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

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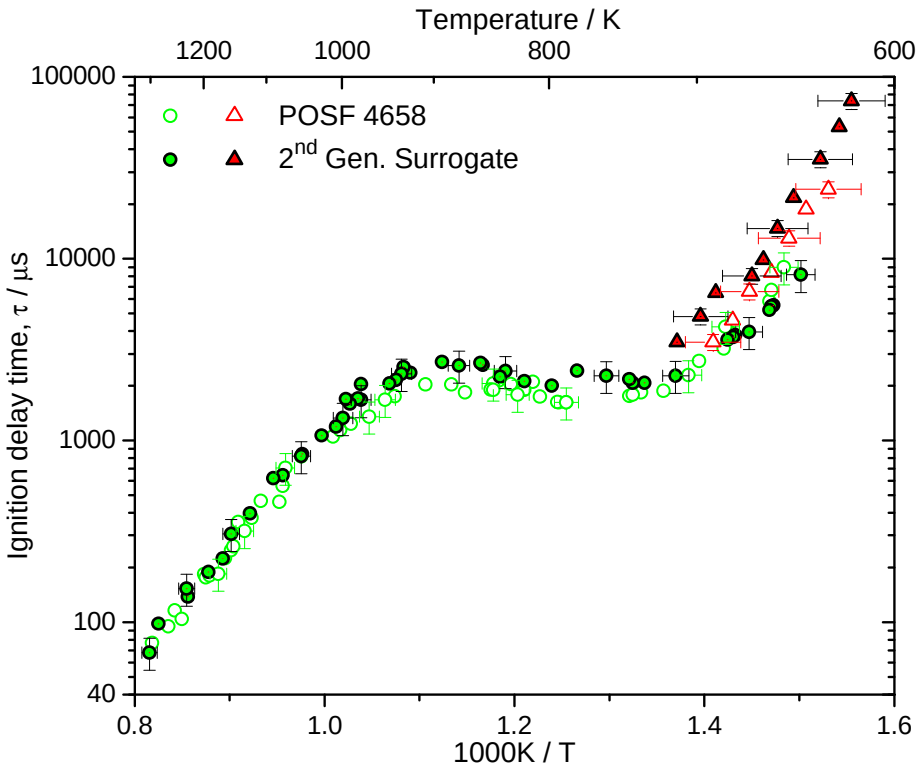
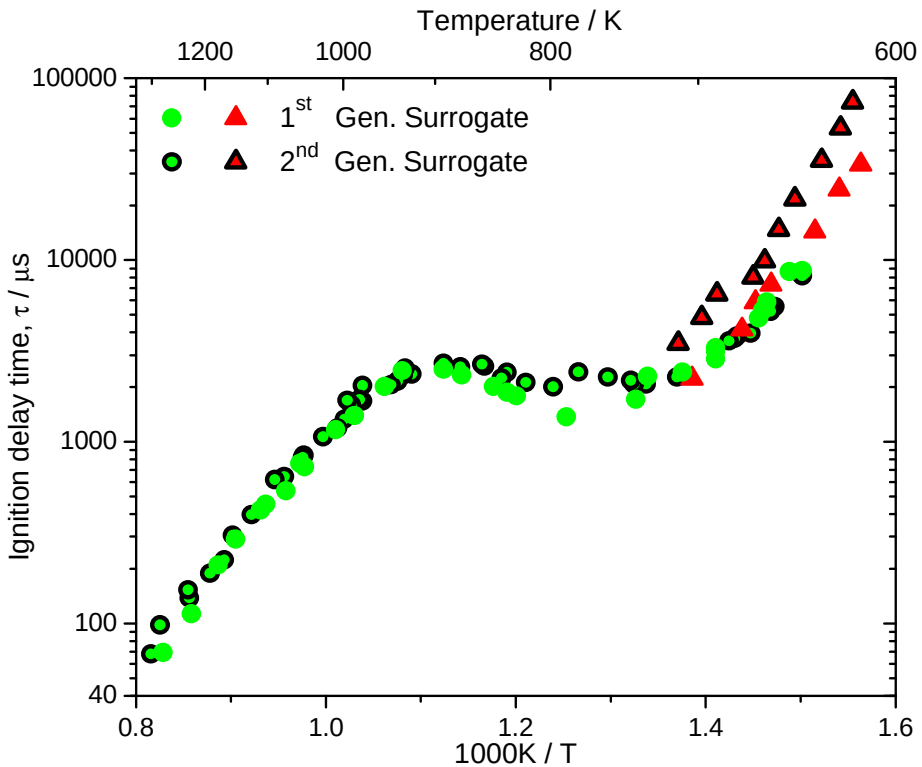
Outline of Presentation

- Fundamental Combustion Properties

  Comparison of Real Jet Fuel and 1st / 2nd Generation Surrogate Mixtures
- Autoignition of Aromatic Hydrocarbons
- Laminar Flame Speeds and Premixed Extinction Stretch Rates of Aromatic Hydrocarbons
- Summary and Future Work

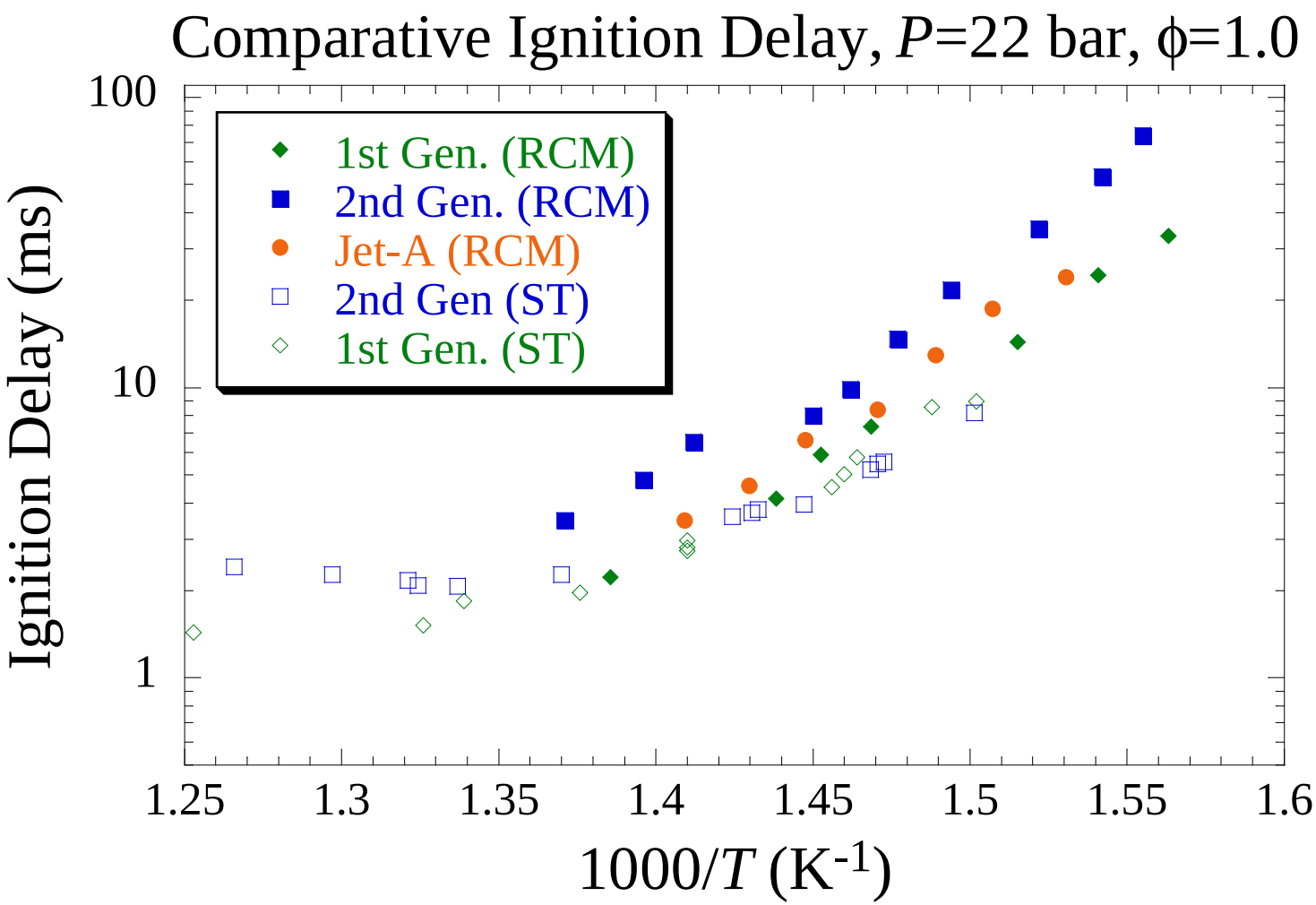
Autoignition Comparison: Jet-A vs. Surrogate Mixtures (1)



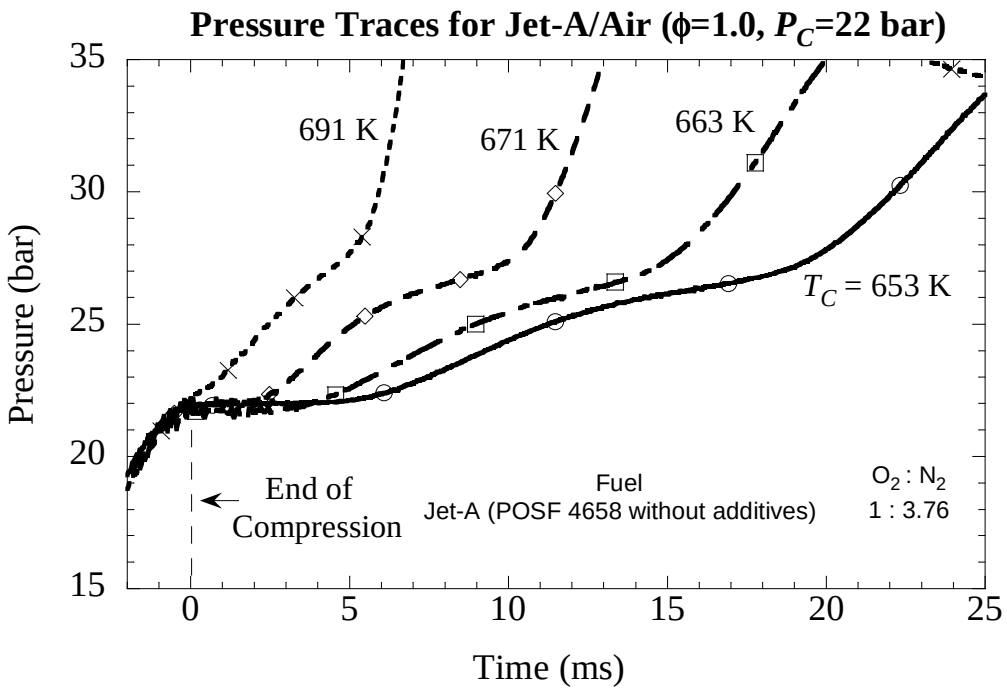


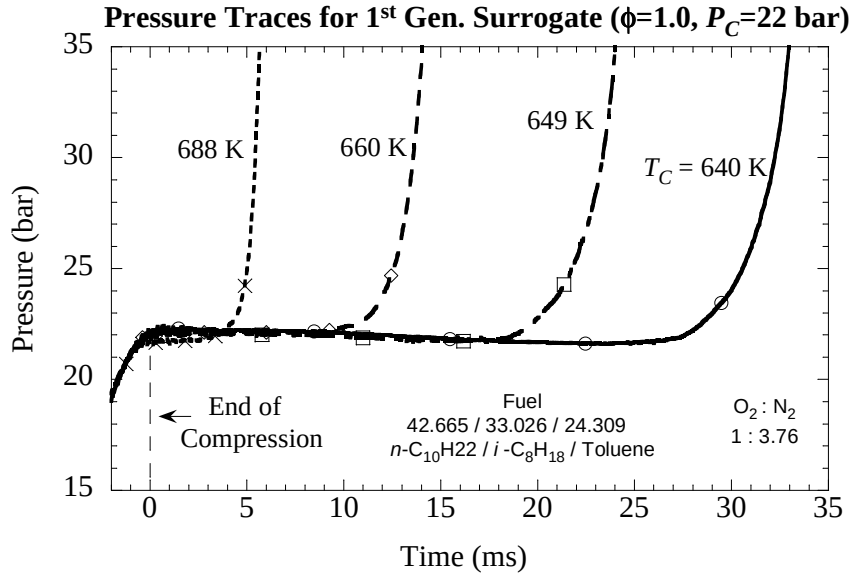
- 1st generation: *n*-decane/*iso*-octane/toluene 42.7/33.0/24.3 mole %.
- 2nd generation: *n*-dodecane/*iso*-octane/*1,3,5* trimethyl-benzene/*n*-propyl-benzene 40.41/29.48/7.28/22.83 mole %.

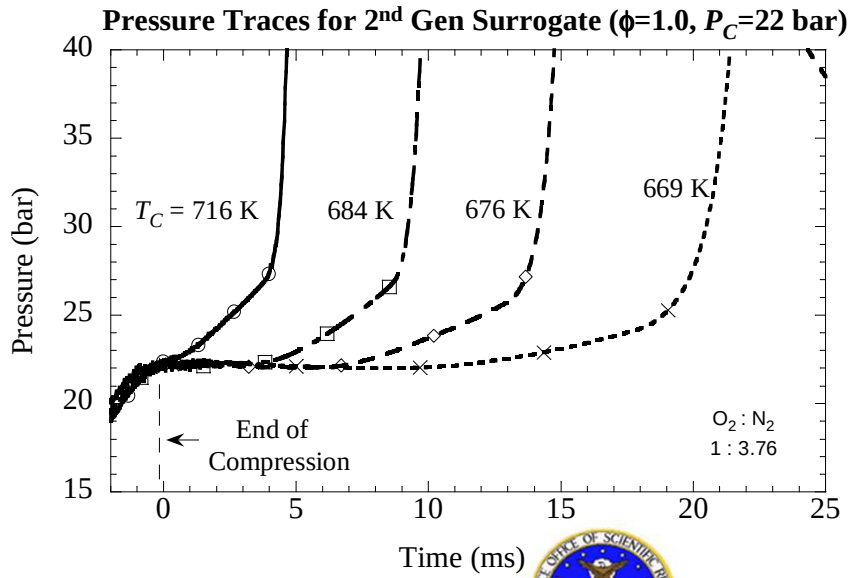
Autoignition Comparison: Jet-A vs. Surrogate Mixtures (2)



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

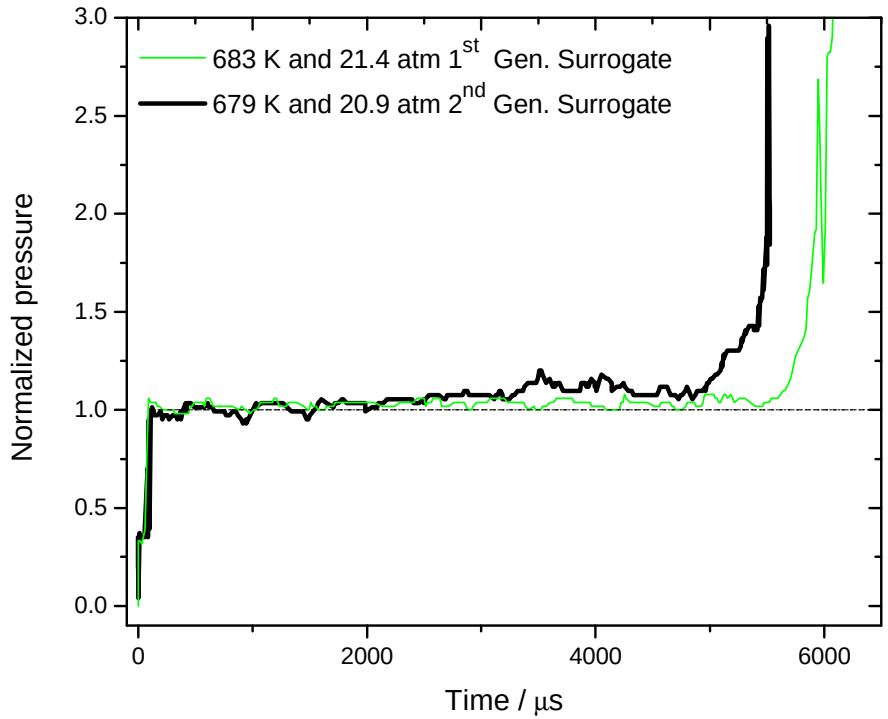


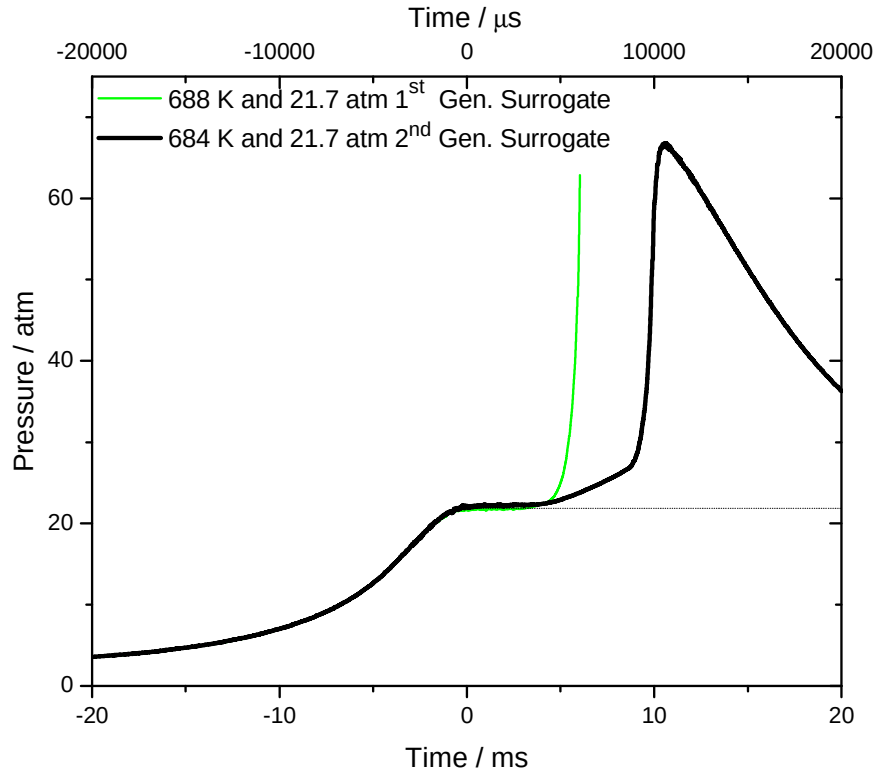




Autoignition Comparison: RCM vs. Shock-Tube (1)

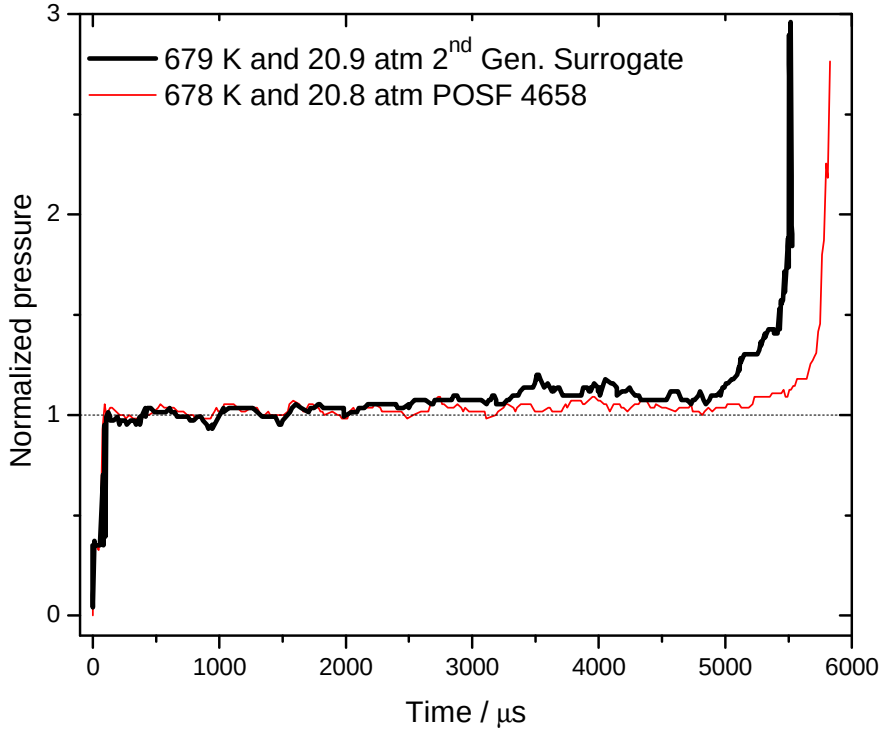
1st Generation Surrogate vs. 2nd Generation Surrogate

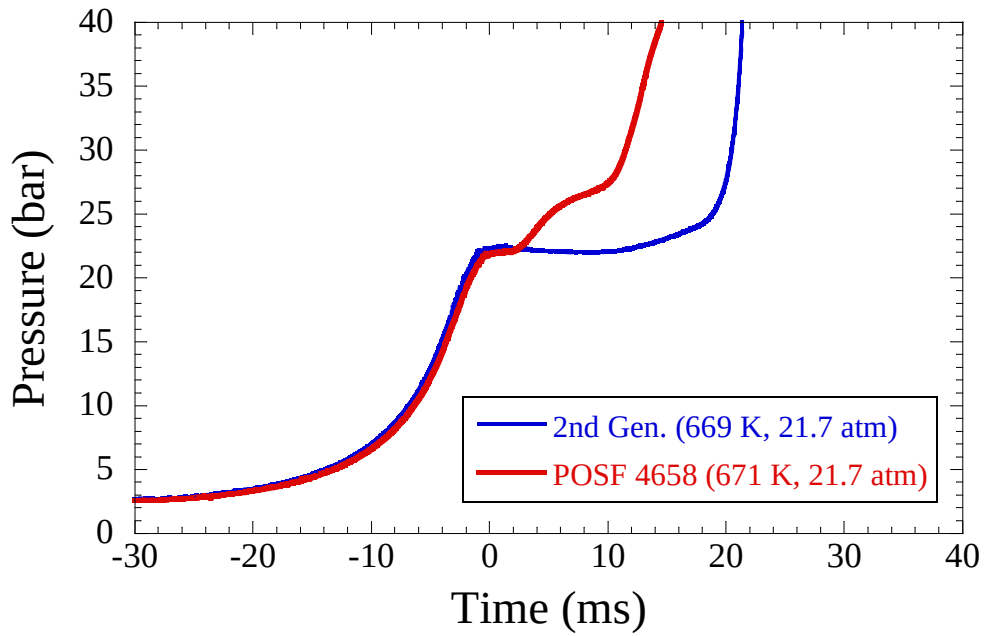




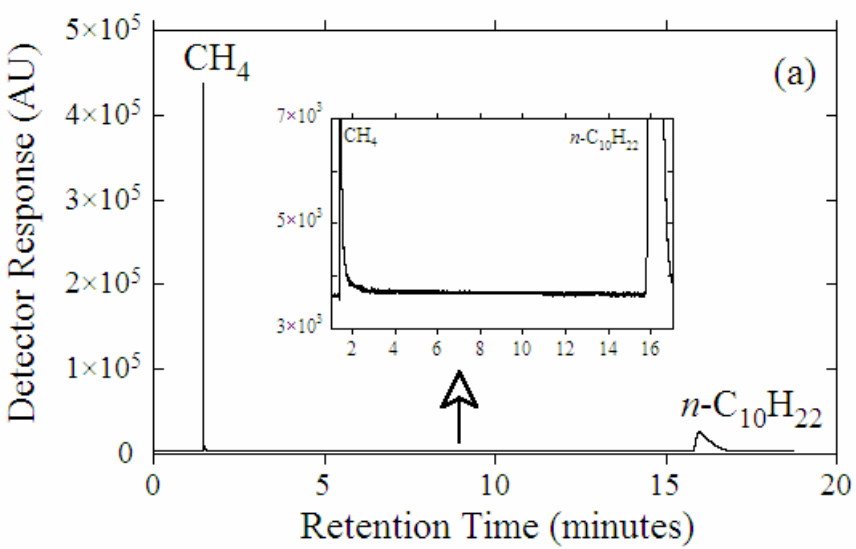
Autoignition Comparison: RCM vs. Shock-Tube (2)

Jet-A vs. 2nd Generation Surrogate



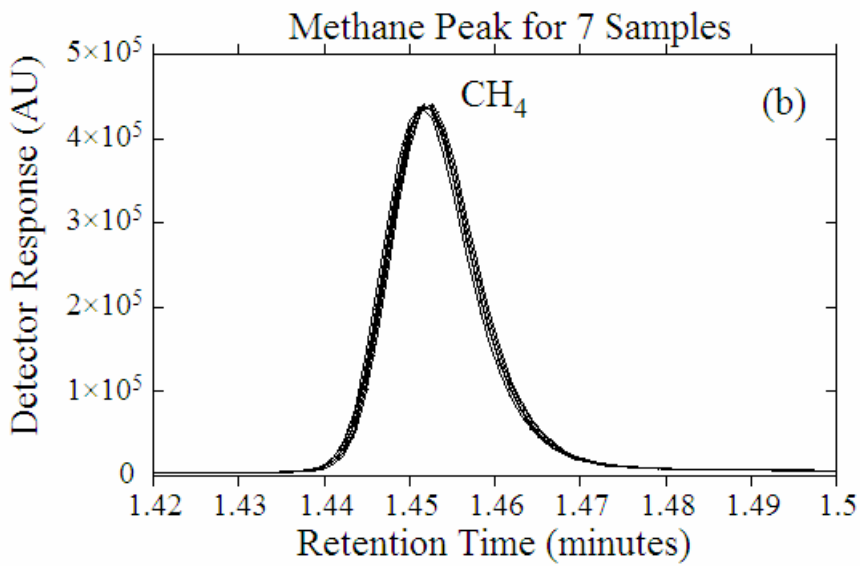


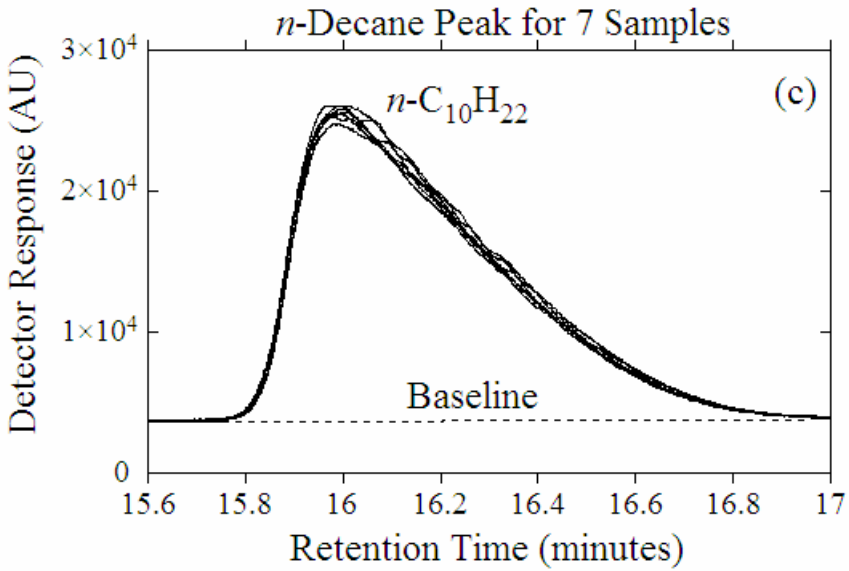
Composition Confirmation



Mixture Molar Percentages:

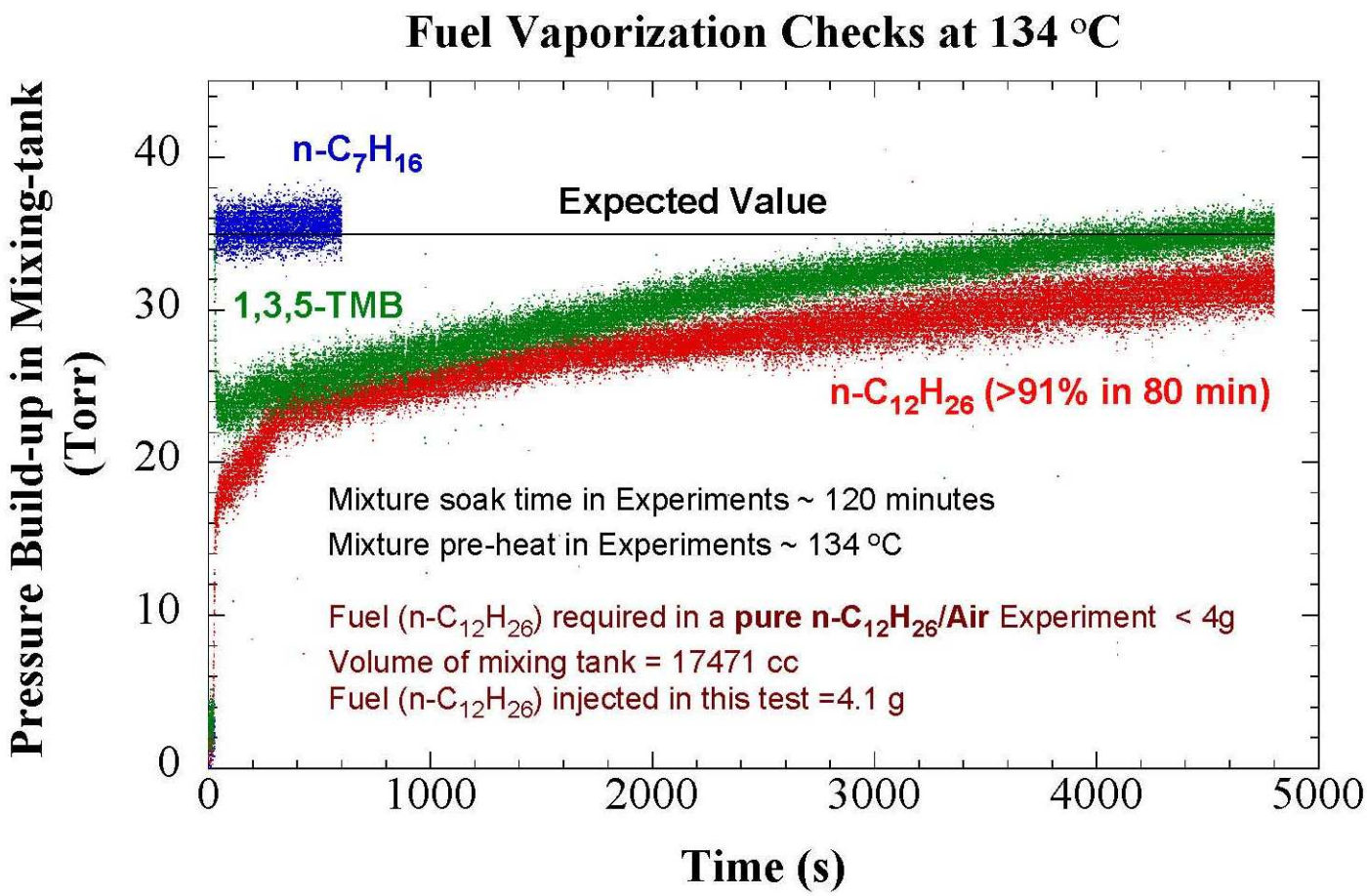
n-decane (0.49%), oxygen (20.91%), nitrogen (76.24%), and methane (2.36%)



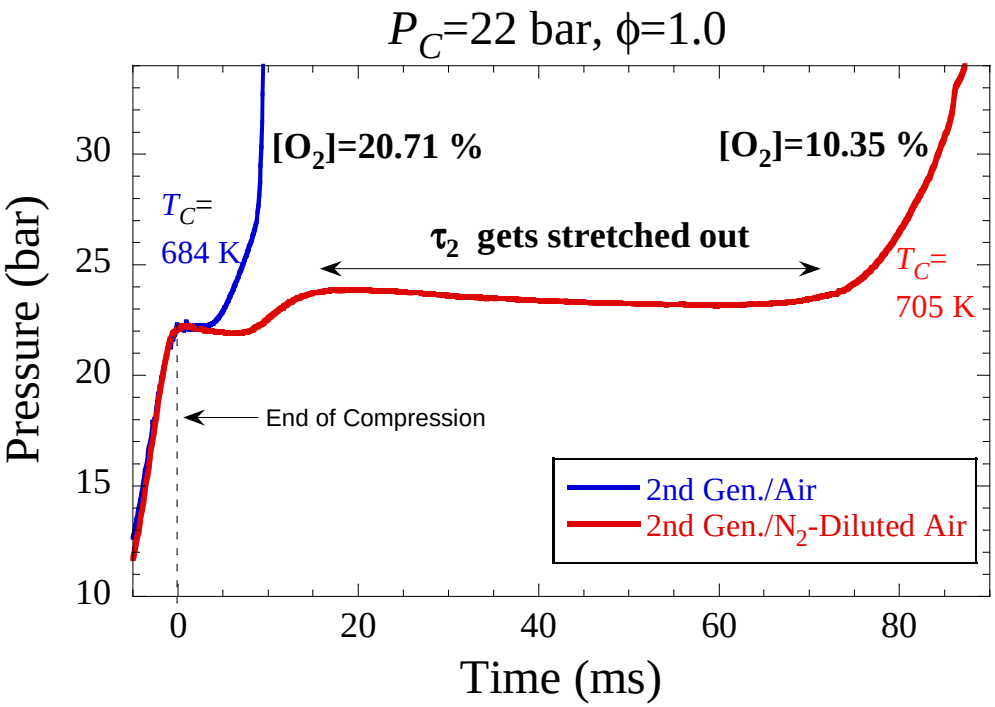


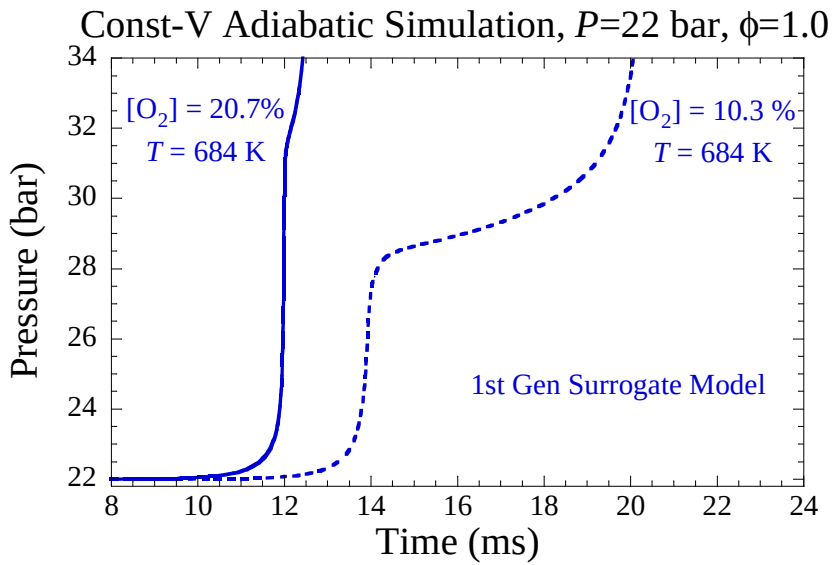
Fuel Vaporization Check

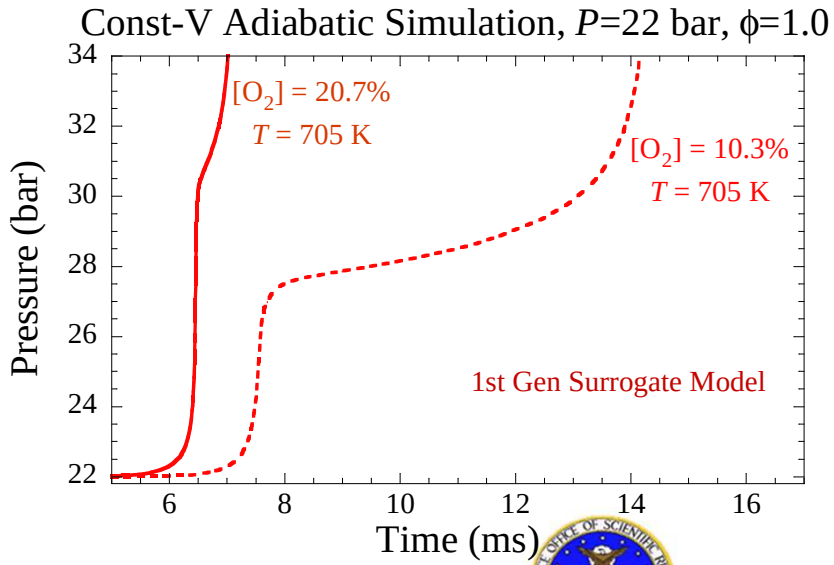
Component	Grams Injected	Gram/mol	Moles Injected	T (K)	Expected Pressure Rise (Torr)
n-Heptane	2.412	100.21	0.02407	407.2	34.98
n-Dodecane	4.100	170.34	0.02407	407.2	34.98
1,3,5-TMB	2.893	120.19	0.02407	407.2	34.98



Effect of Dilution (1)

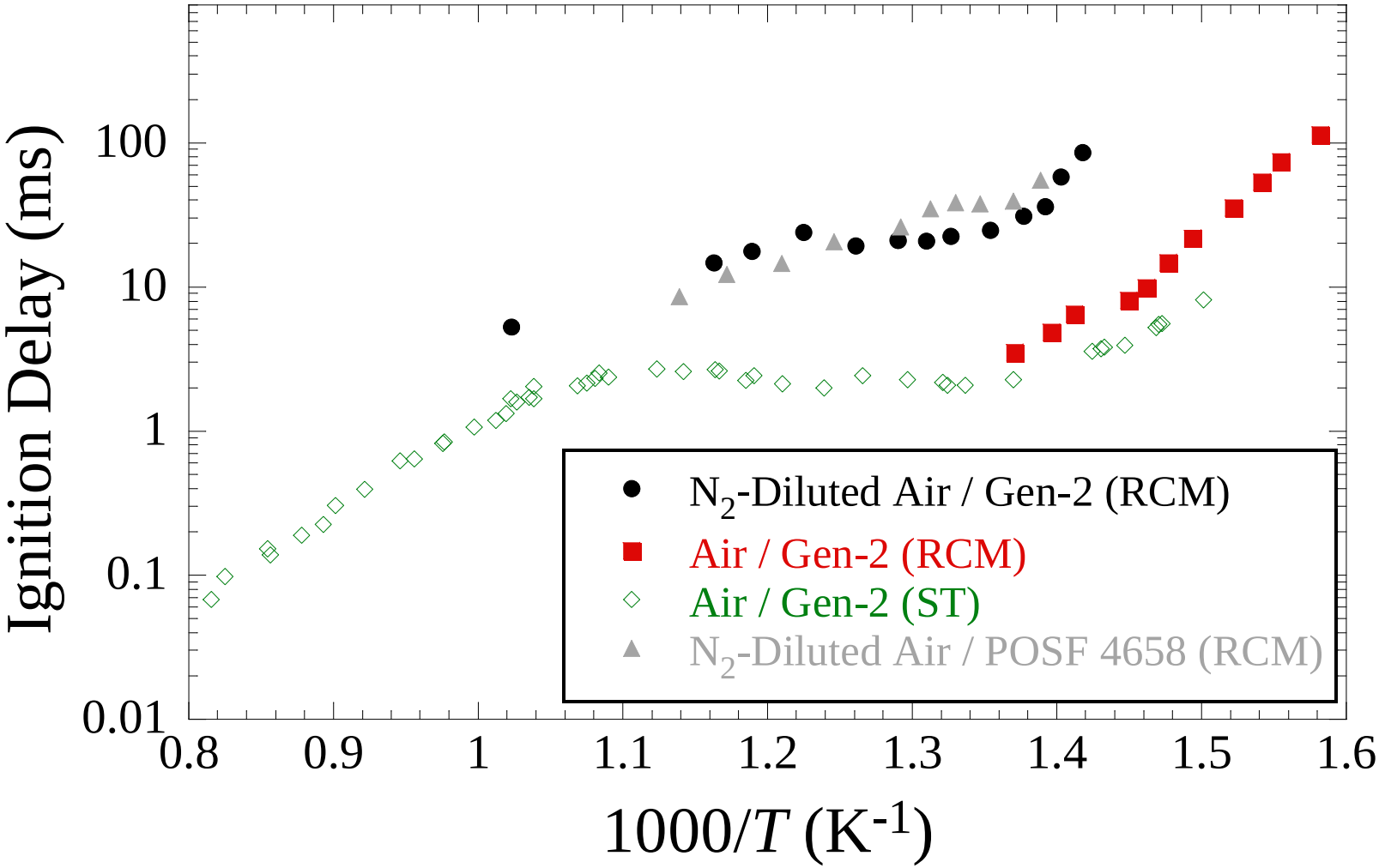




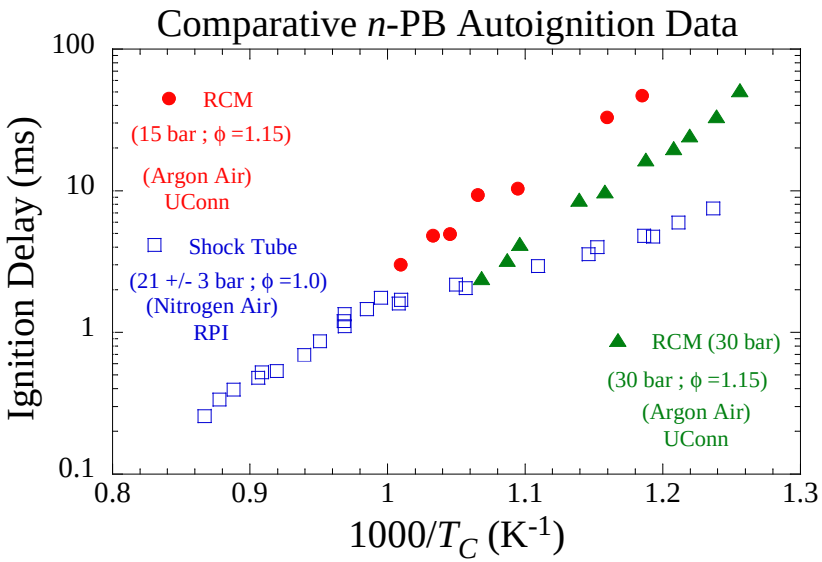


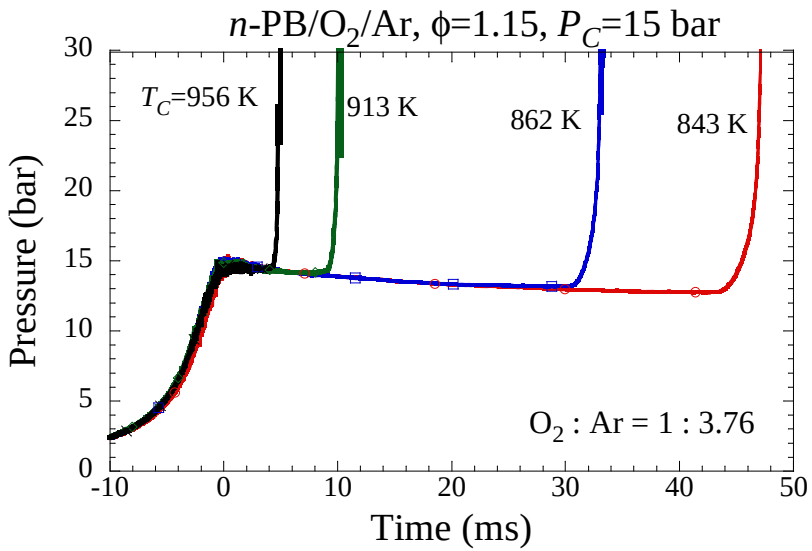
Effect of Dilution (2)

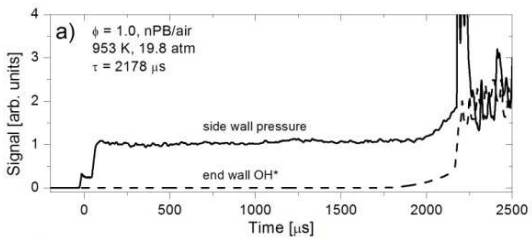
P=22 bar, ϕ=1.0

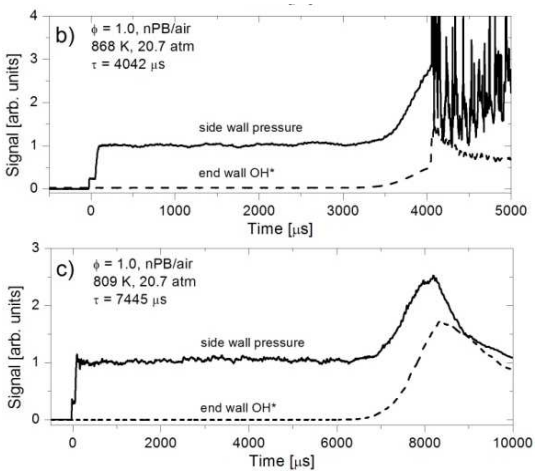


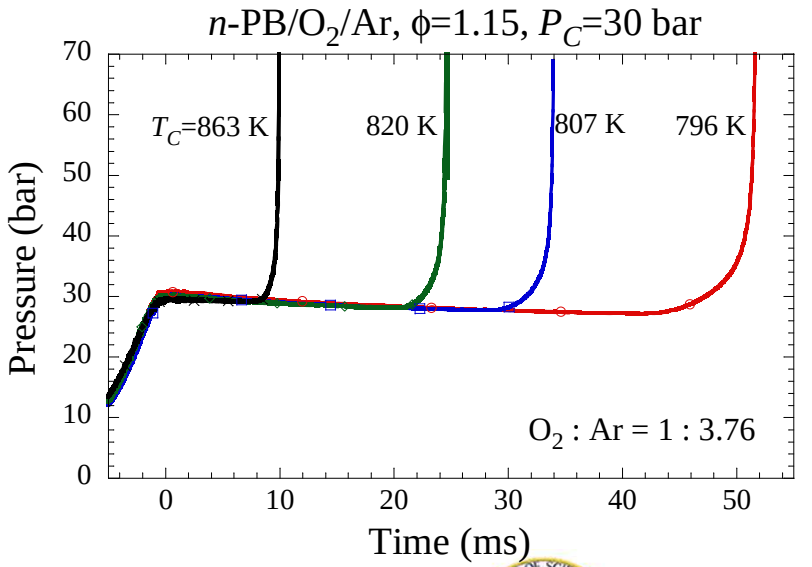
Autoignition of Aromatics (1)



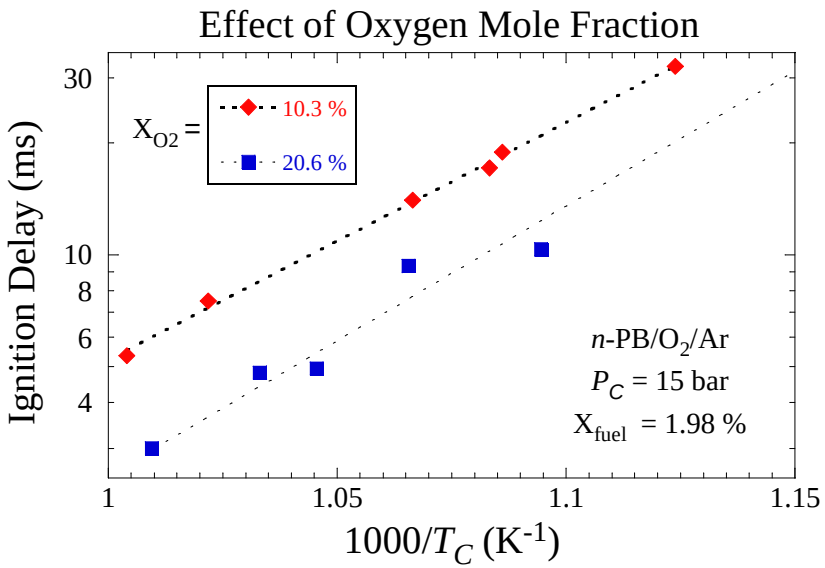


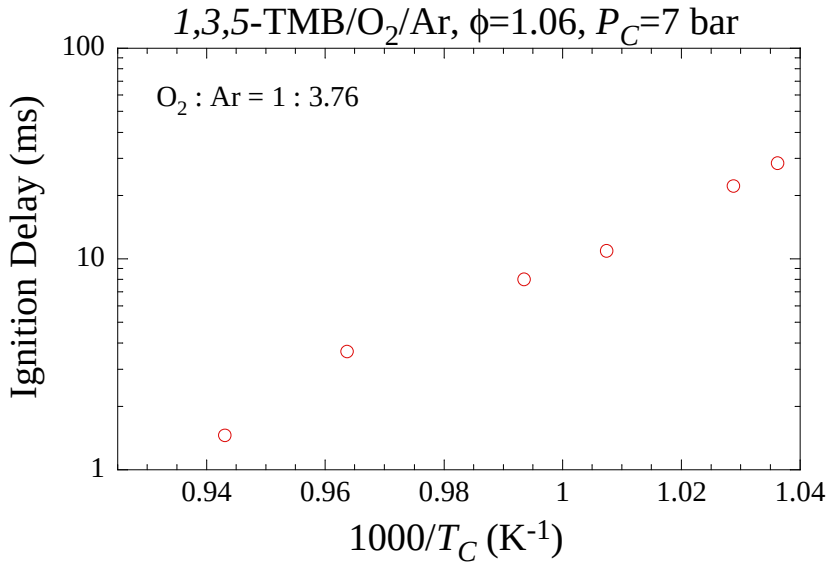


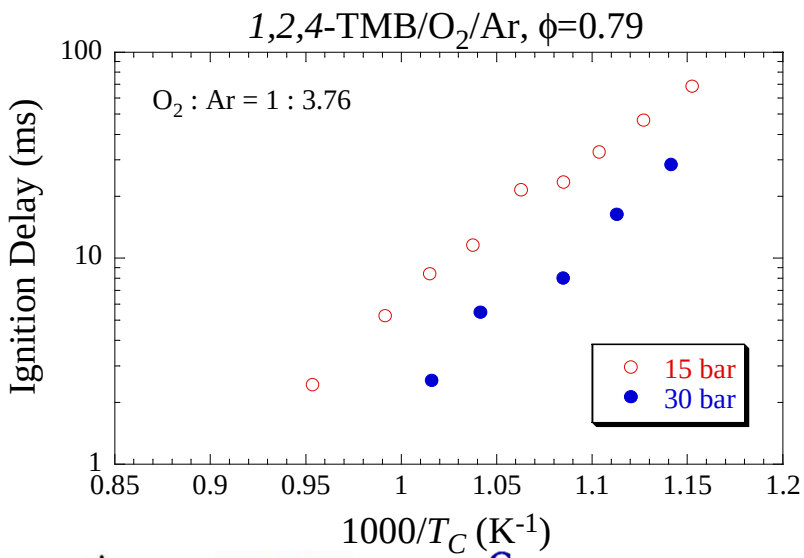


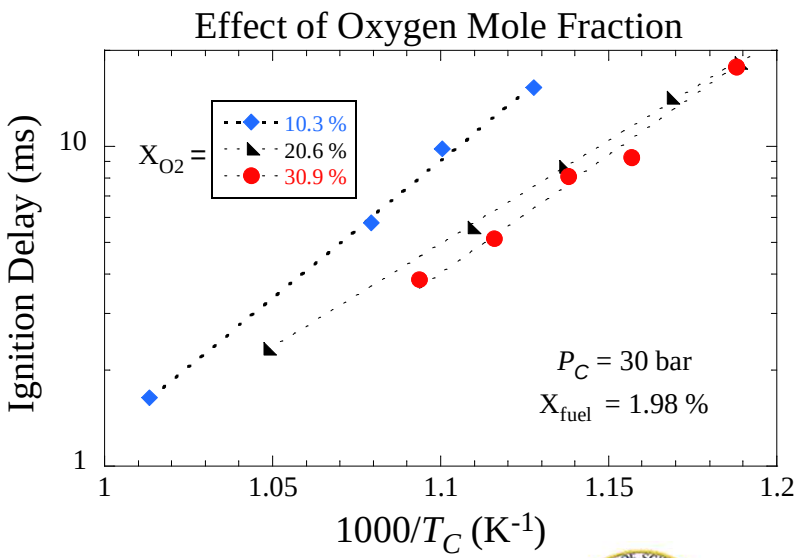


Autoignition of Aromatics (2)



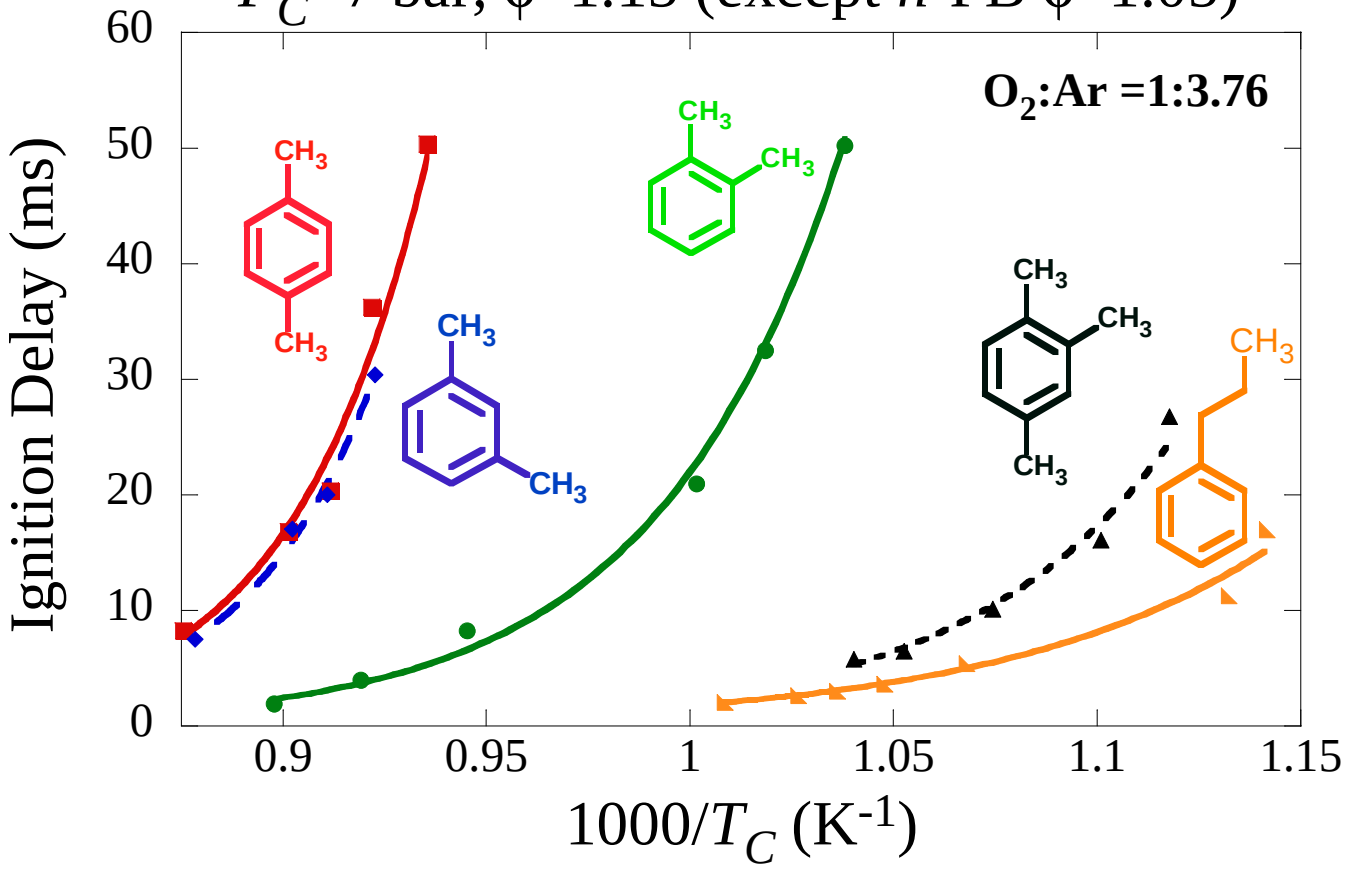






Autoignition of Aromatics (2)

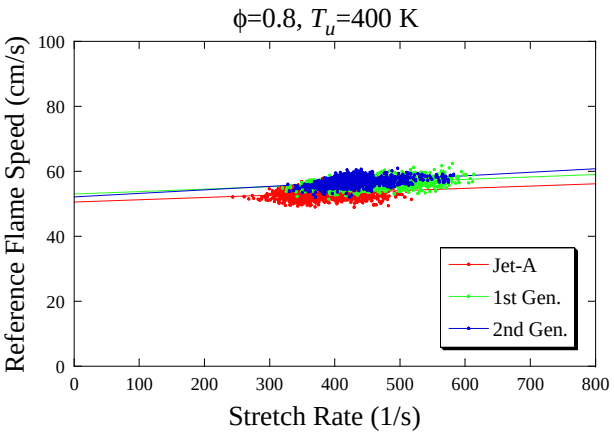
P_C=7 bar, ϕ~1.15 (except *n*-PB ϕ=1.05)

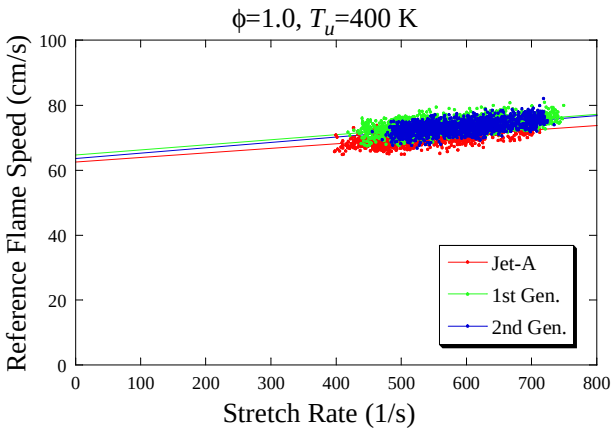


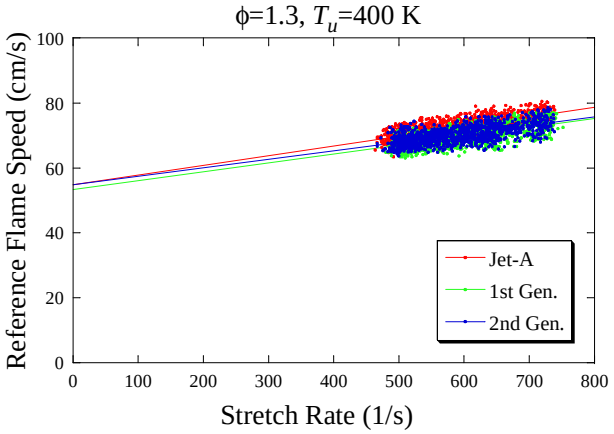
Autoignition Propensity Comparison:

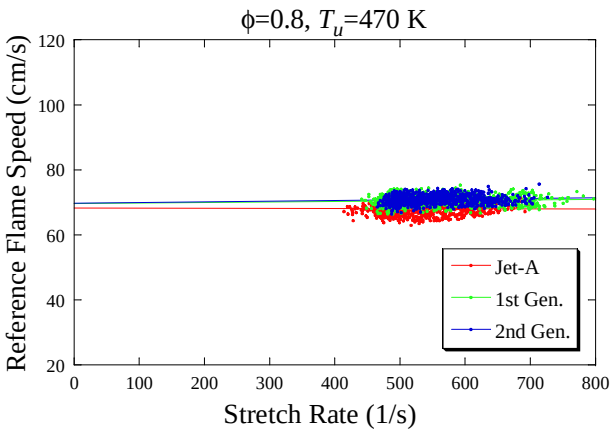
n-PB > *1,2,4*-TMB > *o*-Xylene > *m*-Xylene ≈ *p*-Xylene

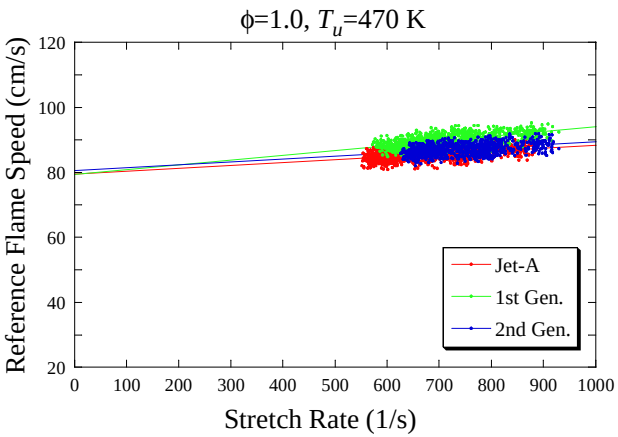
Laminar Flame Speeds:
Jet-A vs. 1st and 2nd Generation Surrogates (1)

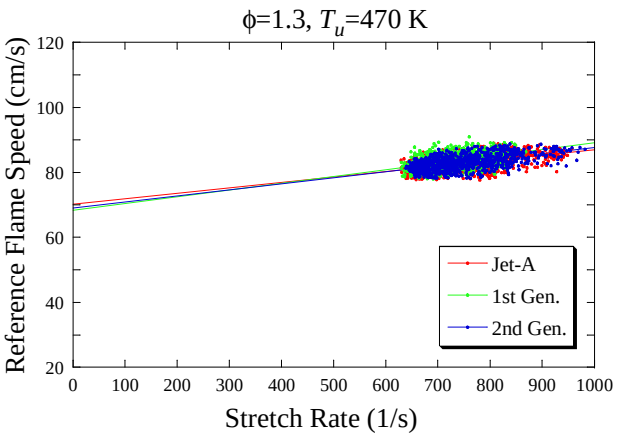




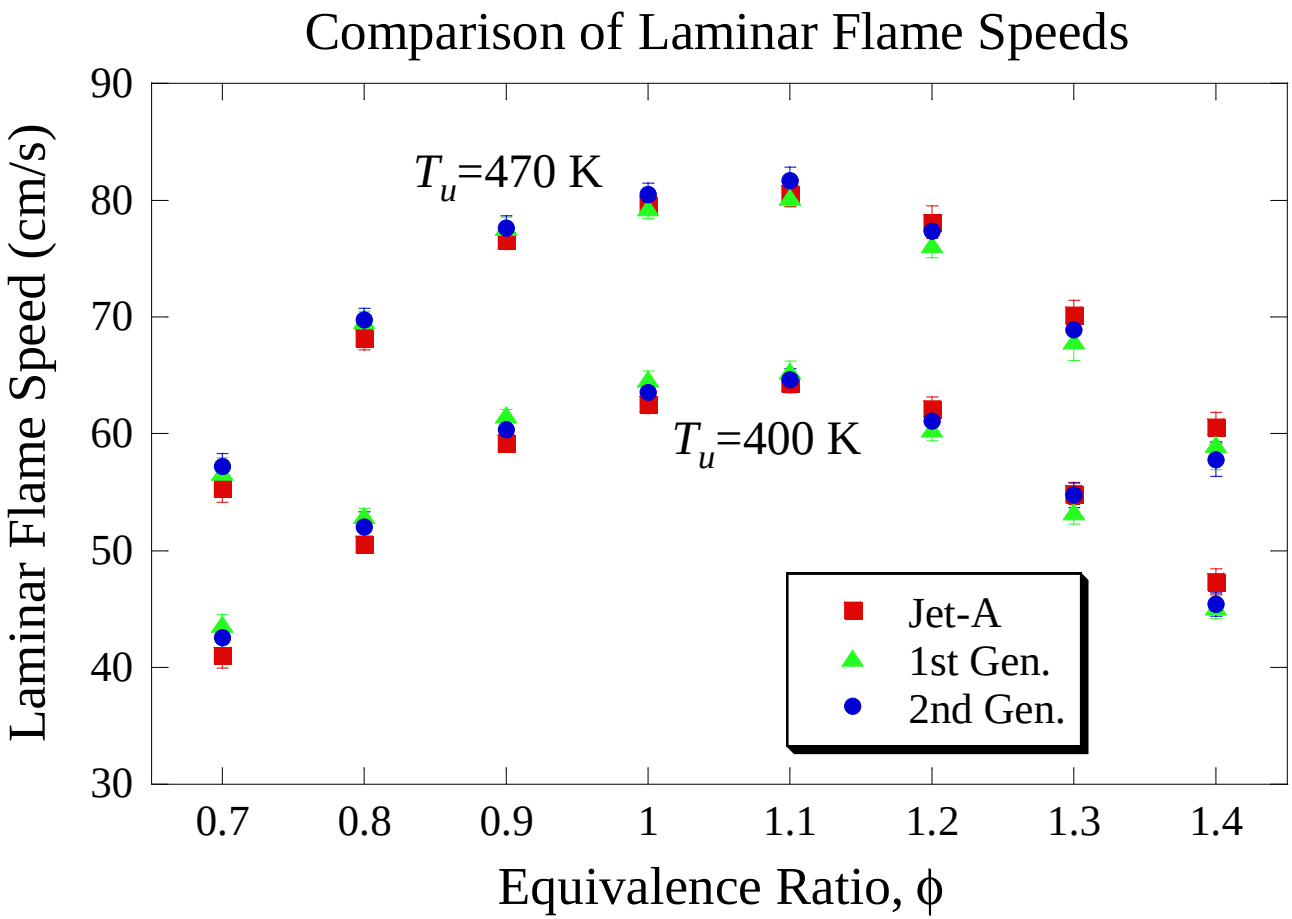




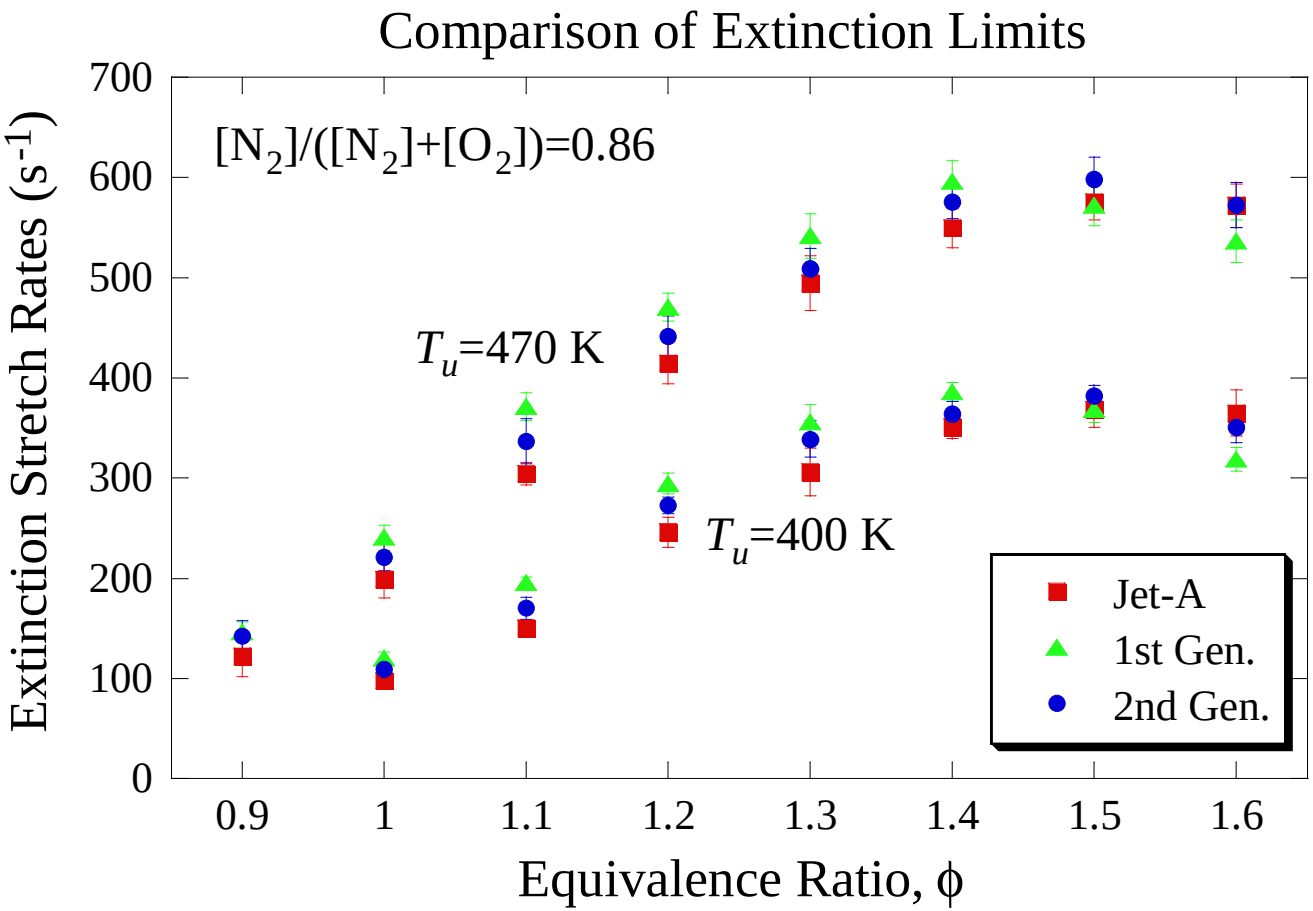




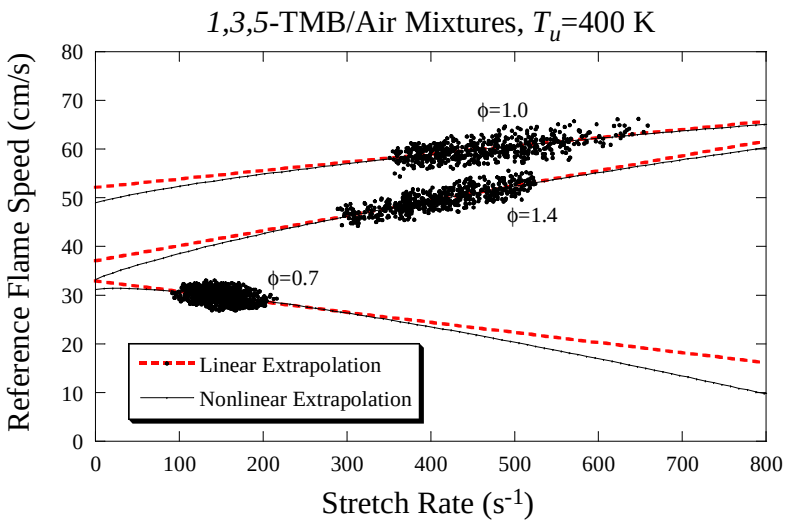
Laminar Flame Speeds:
Jet-A vs. 1st and 2nd Generation Surrogates (2)

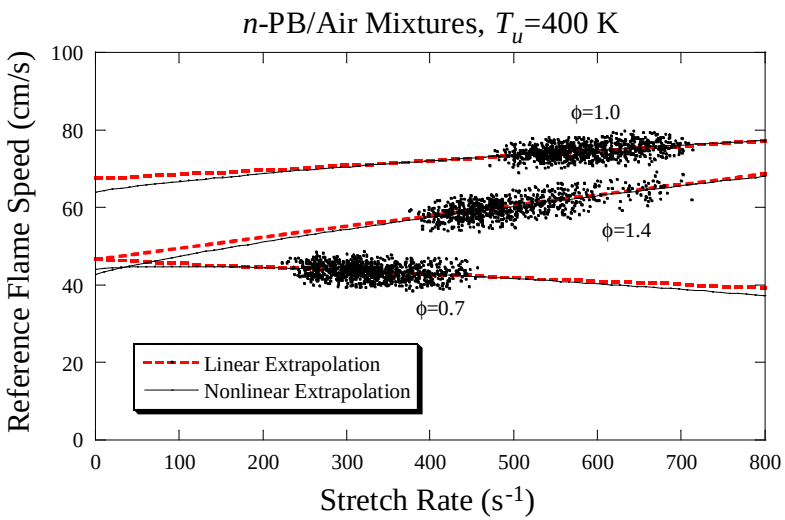


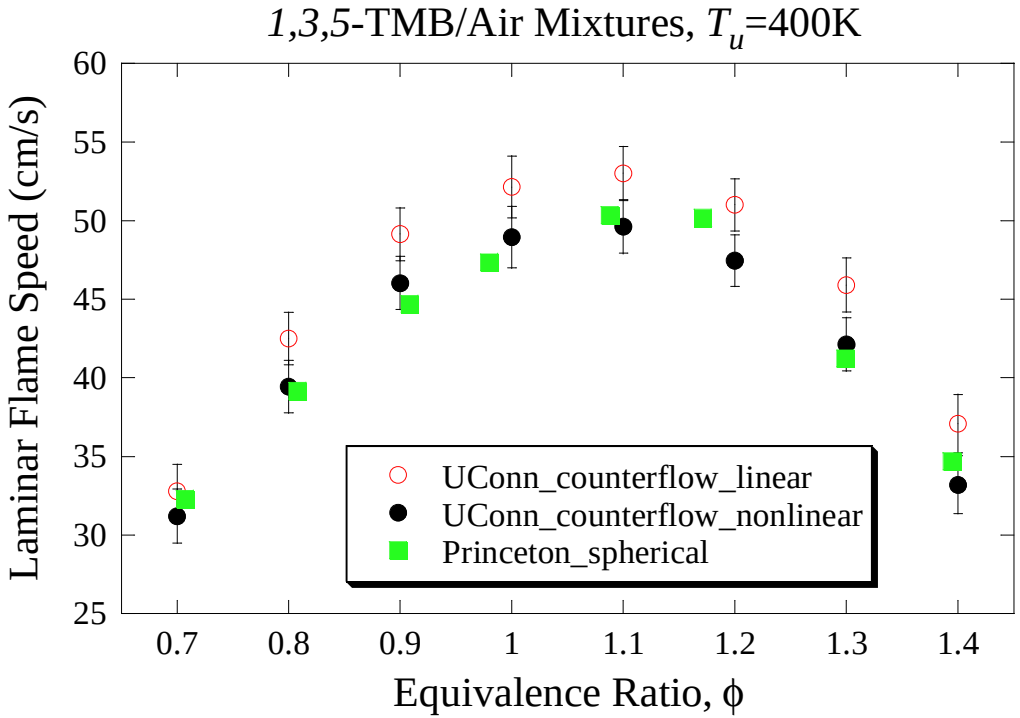
Premixed Extinction Limits:
Jet-A vs. 1st and 2nd Generation Surrogates



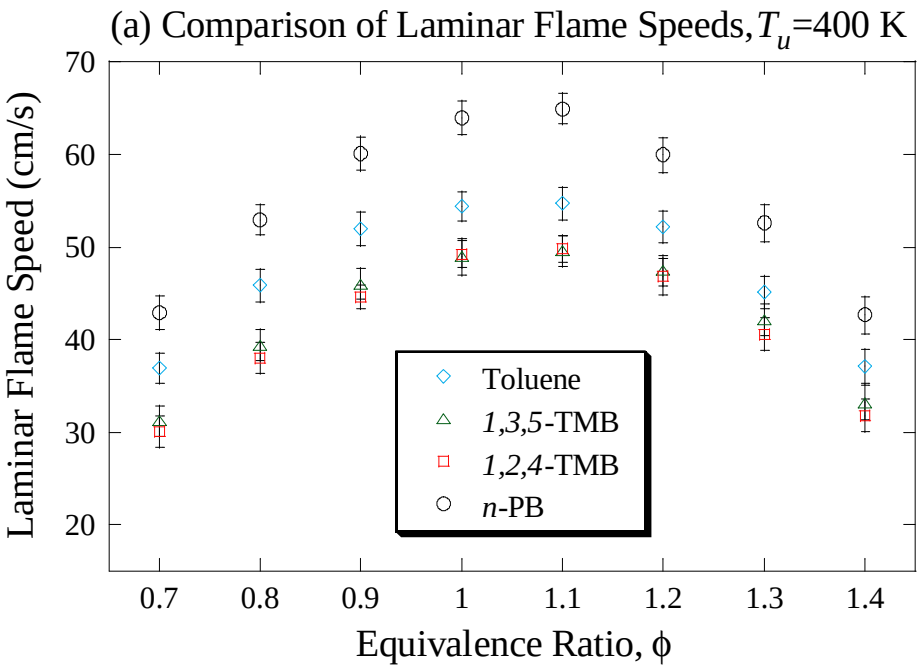
Laminar Flame Speeds of Aromatics: Experimental Results (1)

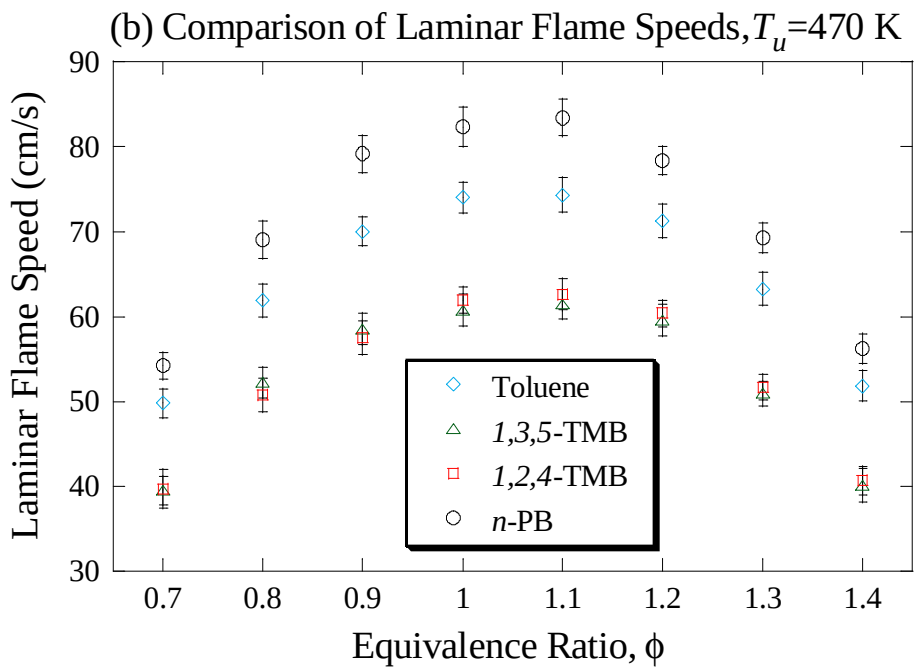






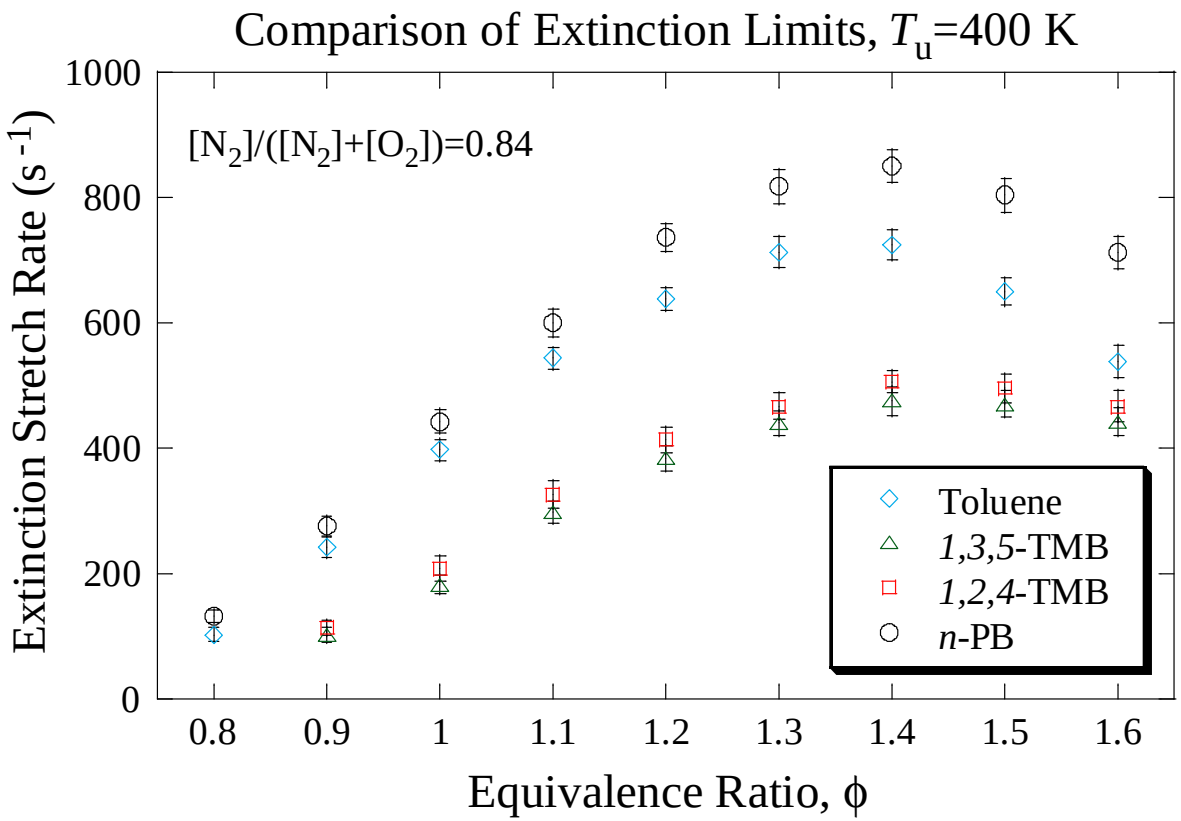
Laminar Flame Speeds of Aromatics: Experimental Results (2)





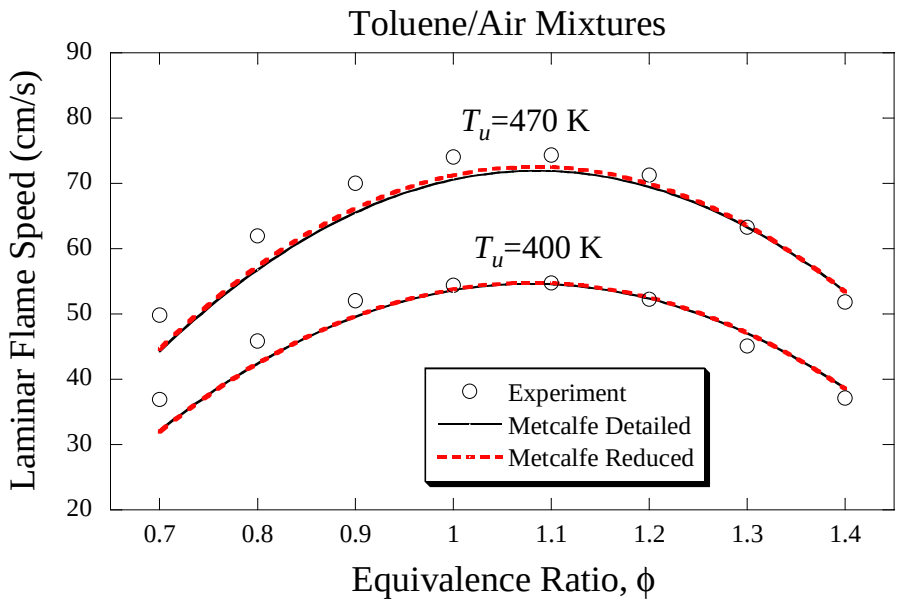
- All laminar flame speeds increase by ~30% with T_u increased from 400 K to 470 K.
- Laminar Flame Speed Comparison: *n*-PB > Toluene > *1,2,4*-TMB ≈ *1,3,5*-TMB.
- T_{ad} ranking is in the order of toluene > *n*-PB > TMBs, but the difference is insignificant.
- Also similar diffusive characteristics ⇒ the difference in laminar flame speeds is largely caused by their different oxidation kinetics due to their different alkyl substitution.

Premixed Extinction Limits of Aromatics: Experimental Results

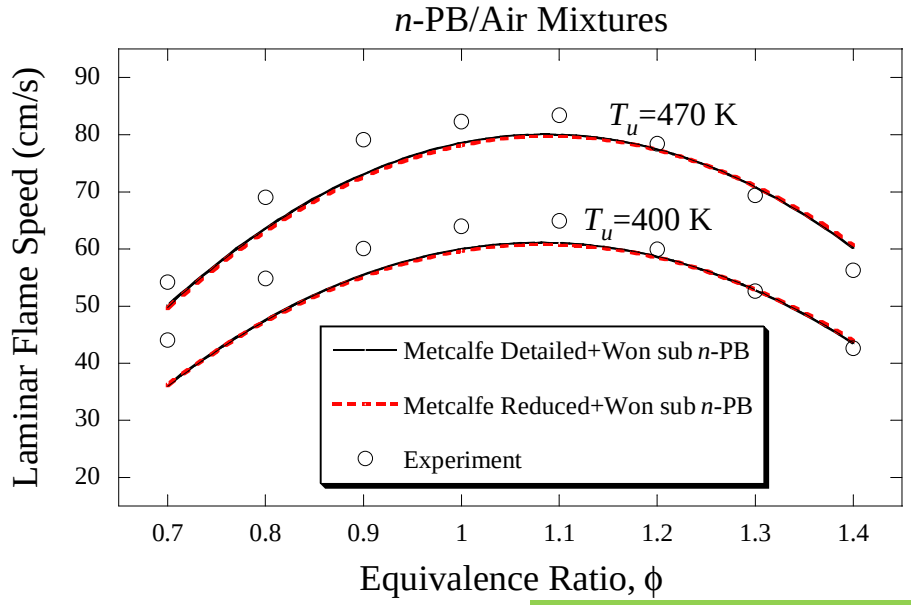


- All the extinction stretch rates peak on the fuel rich side at ϕ~1.4.
- Extinction Stretch Rate Comparison: *n*-PB > Toluene > *1,2,4*-TMB > *1,3,5*-TMB.

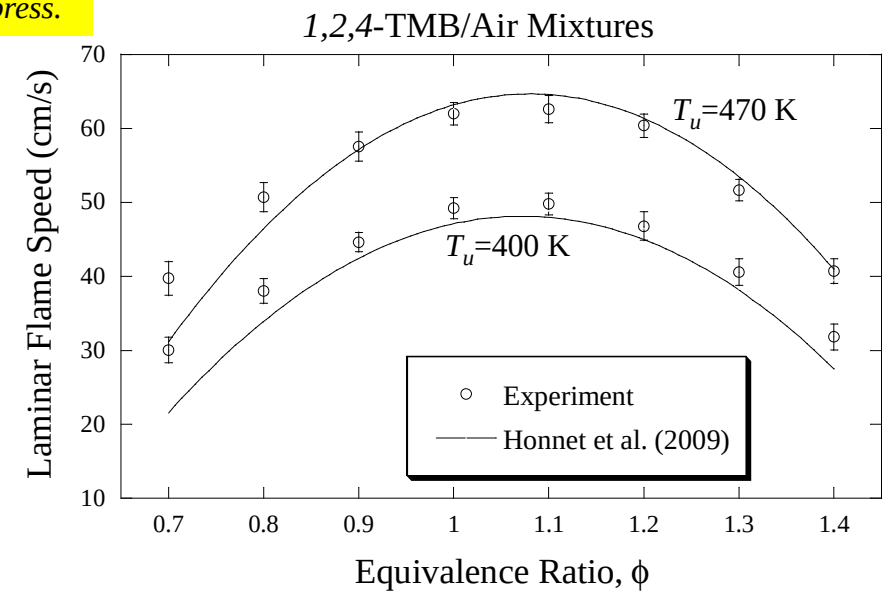
Laminar Flame Speeds of Aromatics: Model Validation



Metcalfe, Dooley, Dryer, E&F, in press.

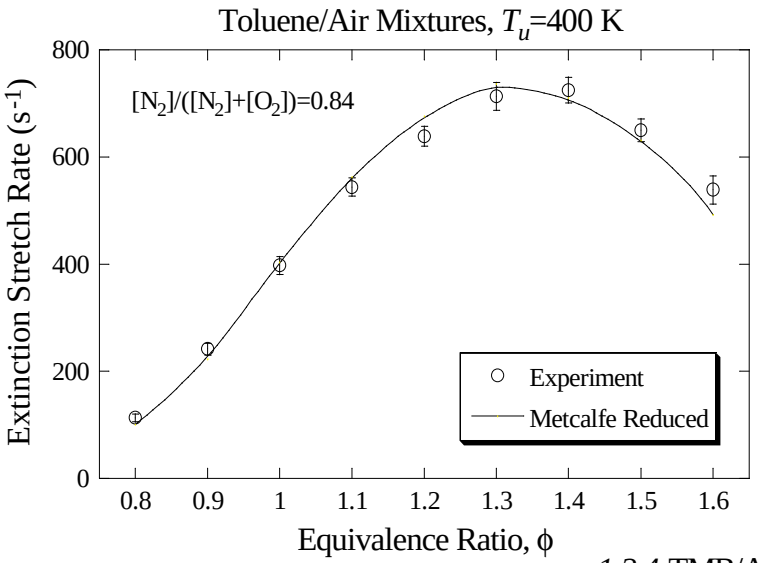


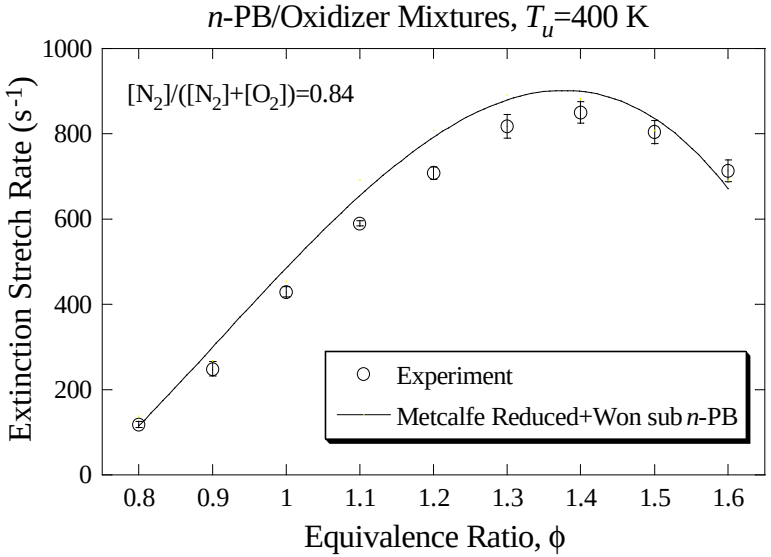
Won, Dooley, Dryer, Ju, PCI 33, 1163-1170, 2011.

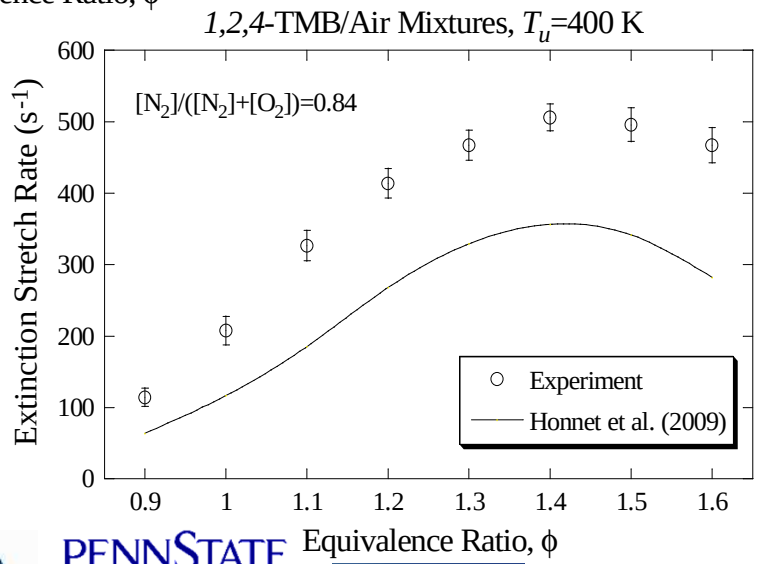


Honnet, Seshadri, Niemann, Peters, PCI 32, 485-492, 2009.

Premixed Extinction Limits of Aromatics: Model Validation





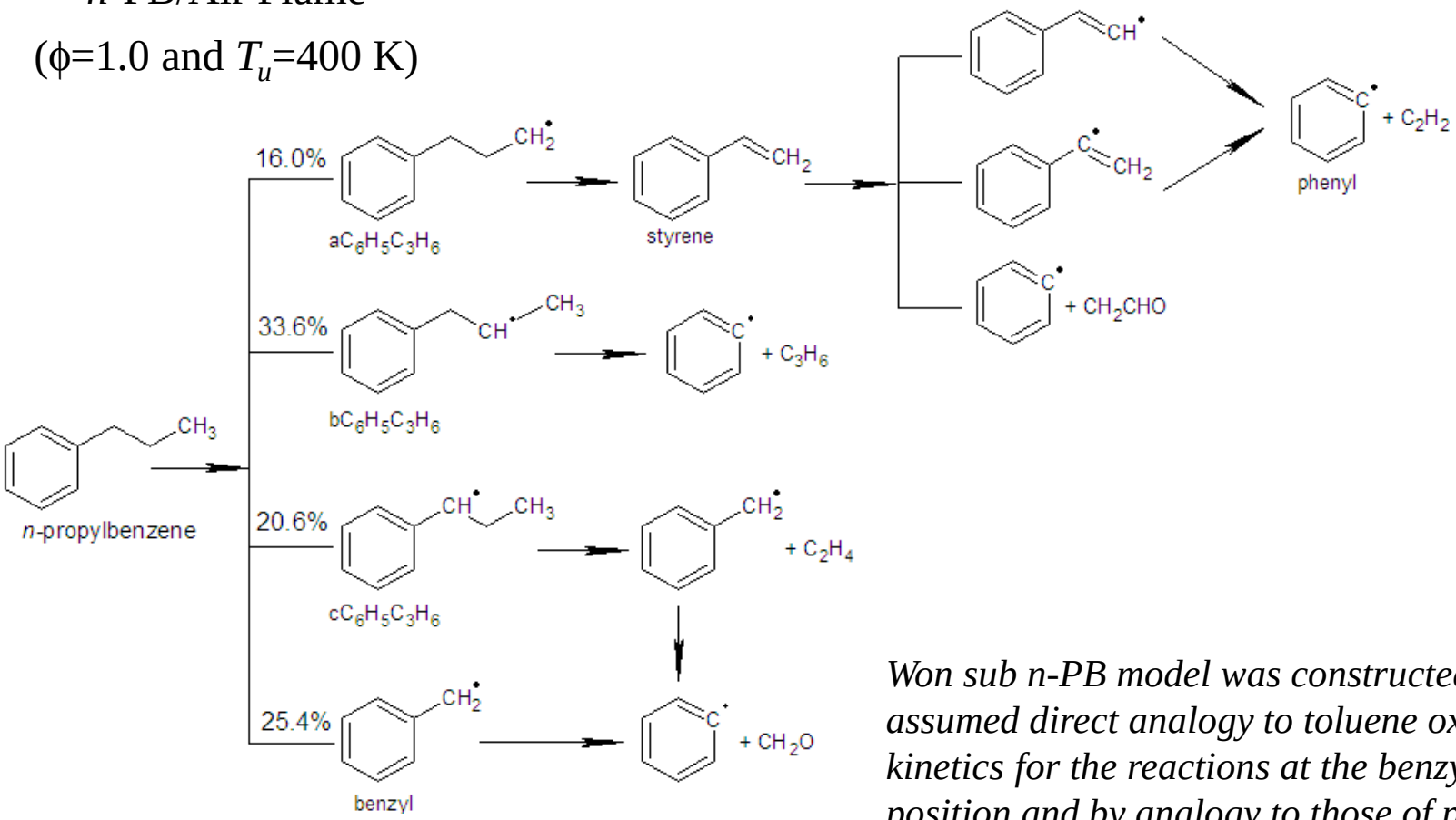


- Won *et al.* (2011) suggested that the under-prediction of *1,2,4*-TMB model is mainly due to the deficiency in the toluene sub-mechanism.

Kinetic Analysis of Aromatic Flames (1)

n-PB/Air Flame

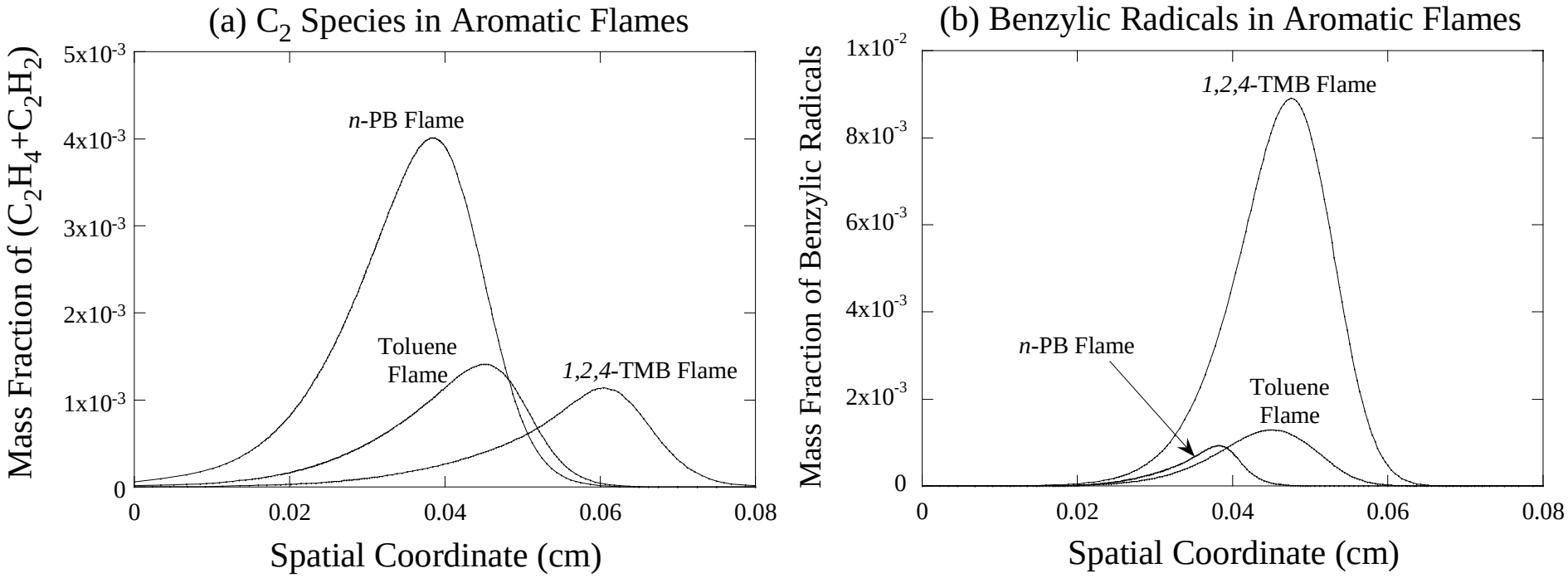
(ϕ=1.0 and T_u=400 K)



Won sub n-PB model was constructed by an assumed direct analogy to toluene oxidation kinetics for the reactions at the benzyl-type position and by analogy to those of propane for the reactions occurring at the alkyl positions.

Kinetic Analysis of Aromatic Flames (2)

ϕ=1.0, T_u=400 K



Summary and Future Work

- A team effort on surrogate mixtures and aromatics.
- Surrogate formulation strategy is demonstrated.
- Need to understand the differences among various datasets.
- Refinement of alkane and aromatic oxidation kinetic models for surrogate mixtures is needed.
- Expand autoignition and flame data of aromatics over a wider range of relevant conditions.
- Provide validation data for MURI-targeted surrogate components.
- Test solvent surrogate formulation approach.

Acknowledgements

- Work supported by AFOSR/MURI, Dr. Julian Tishkoff.
- Tim Edwards of AFRL for jet fuel supplies.
- Research Associate: Dr. Kamal Kumar.
- Graduate Students: Xin Hui, Apurba Das, and Pradeep Singh.