties (1)

POSF 4658 (CHN analyzer with ASTM D5291): $C_{10.174}H_{19.913}$, MW=142.01

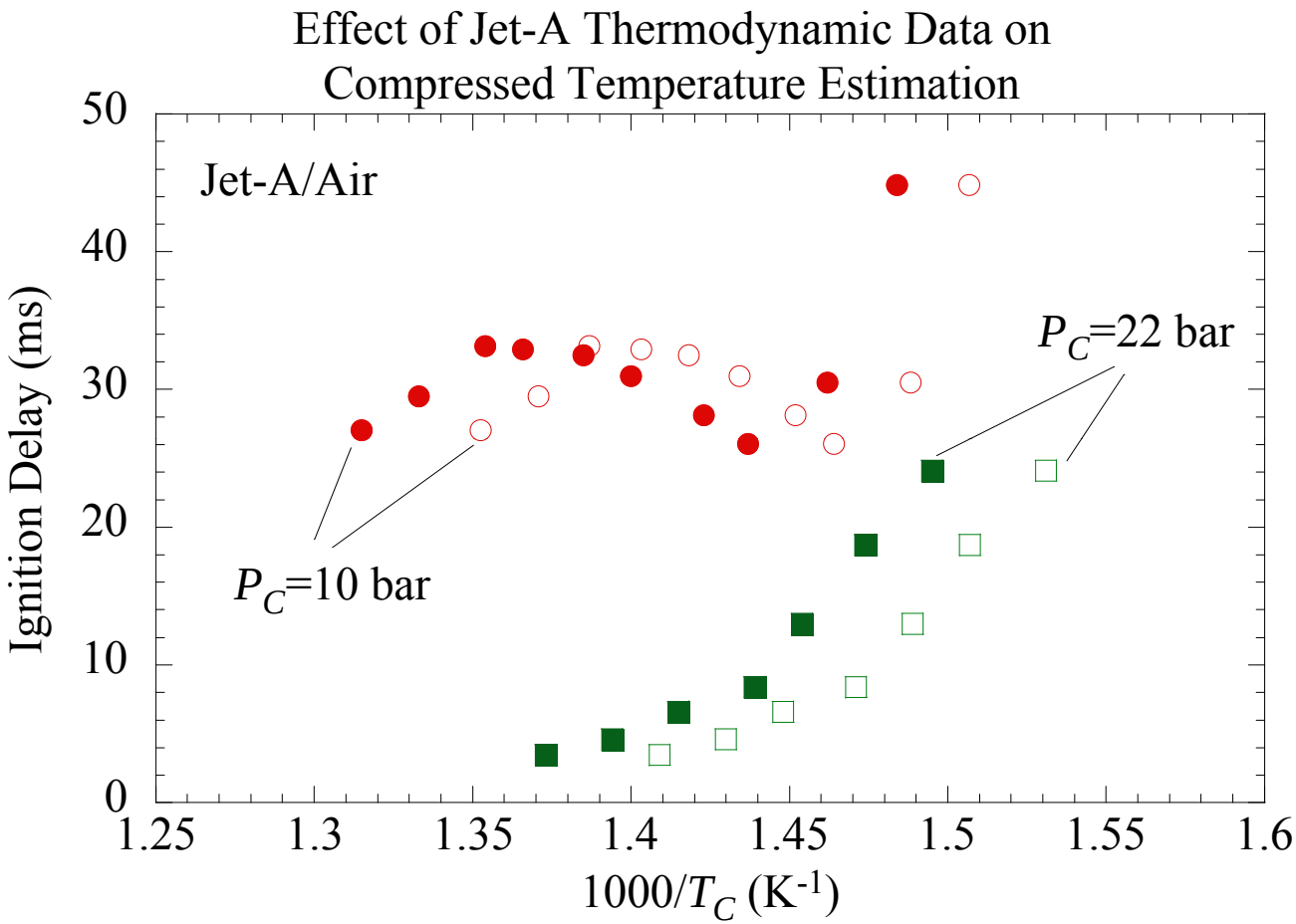
Schulz: $C_{10.632}H_{20.253}$, MW=147.8



Mass Percentage in Fuel

Burcat: $C_{12}H_{23}$, MW=167

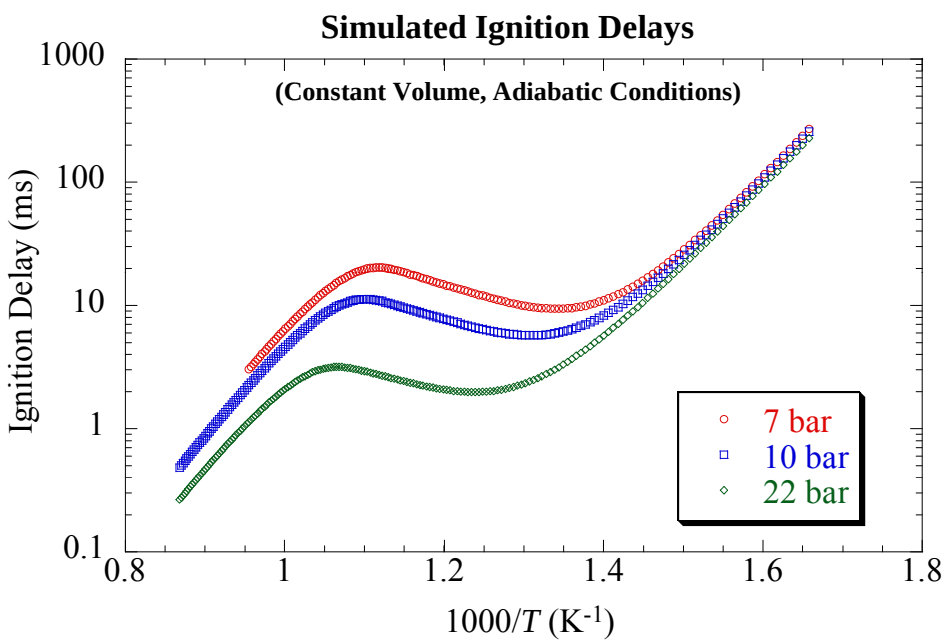
Uncertainty of Jet-A Thermodynamic Properties (2)

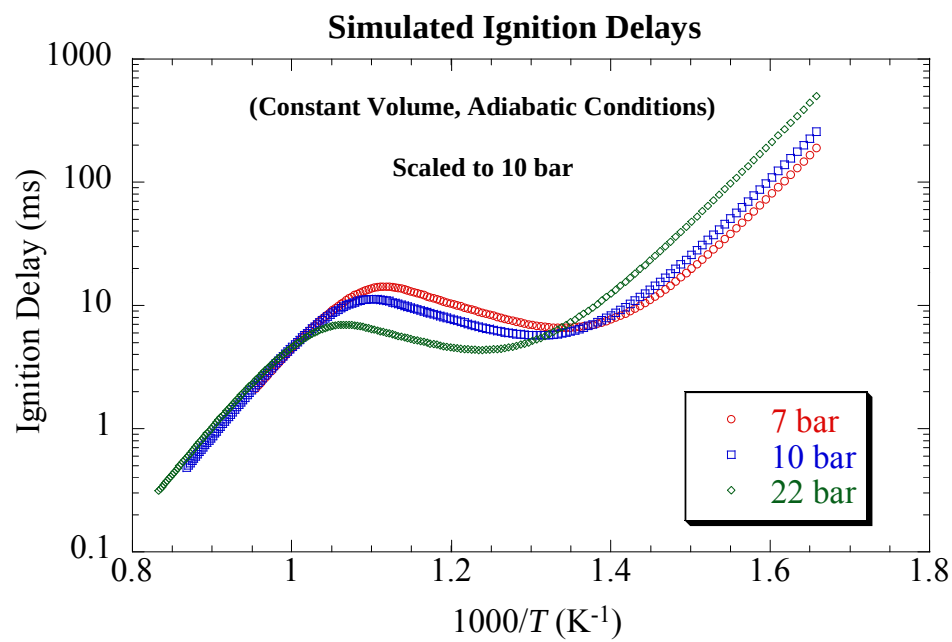


Filled Symbols: Schulz with A/F mass ratio of 14.6

Open Symbols: Burcat with 1.37 mol % of Jet-A

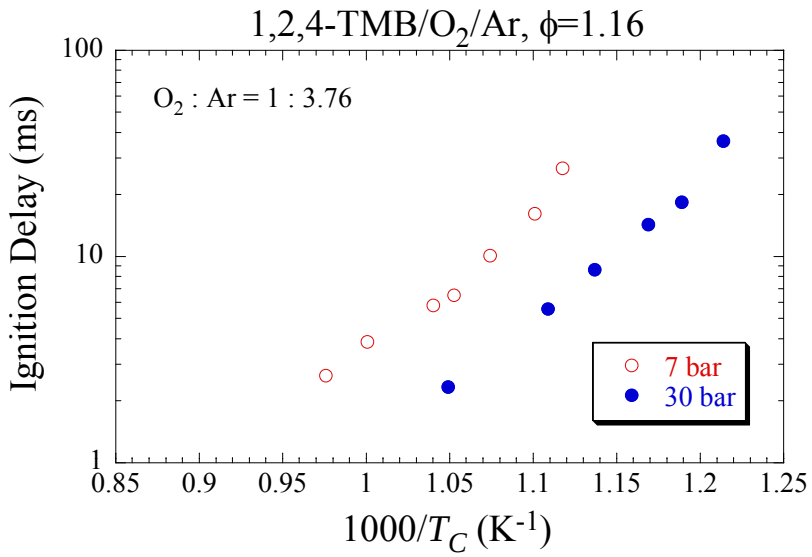
Pressure Scaling

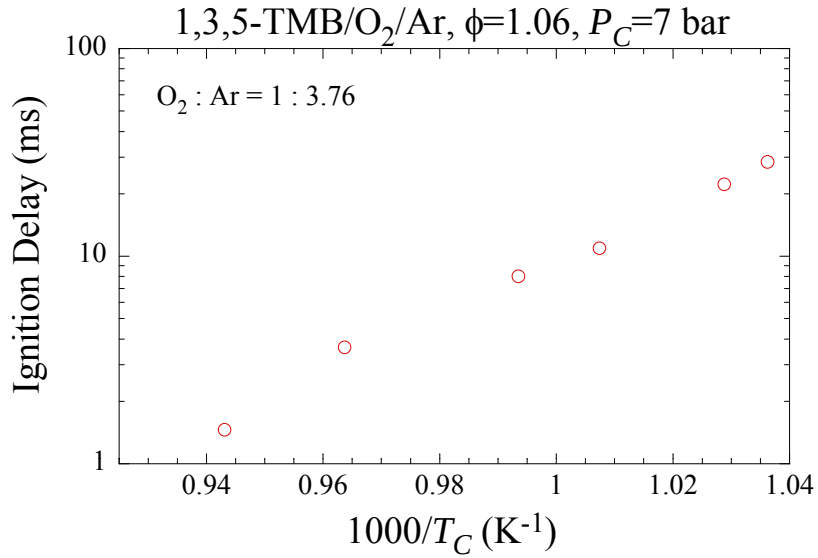


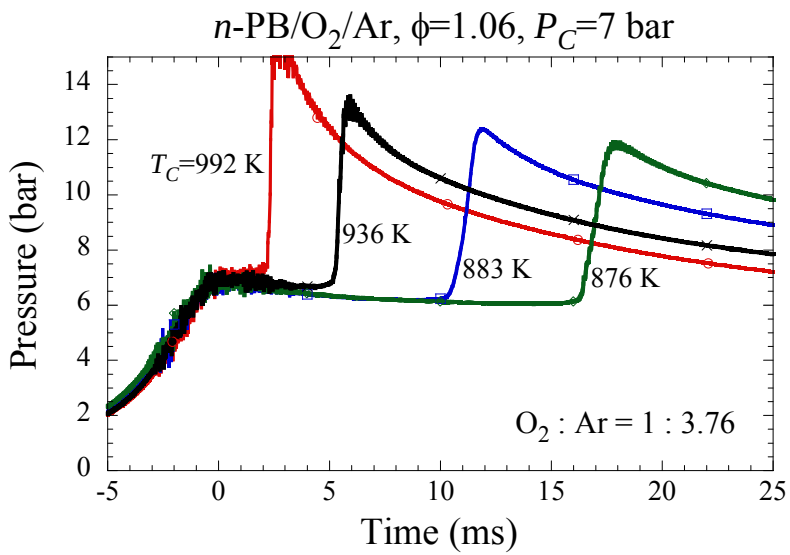


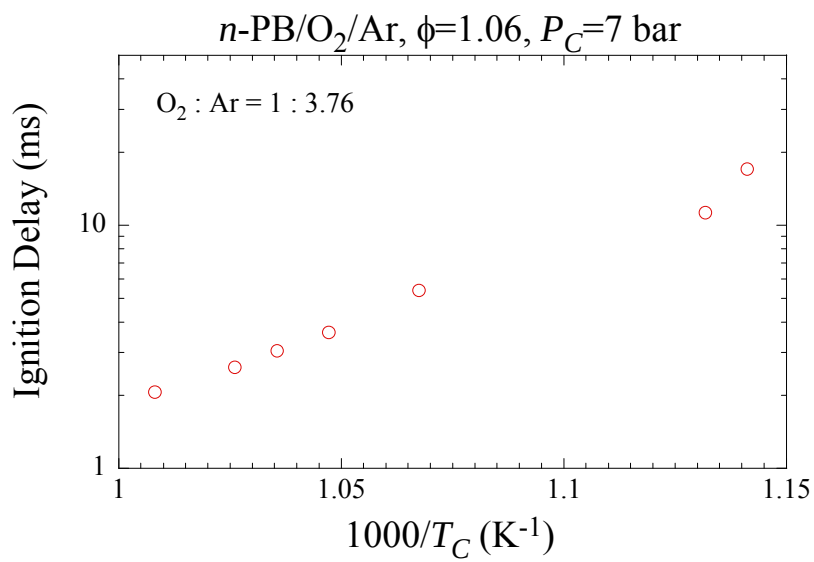
Computational Results using 1st Generation Surrogate Kinetic Model

Autoignition of Aromatics

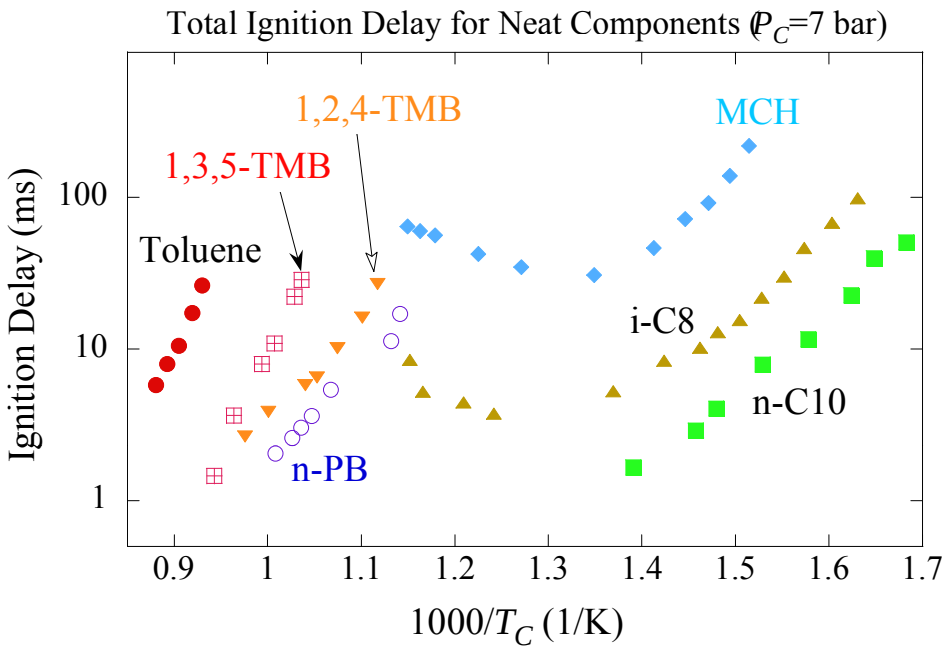


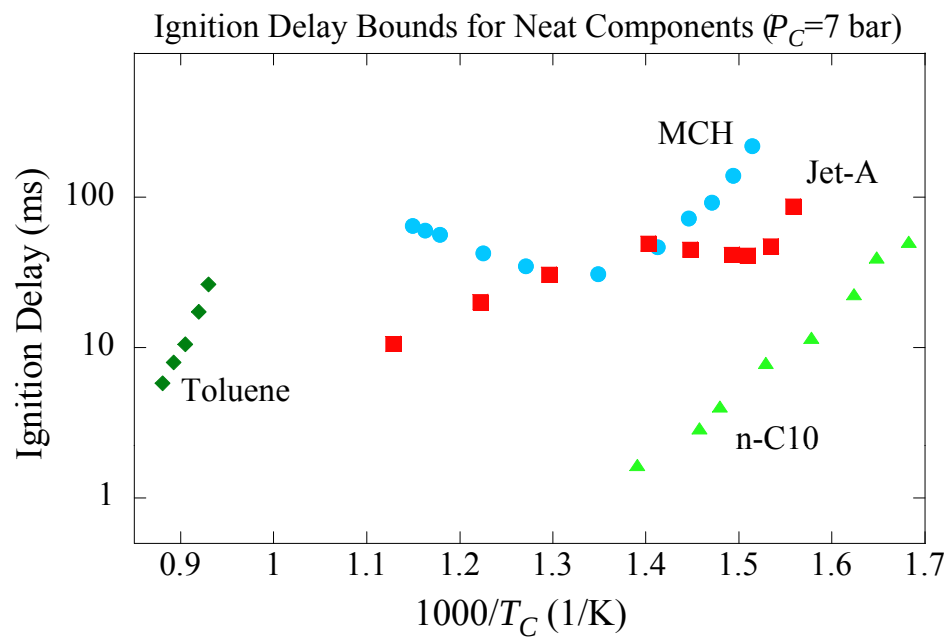






Autoignition Comparison: Jet-A vs. Neat Components

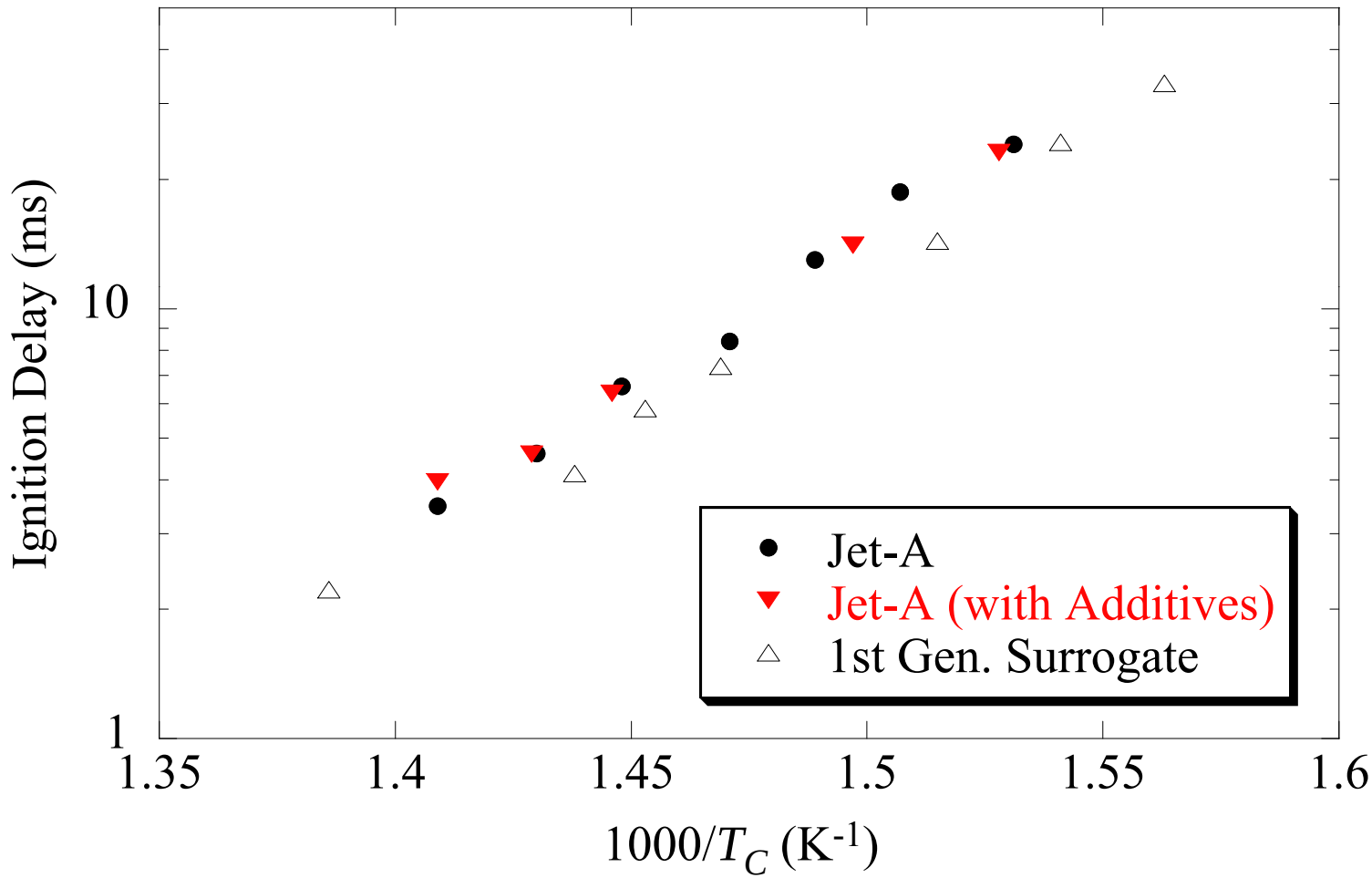




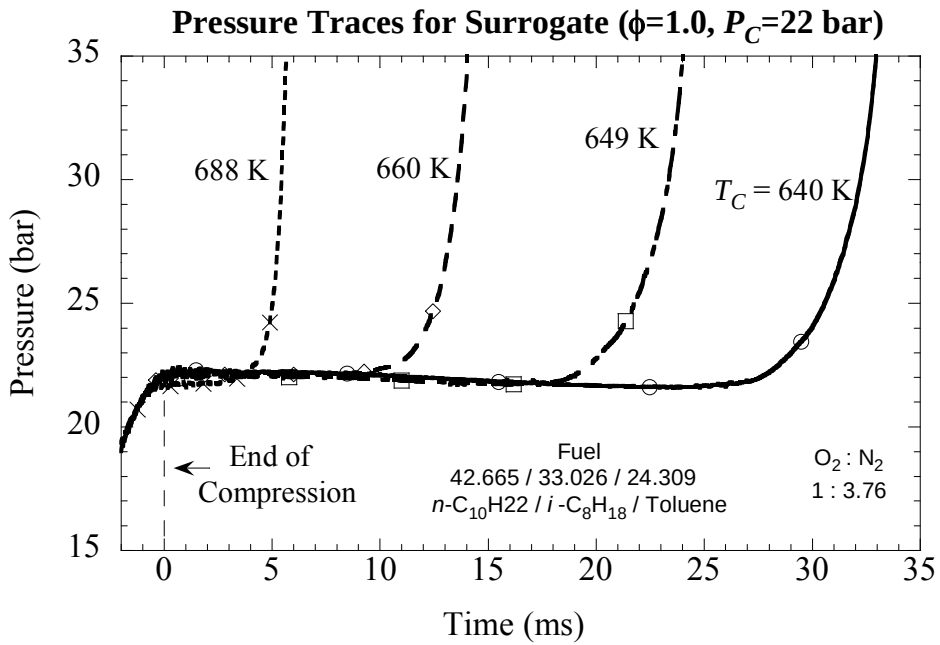
Fuel	**A/F Mass Ratio**	**ϕ**	**Diluent**
iso-Octane	*13.0*	*1.16*	N_2
n-Decane	*13.0*	*1.15*	N_2
Methylcyclohexane	*12.7*	*1.16*	N_2
Toluene	*15.4*	*1.16*	*Ar*
1,3,5- (1,2,4) Trimethyl Benzene	*17.2 (15.8)*	*1.06 (1.16)*	*Ar*
n-Propylbenzene	17.2	1.06	*Ar*
Jet-A (04POSF4658)	*13.0*	*1.12*	N_2
Diluent : Oxygen = 3.76 : 1			

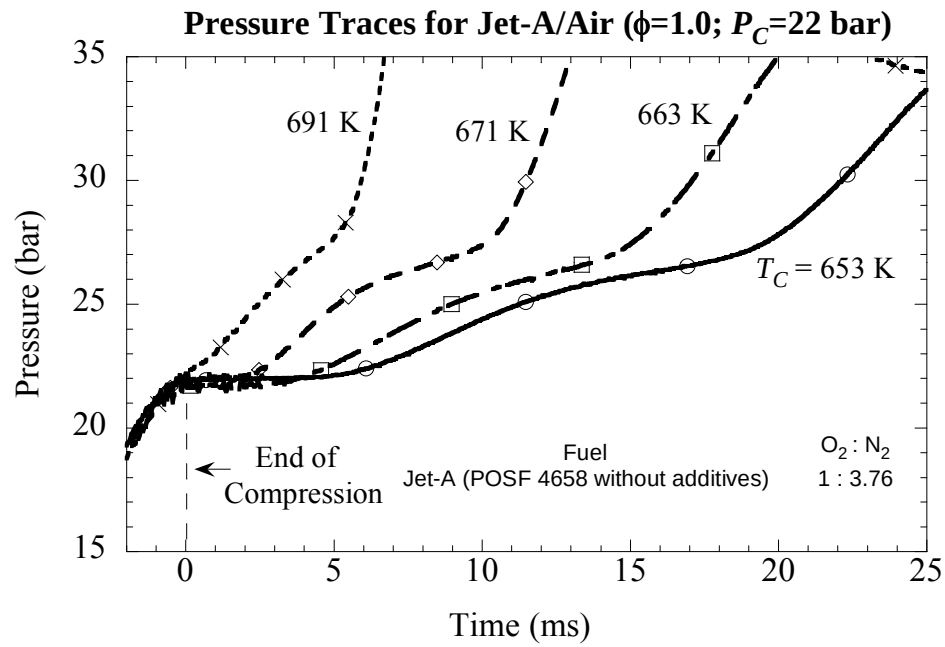
Effect of Additives

Comparative Ignition Delays for Stoichiometric Fuel/Air Mixtures



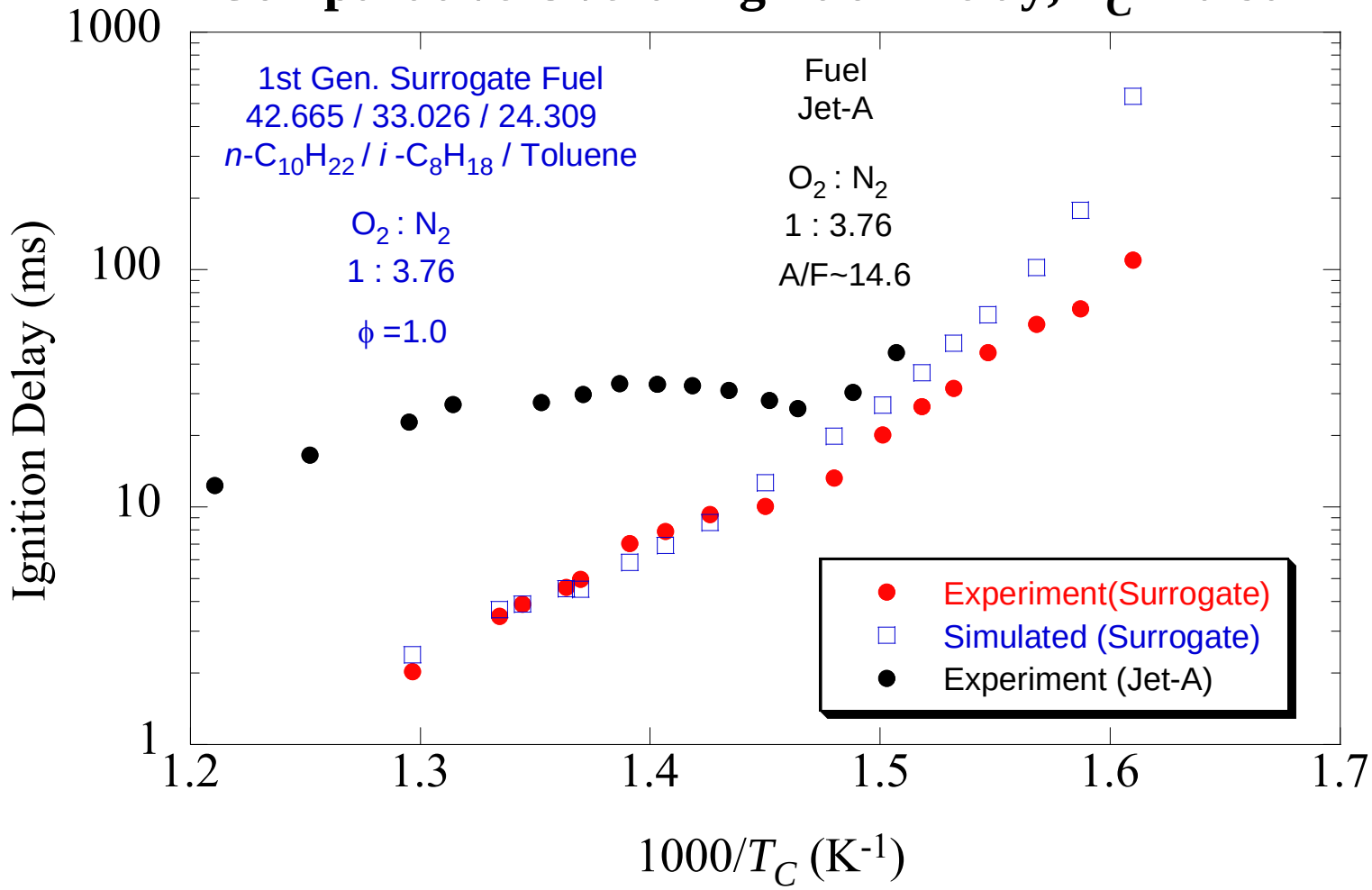
Autoignition Comparison:
Jet-A vs. 1st Gen. Surrogate Mixture (P_C=22 bar)



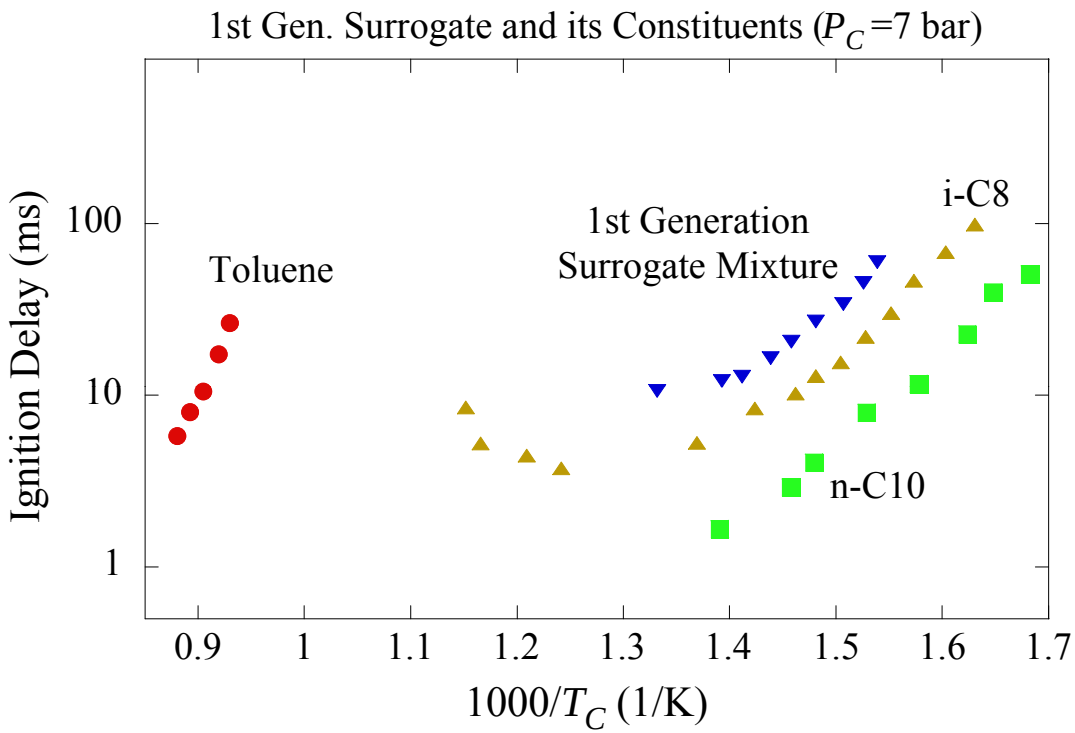


Autoignition Comparison:
Jet-A vs. 1st Gen. Surrogate Mixture (P_C=10 bar)

Comparative Overall Ignition Delay, P_C=10 bar



Autoignition Comparison: Surrogate Mixtures vs. Neat Components (1)

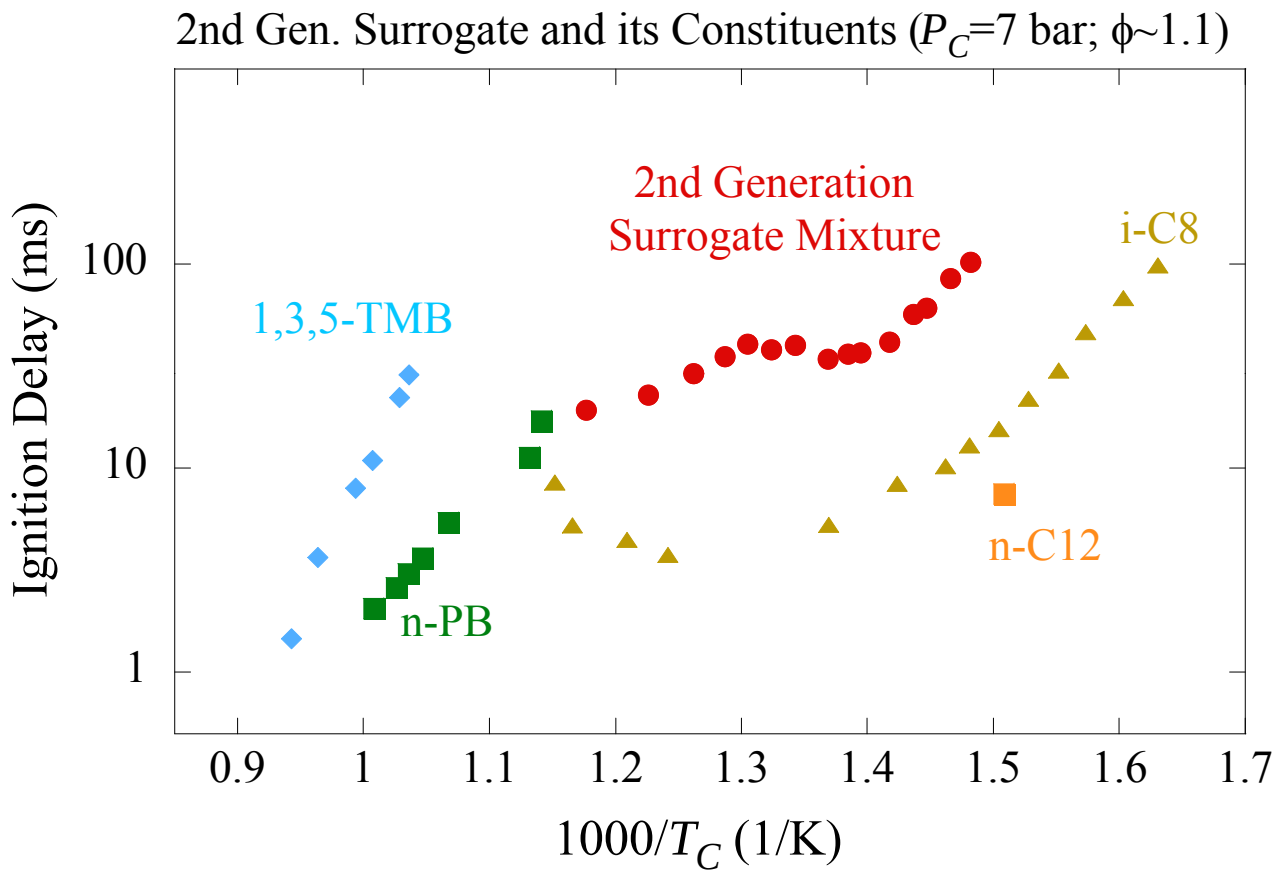


Mole Fraction:

1st Generation surrogate	*n*-decane	*iso*-octane	Toluene
	0.427	0.33	0.243

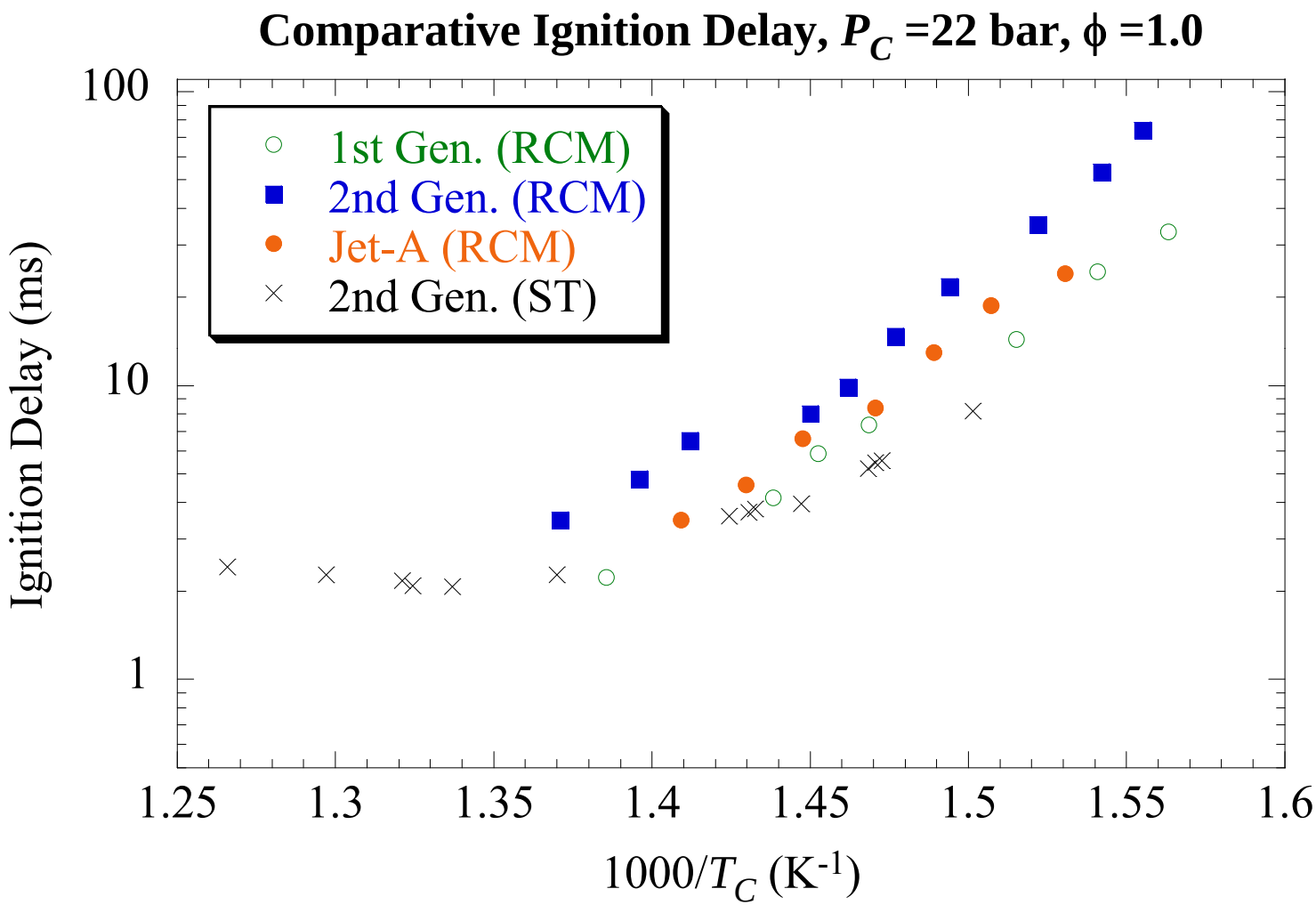
- Surrogate mixtures inherit the traits of the neat constituents
  - NTC trend from i-C_8 in the current range for 1st gen. surrogate

Autoignition Comparison: Surrogate Mixtures vs. Neat Components (2)

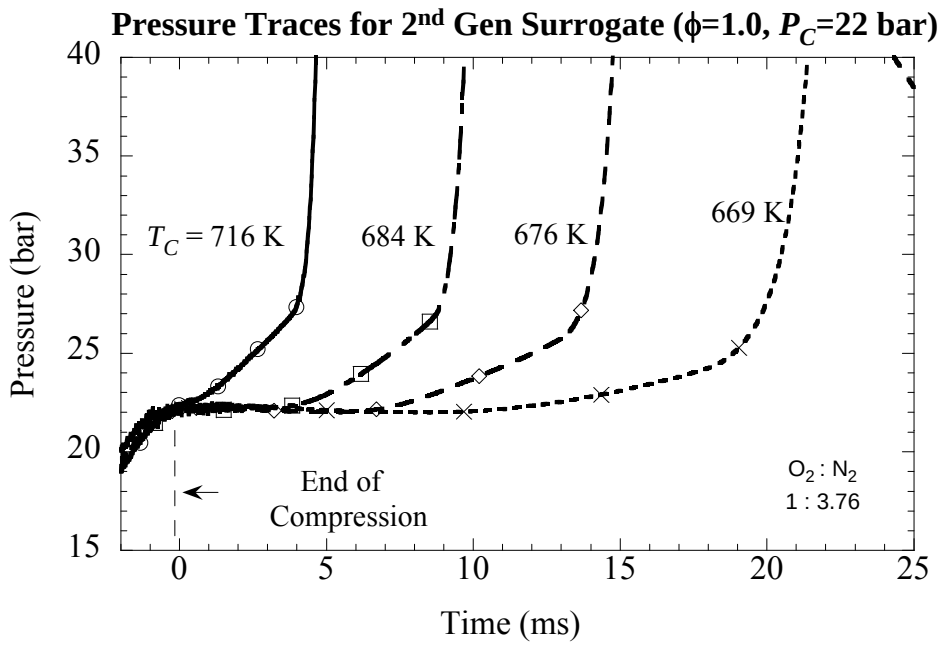


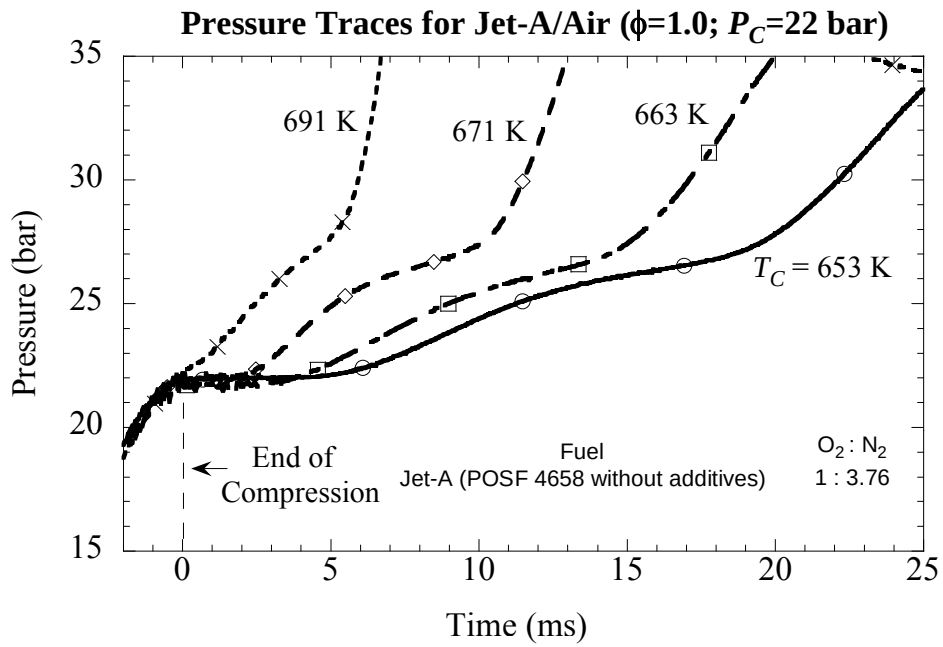
Mole Fraction					DCN	H/C	MW / g mol^{-1}	TSI
Jet-A POSF 4658					47.1	1.957	142.01	21.4
2nd Generation surrogate	*n*-dodecane	*iso*-octane	Mesitylene	n-propyl benzene	48.5	1.95	138.7	20.4
	0.40	029	0.07	0.23				

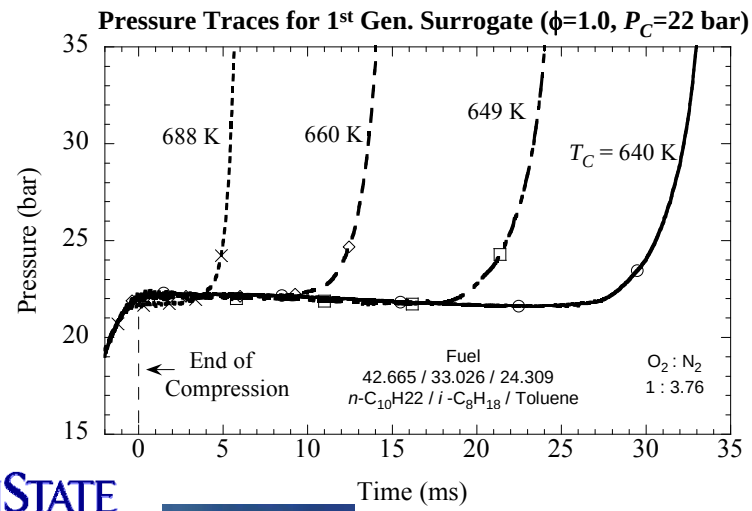
Autoignition Comparison: Jet-A vs. Surrogate Mixtures (1)



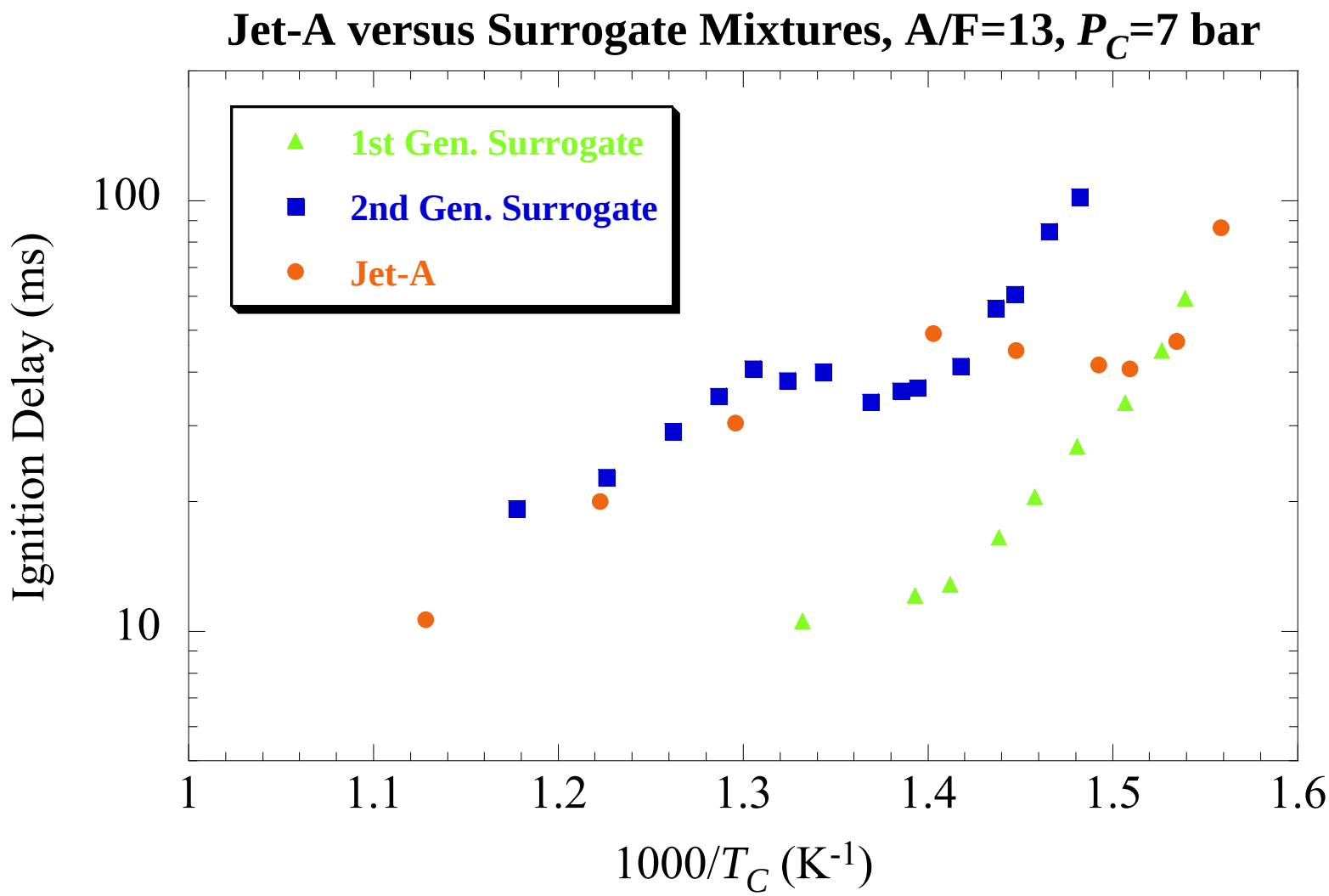
Autoignition Comparison: Jet-A vs. Surrogate Mixtures (2)



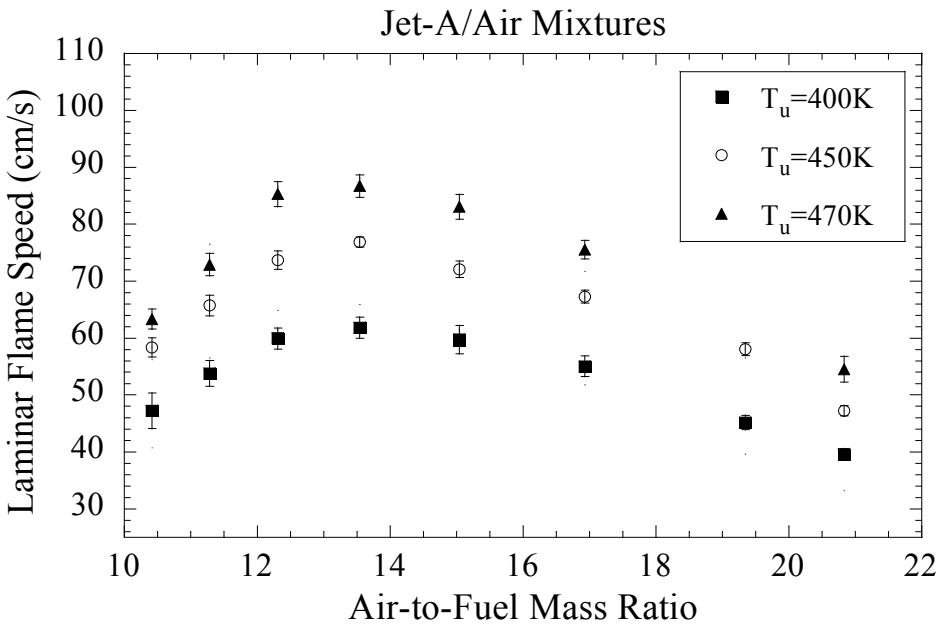


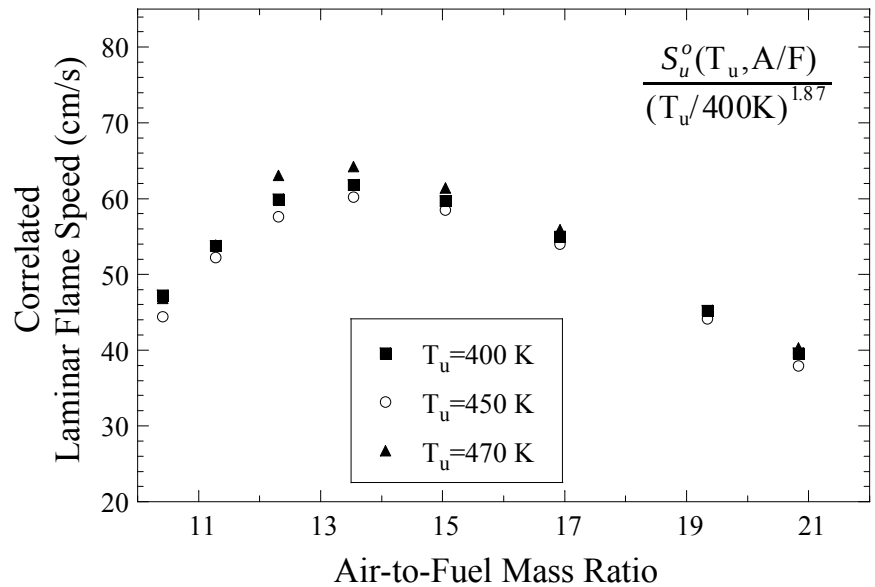


Autoignition Comparison: Jet-A vs. Surrogate Mixtures (3)

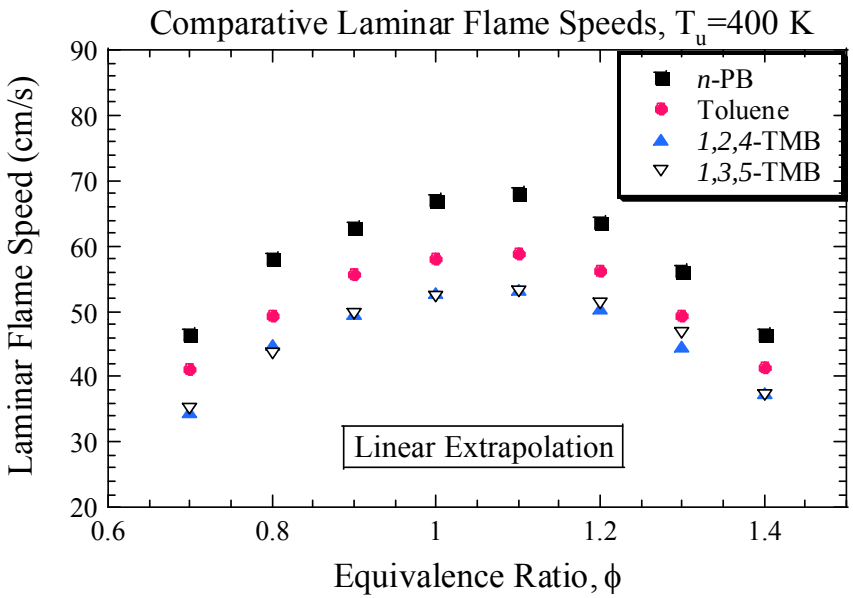


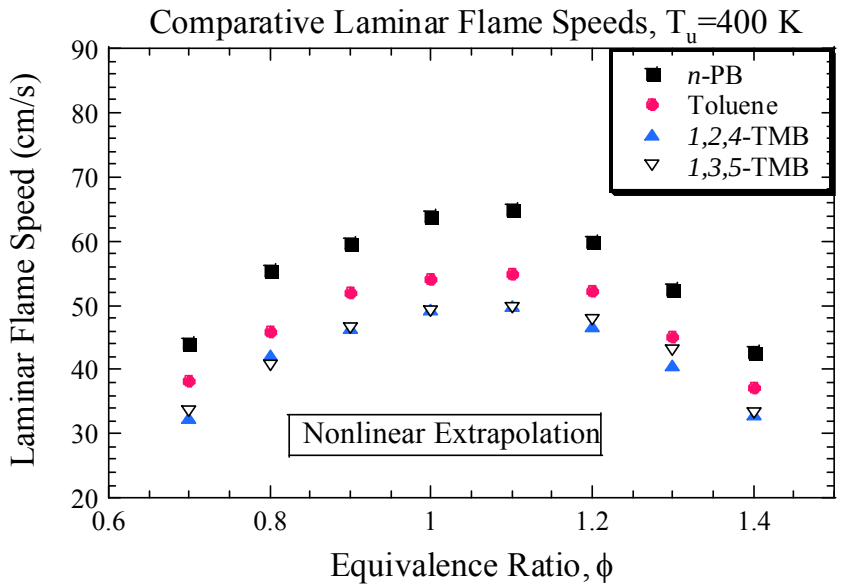
Laminar Flame Speeds of Jet-A





Laminar Flame Speeds of Aromatics

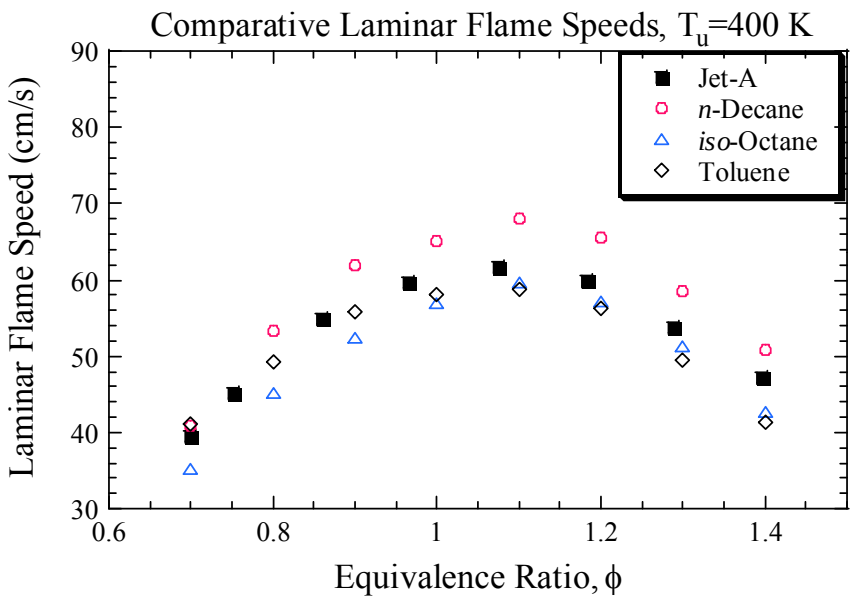


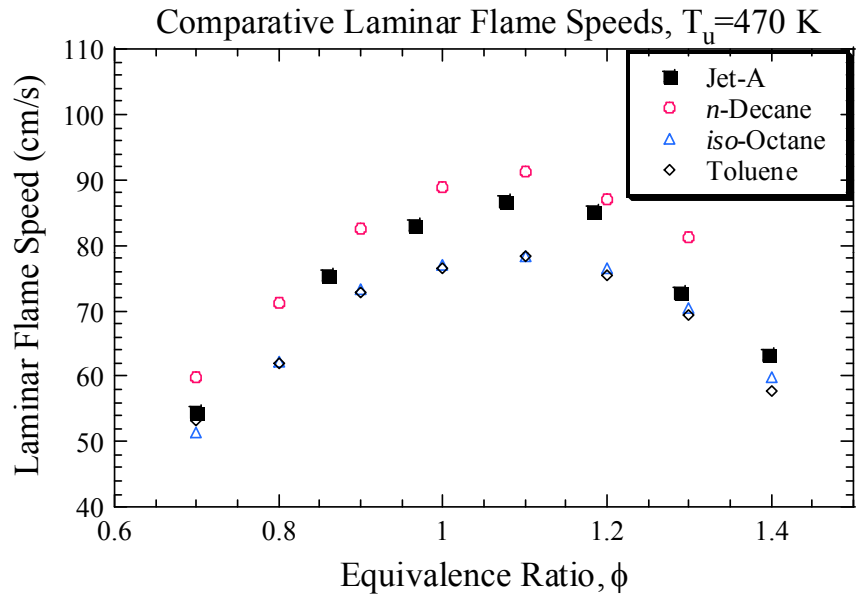


Laminar Flame Speed Comparison:

n-PB > Toluene > *1,2,4*-TMB ≈ *1,3,5*-TMB

Laminar Flame Speed Comparison: Jet-A vs. Neat Components

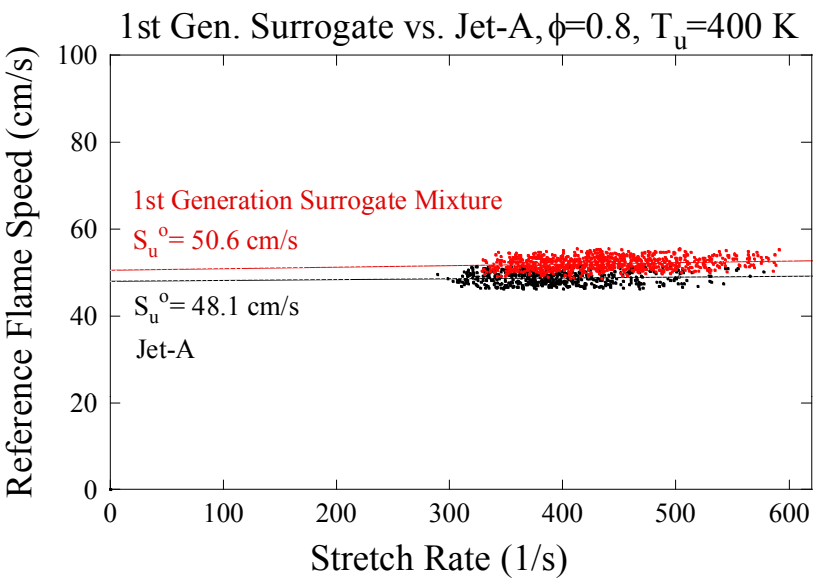


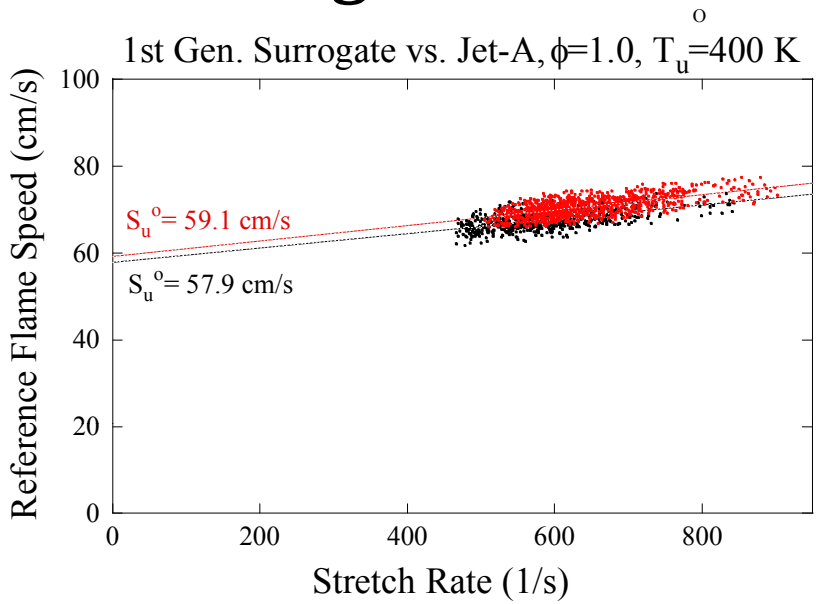


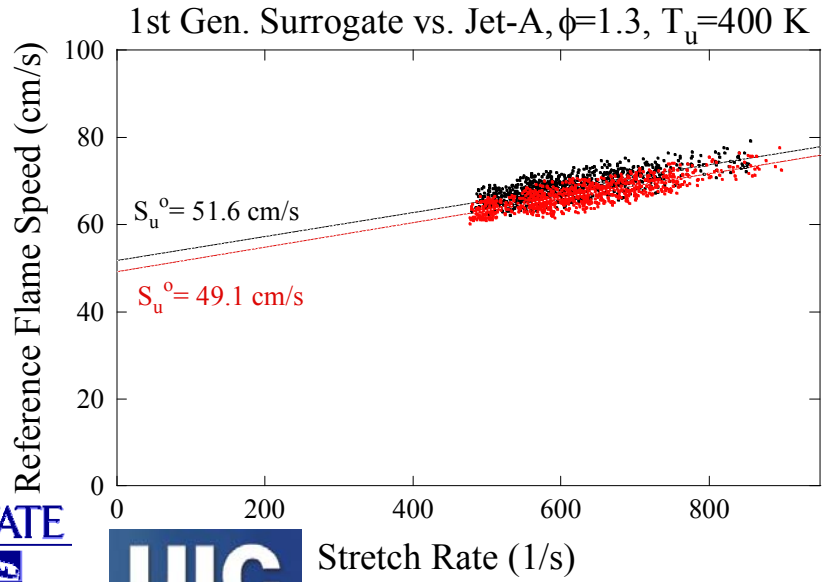
Laminar Flame Speed Comparison:

Linear Alkane > Branched Alkane ≈ Aromatic

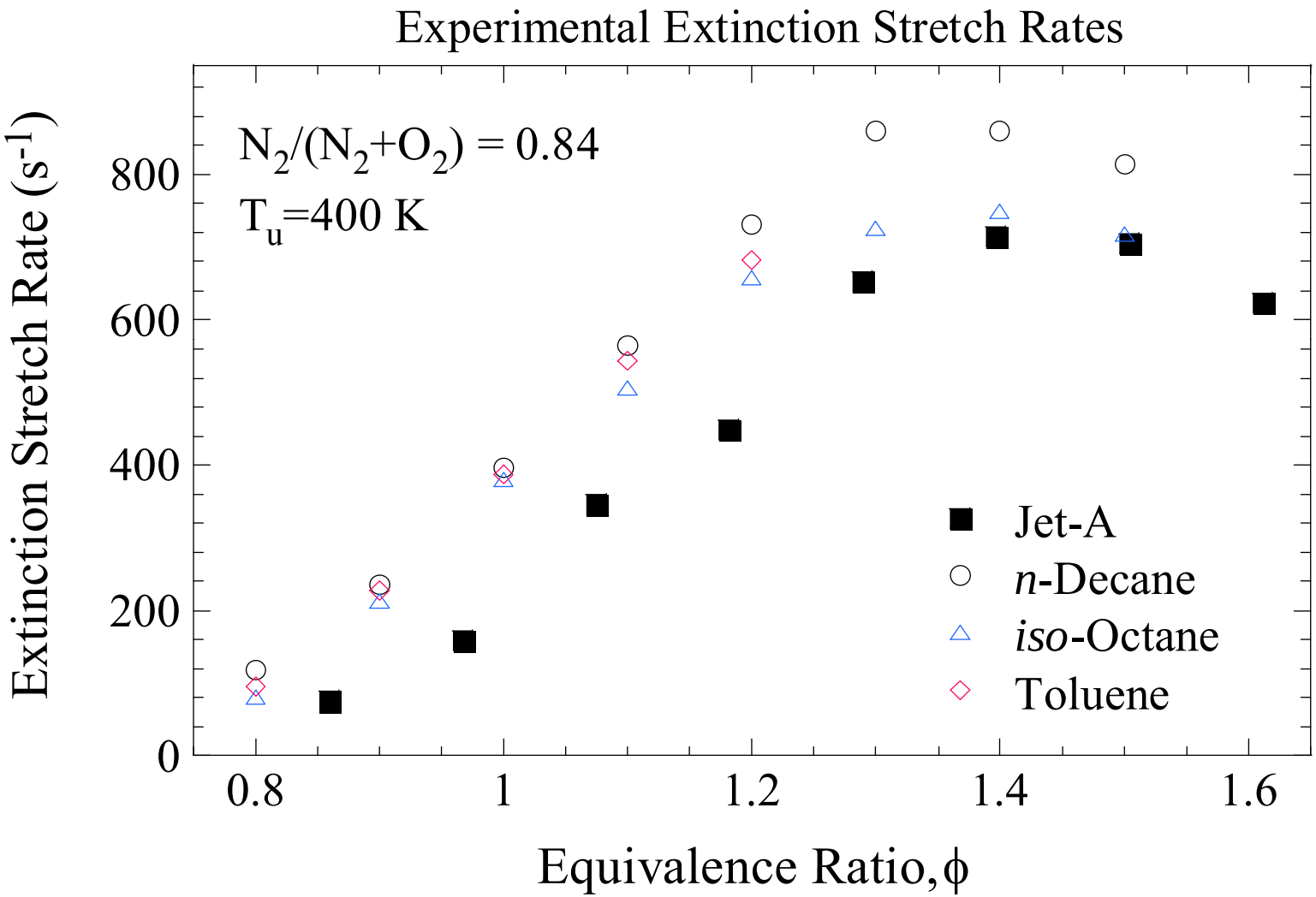
Laminar Flame Speeds:
Jet-A vs. 1st Generation Surrogate



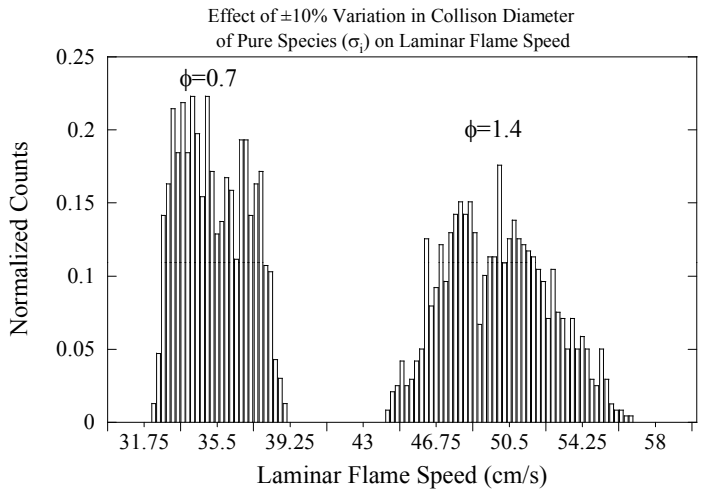




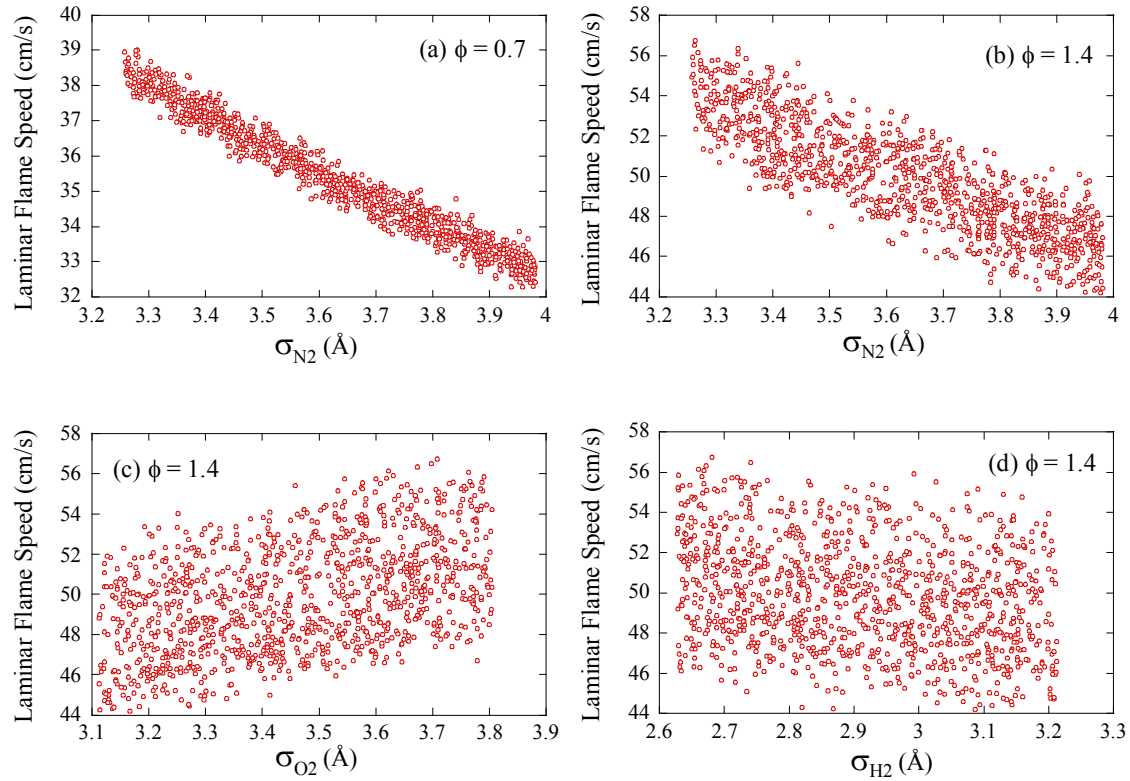
Extinction Limit Comparison: Jet-A vs. Neat Components



Transport Sensitivity (1)

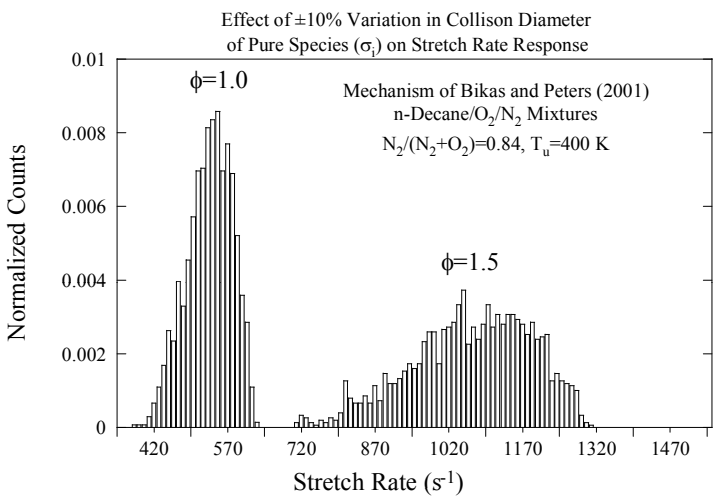


Distribution of laminar flame speed model output to variation in pure species collision diameters for n-decane/air mixtures at T_u=400 K.

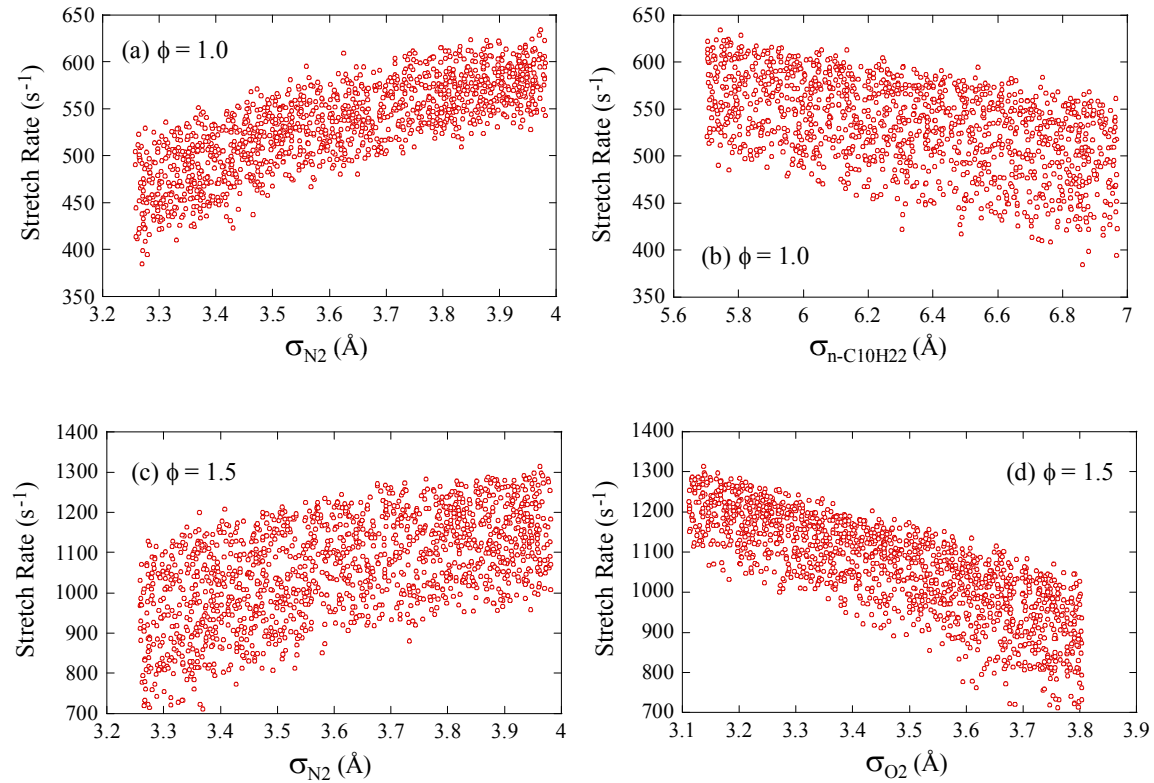


Scatter plot showing laminar flame speed model output to variation in pure species collision diameters for n-decane/air mixtures at T_u=400 K.

Transport Sensitivity (2)



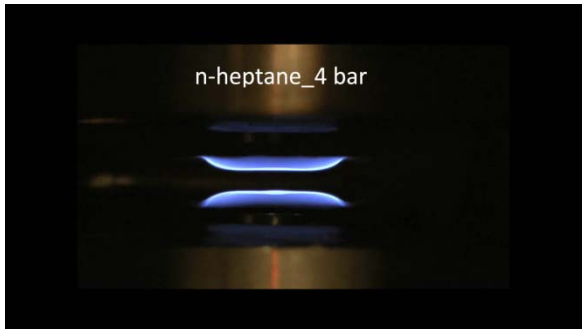
Distribution of counterflow flame model output to variation in pure species collision diameters for n-decane/air mixtures at T_u=400 K. The base case corresponds to a near-extinction flame condition.



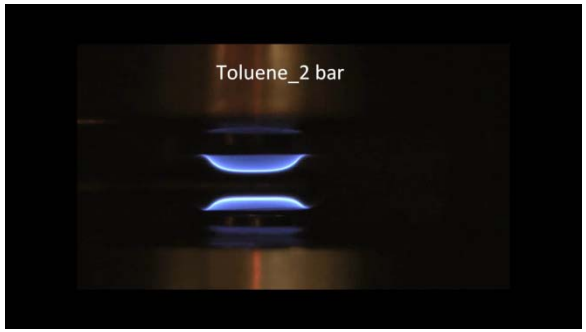
Scatter plot showing laminar flame speed model output to variation in pure species collision diameters for n-decane/air mixtures at T_u=400 K.

High Pressure Counterflow Burners

n-Heptane/Air Flames (ϕ=0.85)

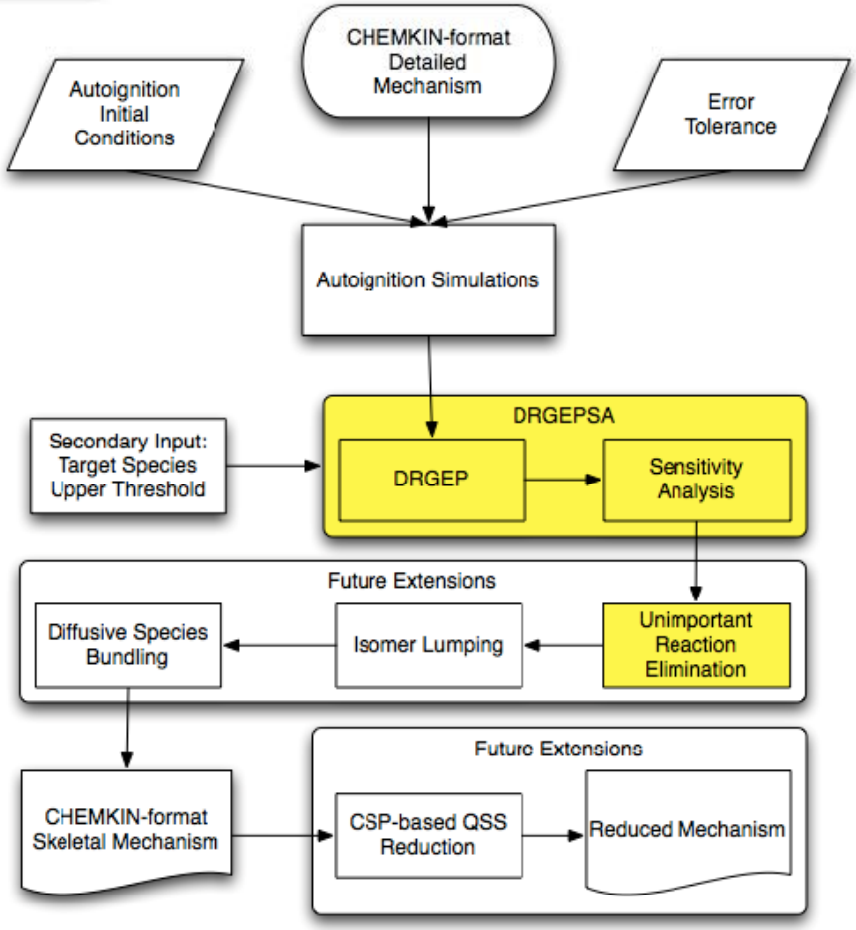


Toluene/Air Flames (ϕ=0.8)

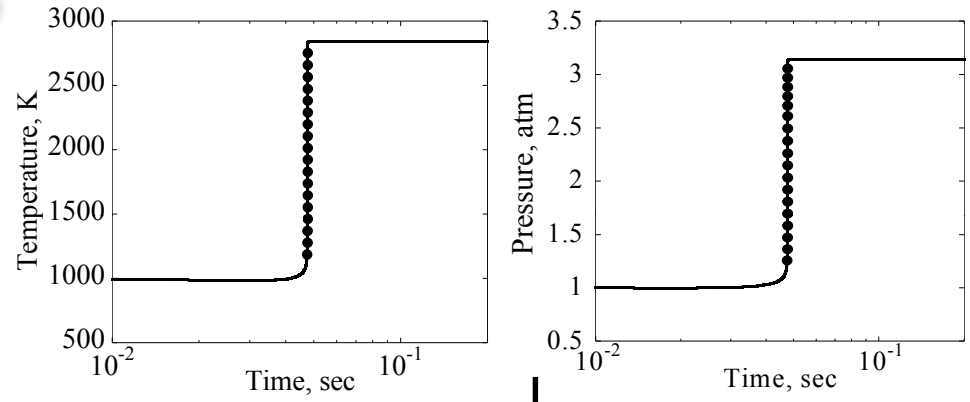


Skeletal Reduction

Mechanism Automatic Reduction Software (MARS)



Wide Range T_0, P_0, ϕ



DRGEP

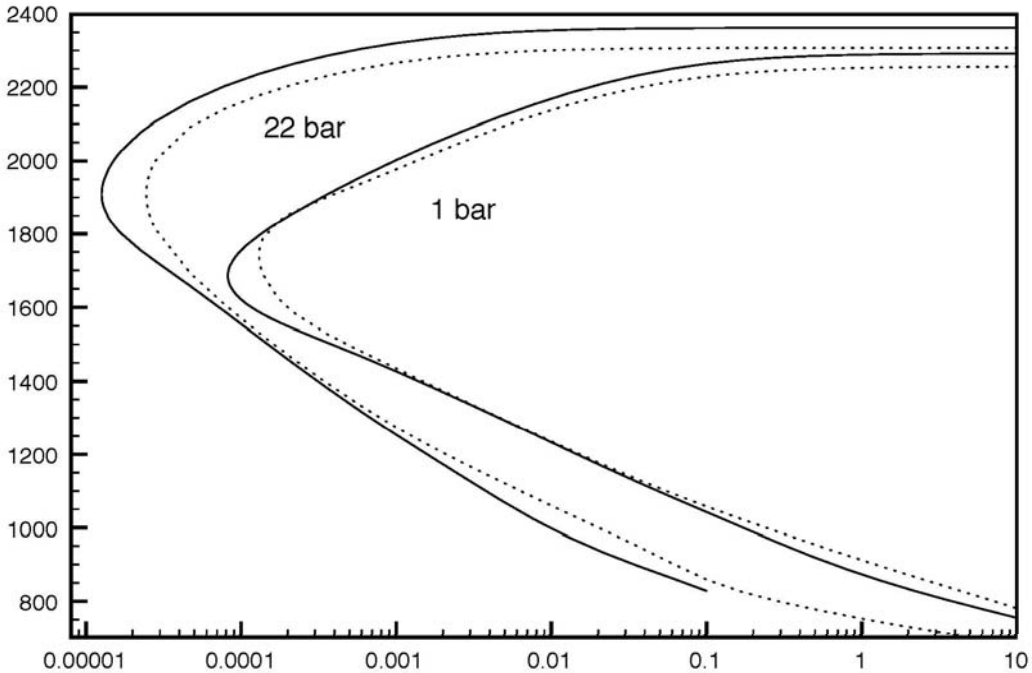
Skeletal Mechanism

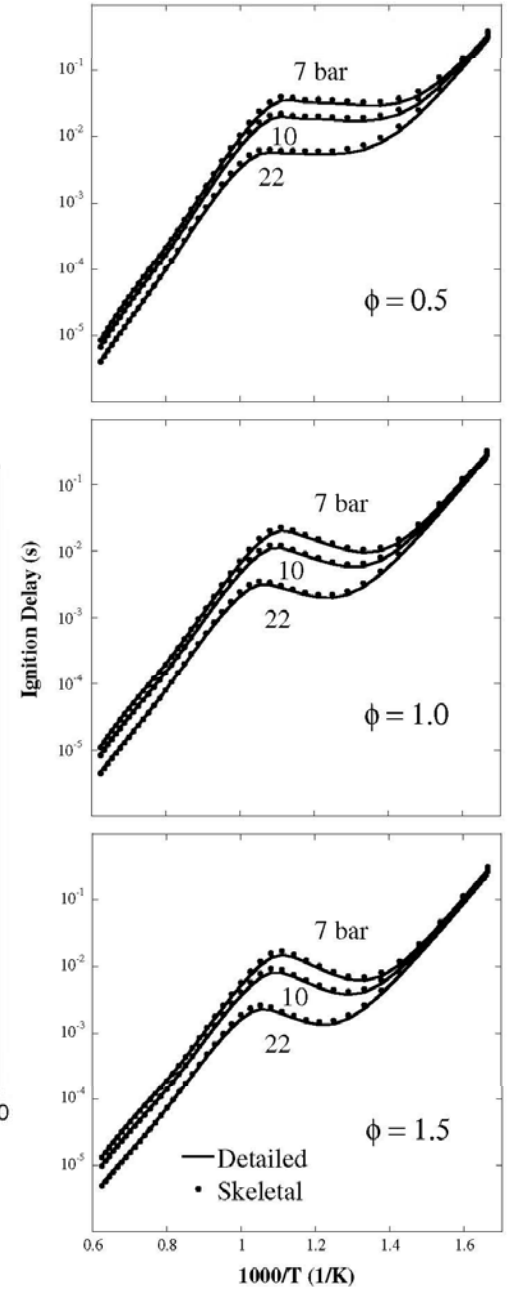
SA

Final Skeletal Mechanism

Skeletal Mechanism of 1st Generation Surrogate

- Detailed: 1599 species and 6633 reactions
- Skeletal: 297 species and 1360 reactions





Summary and Future Work

- Surrogate formulation strategy is demonstrated.
- Refinement of formulation and kinetic model is needed.
- Acquire autoignition and flame data of aromatics relevant to jet fuel surrogates over a range of conditions.
- Acquire autoignition data of next generation surrogate.
- Measure and compare extinction limits of surrogate mixtures and real jet fuels.
- Conduct high-pressure flame measurements for neat surrogate components and real jet fuels.
- Explore surrogate formulation for alternative jet fuels.

Acknowledgements

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- Research Associate: Dr. Kamal Kumar.
- Graduate Students: Xin Hui, Apurba Das, and Kyle Niemeyer.