Fundamental Combustion Data for Surrogate Components, Blends, and Jet Fuels

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

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

National Institute of Standards and Technology
Gaithersburg, MD 20899

September 8, 2008

Key Tasks

- Acquire extensive and comprehensive experimental validation database for **neat surrogate components**, **binary fuel blends**, and **real jet fuels**.
- *Rapid Compression Machine* Experiments:
  - Obtain experimental data for autoignition delays and pre-ignition species evolutions at elevated pressures and low-to-intermediate temperatures.
- *Counterflow Flame* Experiments:
  - Determine fundamental flame properties, including laminar flame speeds and extinction stretch rates.

Year 1 Progress

- Autoignition of neat hydrocarbon components under high pressure conditions.
  - *n-decane*
  - *dimethyl ether (DME)*
  - *methylcyclohexane (MCH)*
  - *toluene*
  - *iso-octane*
  - *diisobutylene-1 (DIB-1)*
- Chemical kinetic interactions in binary fuel blends.
  - *toluene+iso-octane* and *toluene+DIB-1*.
- Autoignition of real jet fuels, including *Jet-A*, *JP-8*, and *S-8*.
- Laminar flame speeds of preheated *Jet-A/air* and *S-8/air* mixtures.

Outline of Presentation

- Characterization of Rapid Compression Machine
- Autoignition of Jet-A
- Autoignition of Fuel Blends
- Laminar Flame Speeds of Jet-A
- Future Work

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Characterization of Rapid Compression Machine (RCM)

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Issues/Concerns

- *"You don't know anything about gas motion and heat loss inside an RCM!"*
  - A main reason why kinetics people are quite critical, even dismissive, of results from RCMs.
- Much of our effort was expended to make the RCM technique sound and convincing.
  - improved temperature homogeneity using creviced piston
    - Acetone PLIF experiments confirm these attributes
  - model the heat loss effect using *effective volume approach*
- Is zero-dimensional modelling *hunky dory*?
  - need much more sophisticated numerical approaches to model RCM studies?

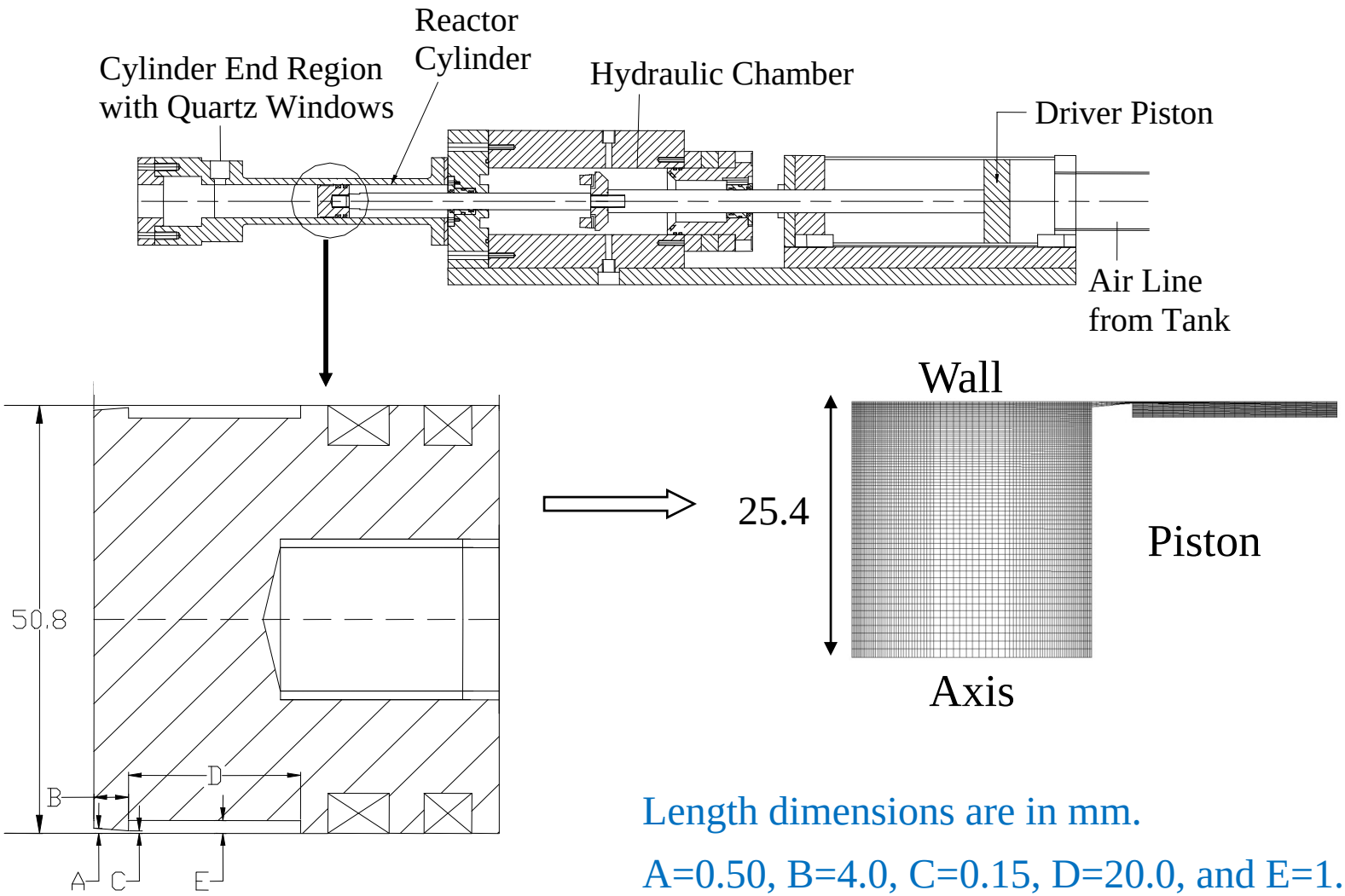
CFD Modeling

- Influence of physical and operating parameters on RCM performance
- Hydrogen ignition in an RCM
  - representing single-stage ignition phenomenon
  - considering conditions above the extended second limit to examine pre-ignition heat release effect on hot ignition event
- *Hydrocarbon fuels with two-stage ignition behavior (in progress)*

Modeling Objectives

- Assess RCM performance over a range of physical and operating conditions
  - Effect of pressure
  - Effect of compression stroke
  - Effect of clearance volume
- Compare CFD simulation and zero-dimensional calculation for reactive mixtures
- Assess various heat loss models

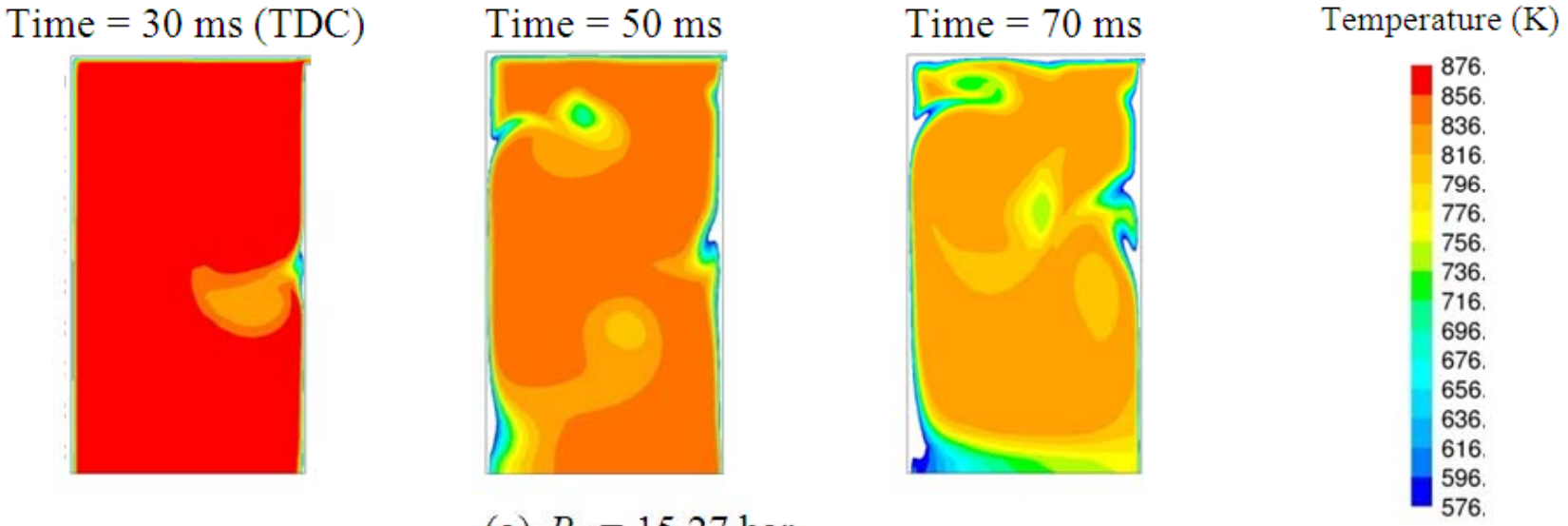
Computational Grids



Length dimensions are in mm.

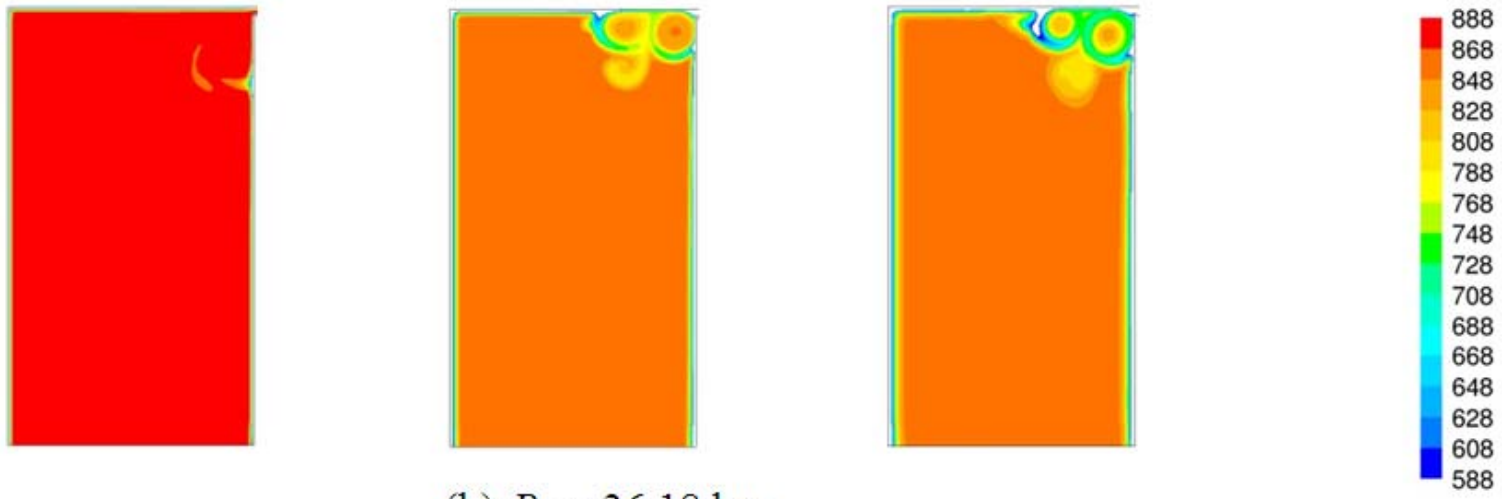
A=0.50, B=4.0, C=0.15, D=20.0, and E=1.50.

Effect of Pressure (1)



(a) P_C = 15.27 bar

Stroke Length = 25.4 cm, Clearance = 1.4 cm

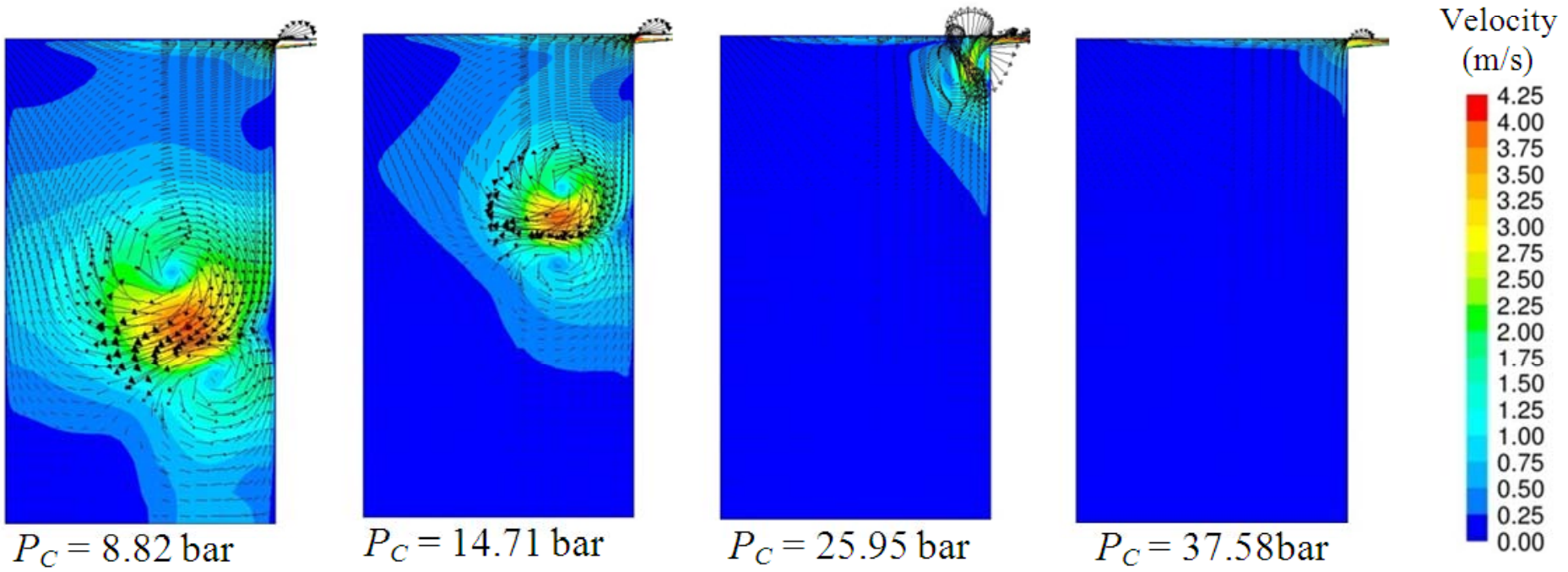


(b) P_C = 36.18 bar

Effect of Pressure (2)

Stroke Length = 25.4 cm, Clearance = 1.4 cm

at TDC (time = 30 ms), T_C = 1070 K



P_C = 8.82 bar	P_C = 14.71 bar	P_C = 25.95 bar	P_C = 37.58bar
0.85 m/s	***0.57 m/s***	***0.18 m/s***	***0.10 m/s***

(mass-weighted average velocity)

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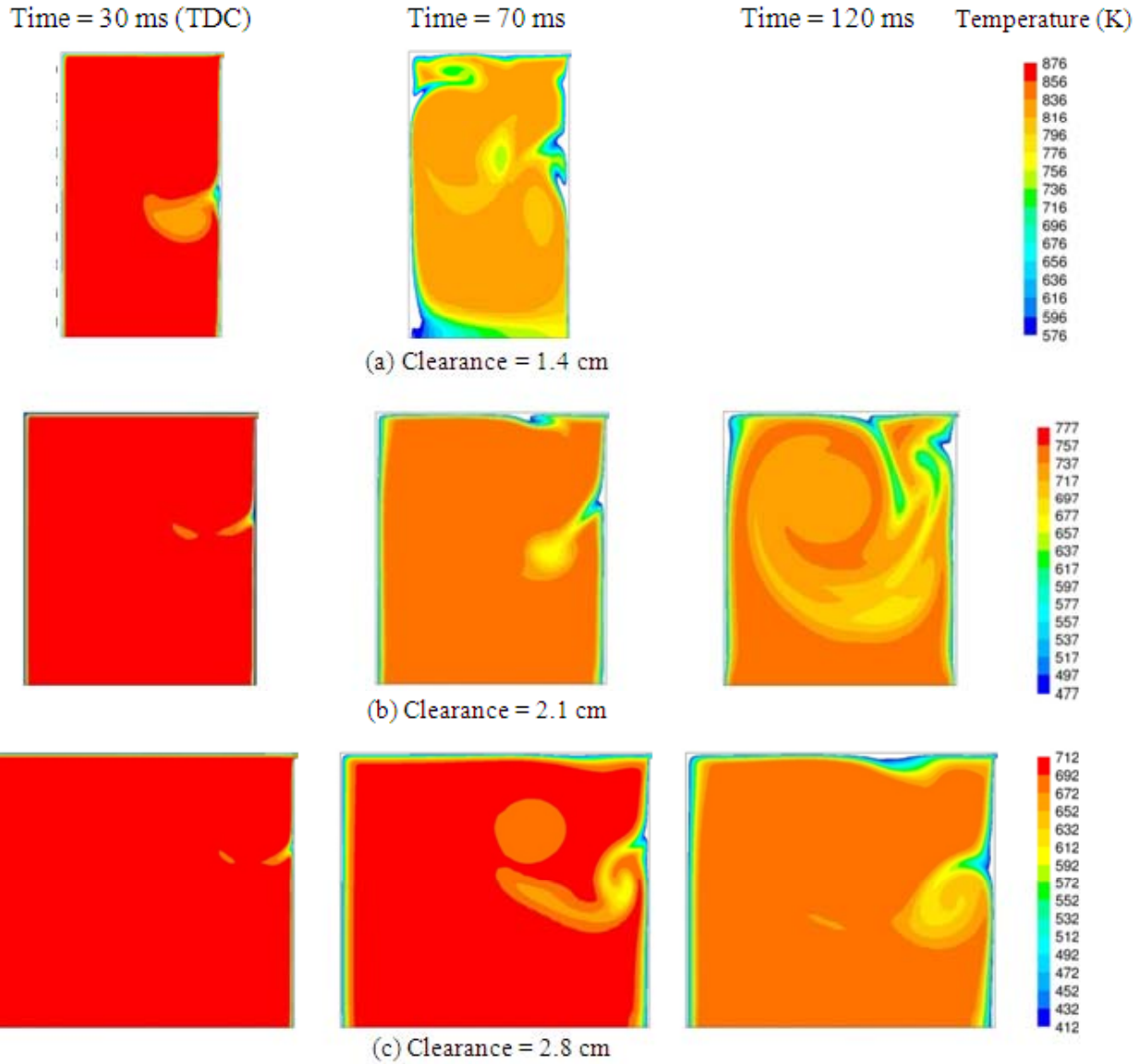
Effect of Clearance

Stroke Length = 25.4 cm, P_C ~ 15.3 bar



(a) Clearance = 1.4 cm

(b) Clearance = 2.1 cm

(c) Clearance = 2.8 cm

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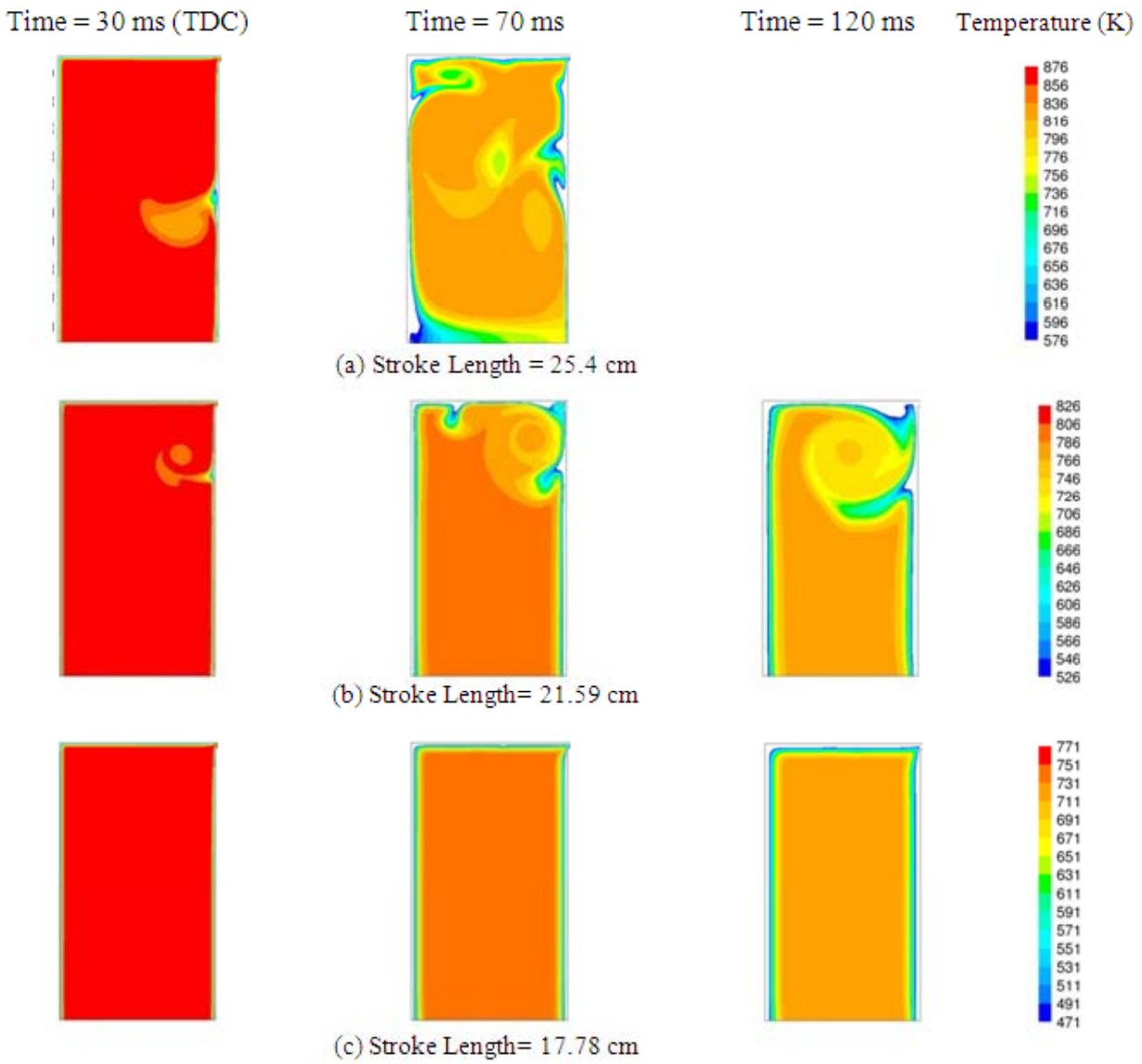
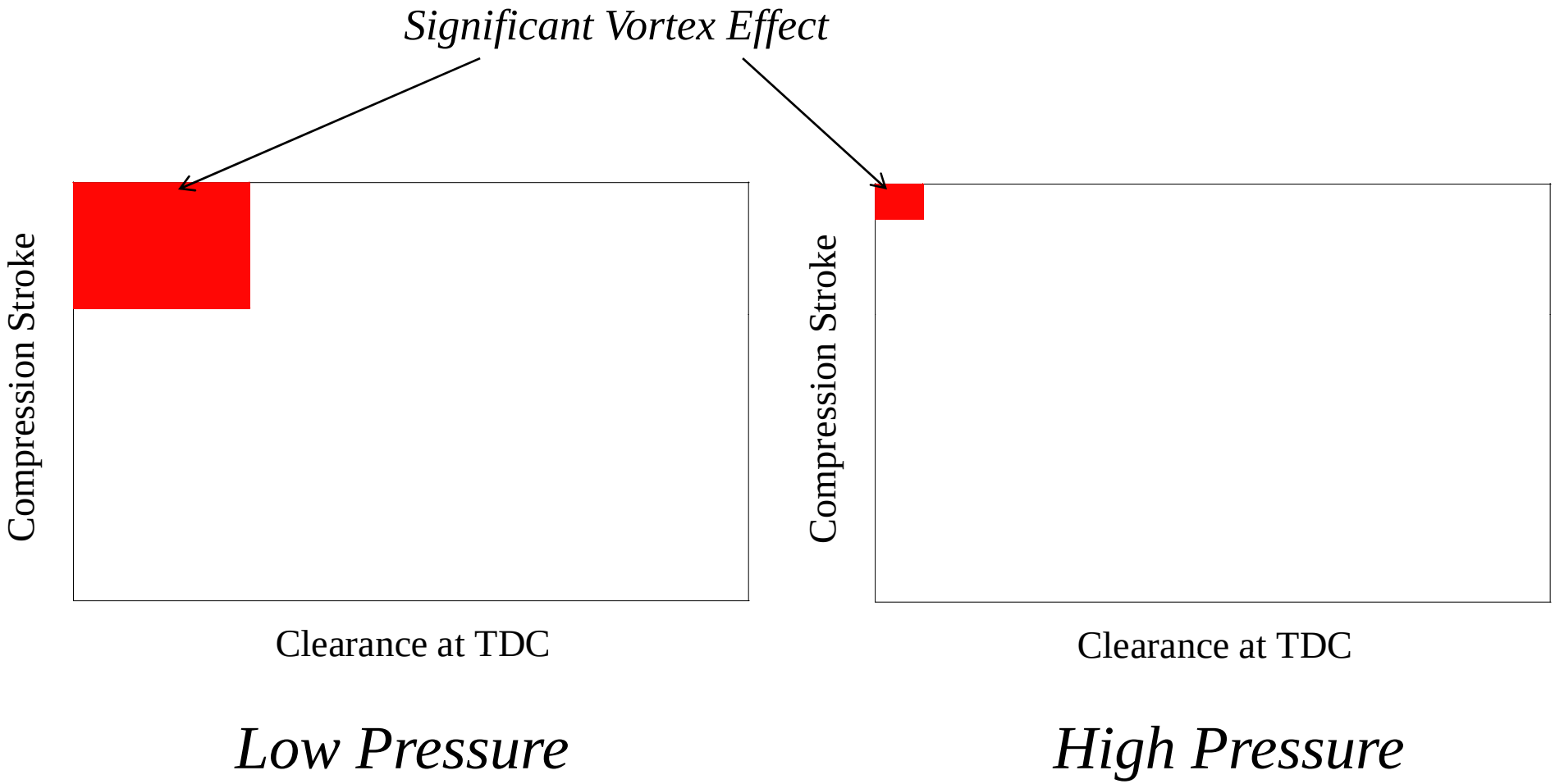
Effect of Compression Stroke

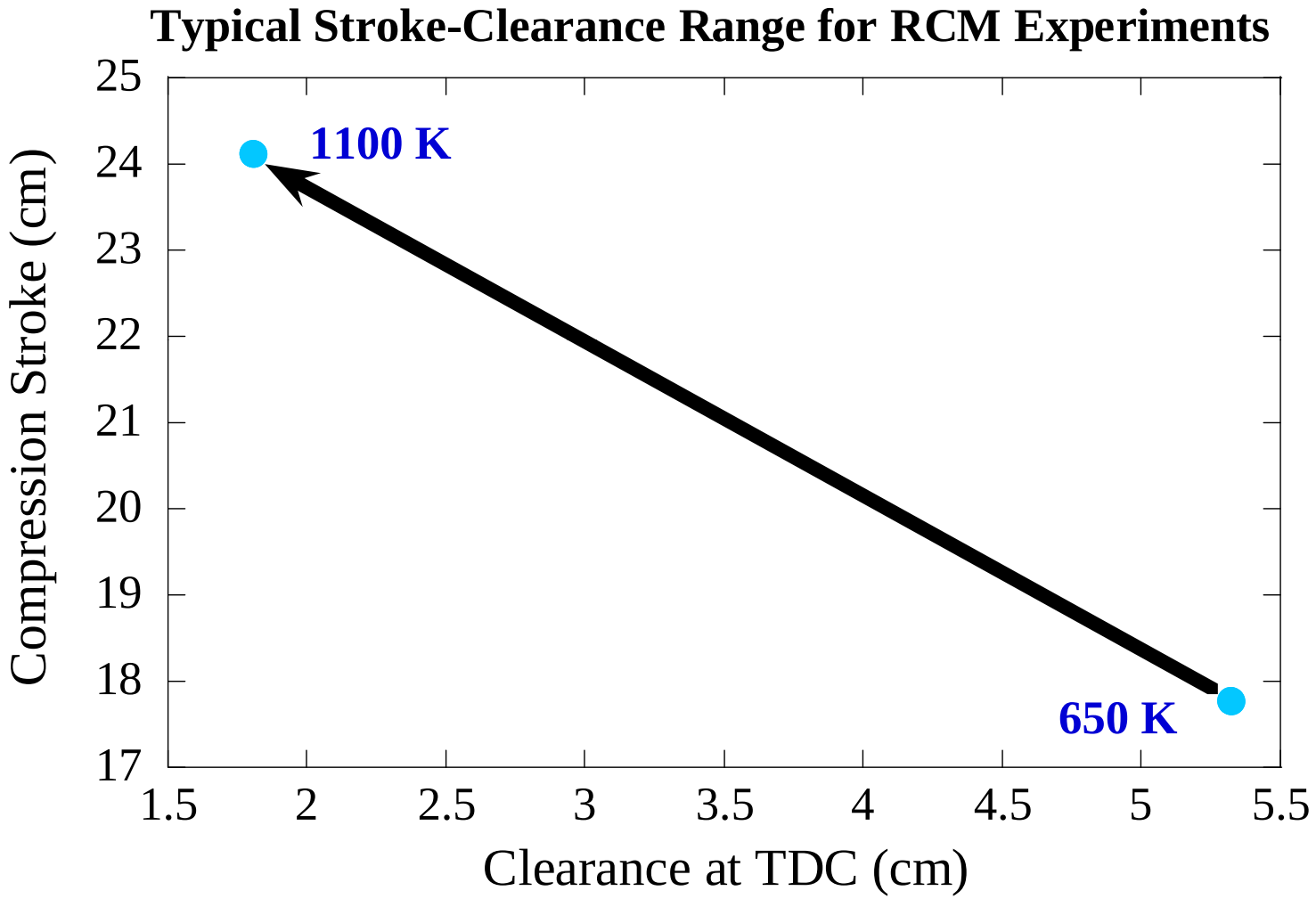
Clearance = 1.4 cm, P_C ~ 15.3 bar



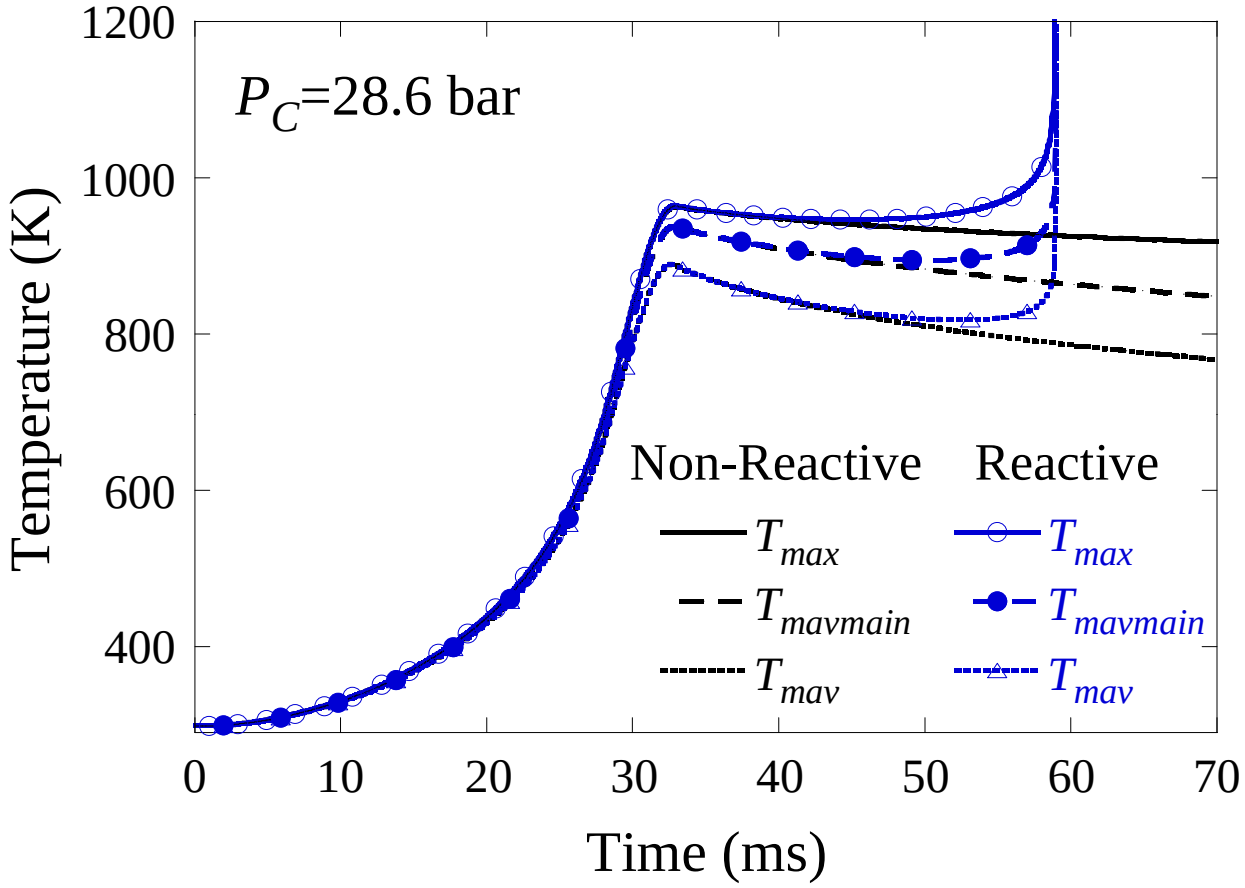
Performance Summary (1)



Performance Summary (2)



Fluent Simulations

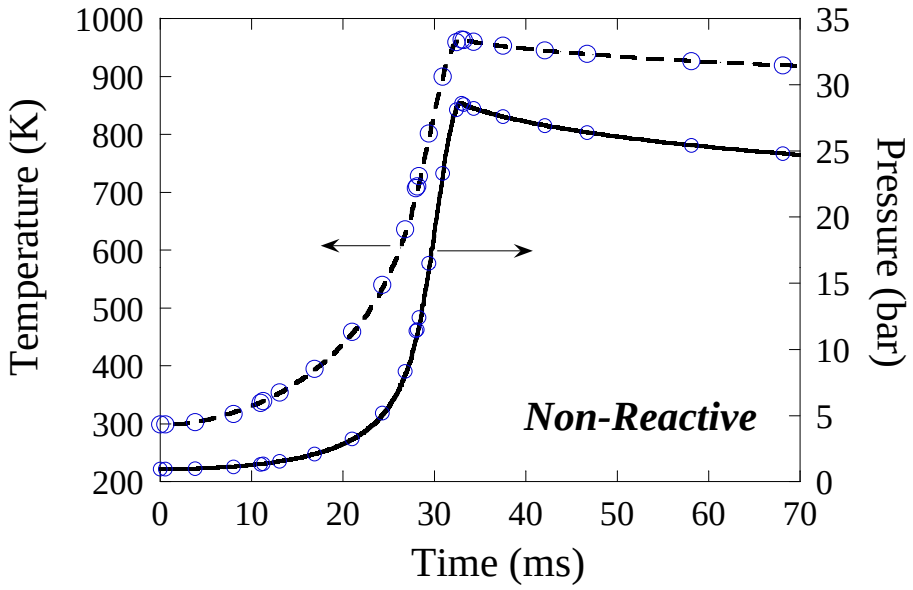


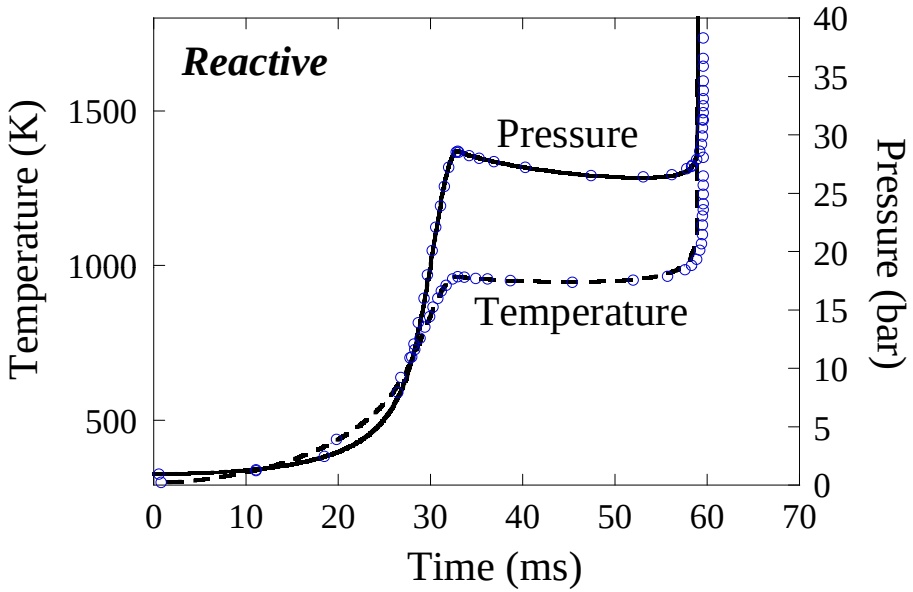
T_{max} = maximum instantaneous temperature

$T_{mavmain}$ = mass averaged temperature of the main reaction chamber (without crevice)

T_{mav} = mass averaged temperature of the entire reaction chamber (including crevice)

FLUENT vs. SENKIN (1)

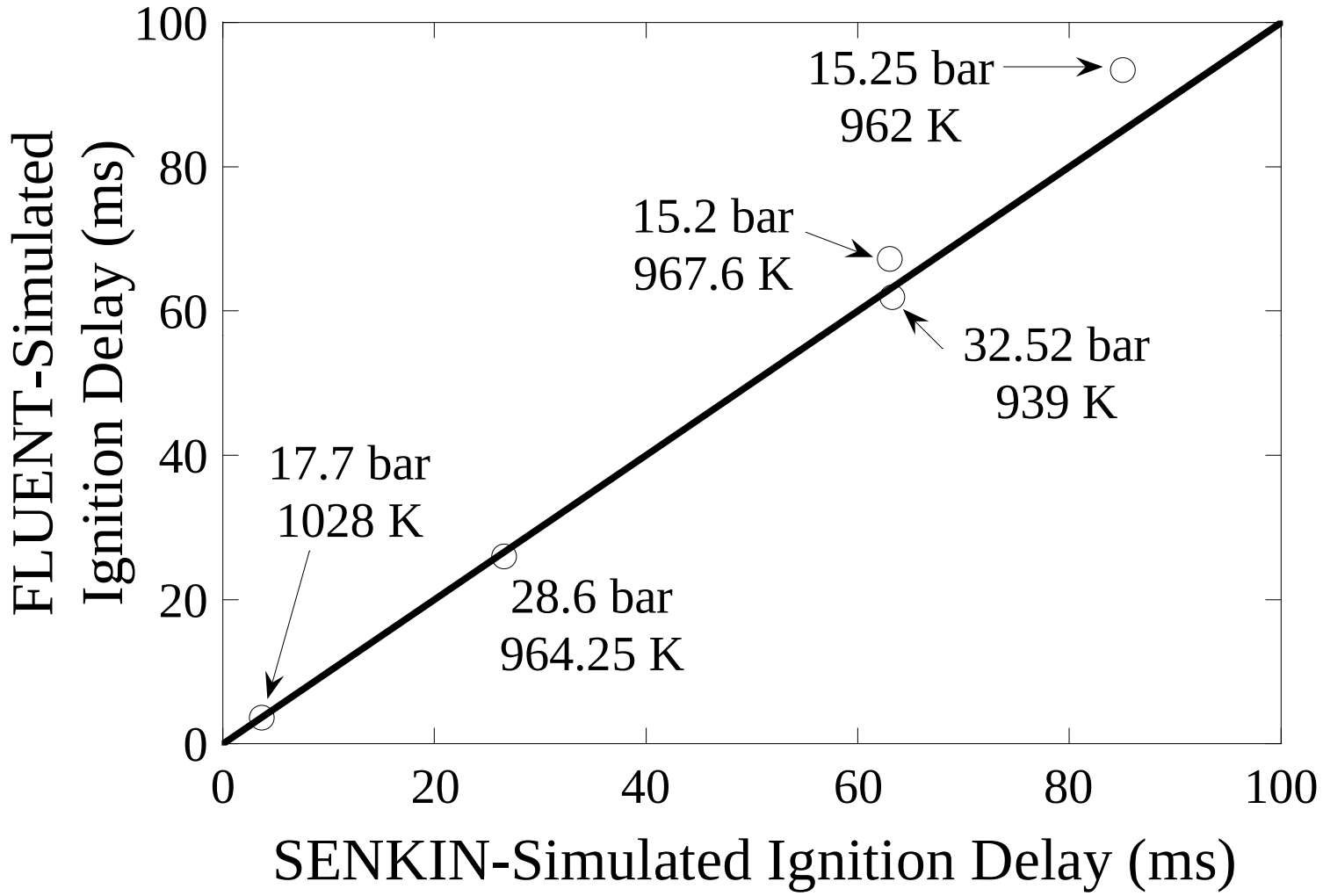




FLUENT (lines)

SENKIN with effective volume specification (circles)

FLUENT vs. SENKIN (2)



Modeling Remarks

- Important to assess RCM performance over the associated range of operating conditions in order to obtain reliable chemical kinetics data.
- For the H_2 cases investigated, zero-dimensional modeling along with the effective volume approach is acceptable in terms of mechanism validation for ignition delays.
  - Expected to be valid for the ignition cases of other hydrocarbons exhibiting single-stage ignition characteristics.
- Preliminary results on two-stage ignition modeling.

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Autoignition of Jet-A under High Pressure Conditions

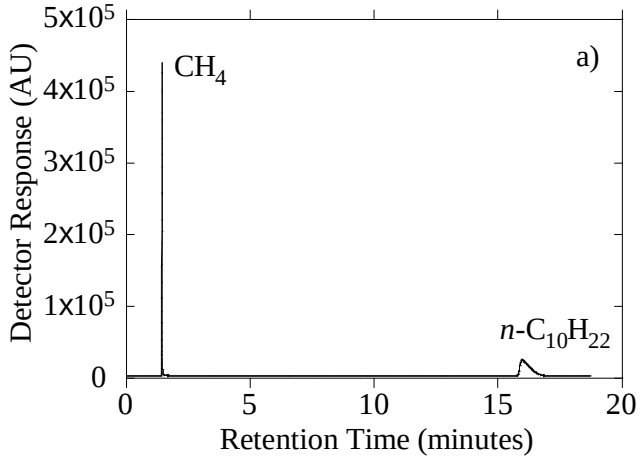

Mixture Preparation

- Homogeneous test mixture prepared in a *stirred*, *heated* stainless steel tank of known volume
  - Gaseous components in the test mixture are determined manometrically
  - Liquid fuel components are added on a gravimetric basis
- Add air/fuel under ambient temperature conditions
- Preheat temperature 97–134 ºC (below the boiling points of the liquid fuel components)
  - Continuous magnetic stirring
  - Soak time ~ 2 hours for complete vaporization of the liquid components



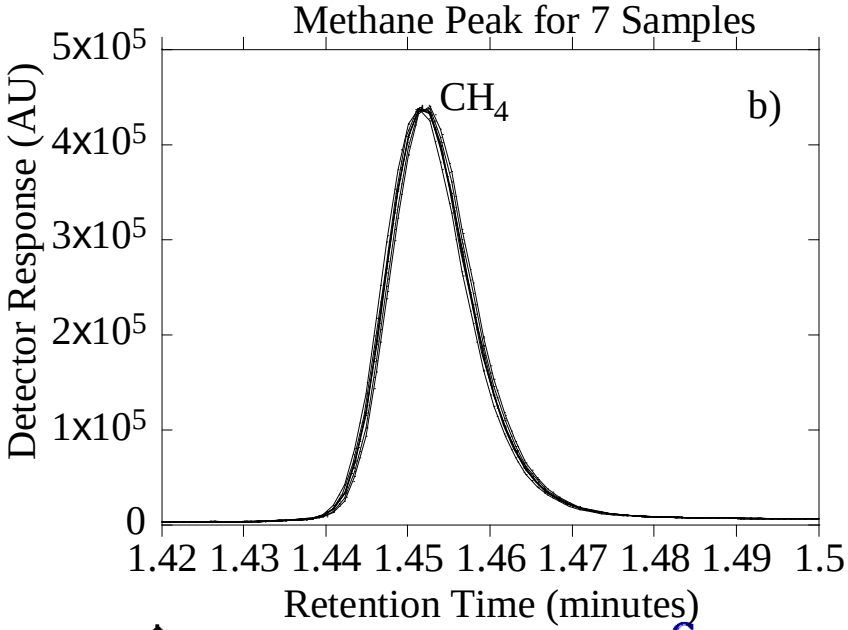


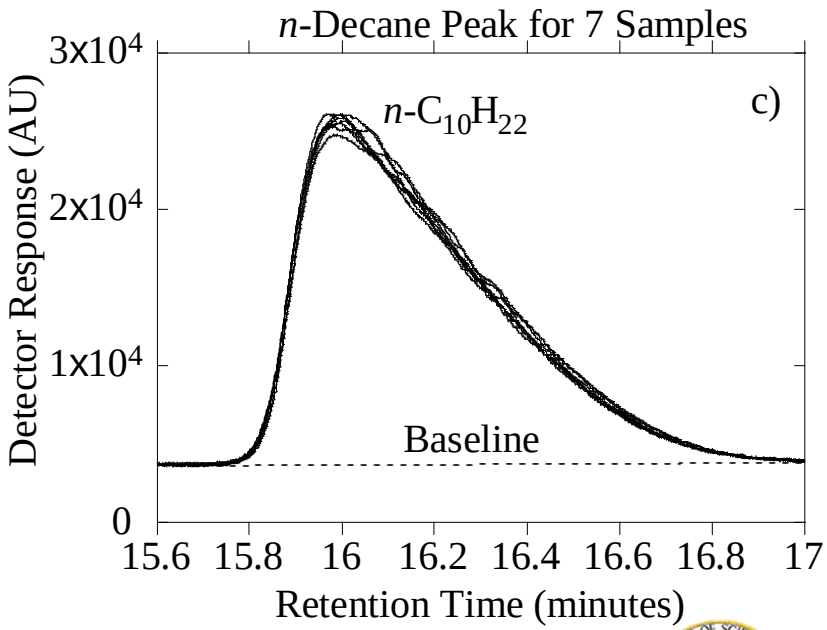
Composition Confirmation



Mixture Molar Percentages:

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





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Test Matrix

Mass Proportion								
Jet-A	***O_2***	***N_2***	***Ar***	***O/F***	***ϕ***	***7 bar***	***15 bar***	***30 bar***
5.00	33.21	61.79	0.00	19.00	0.51		**data available**	
7.14	32.46	60.40	0.00	13.00	0.75			
5.00	22.14	72.86	0.00	19.00	0.77	**to be presented**		
7.14	21.64	71.22	0.00	13.00	1.12			
5.00	11.07	83.93	0.00	19.00	1.53		**data available**	
7.14	10.82	82.03	0.00	13.00	2.24			
1.16	9.50	31.25	58.09	84.85	0.42	**to be presented**		

Jet-A (supplied by Tim Edwards): composite blend, labeled 04POSF4658

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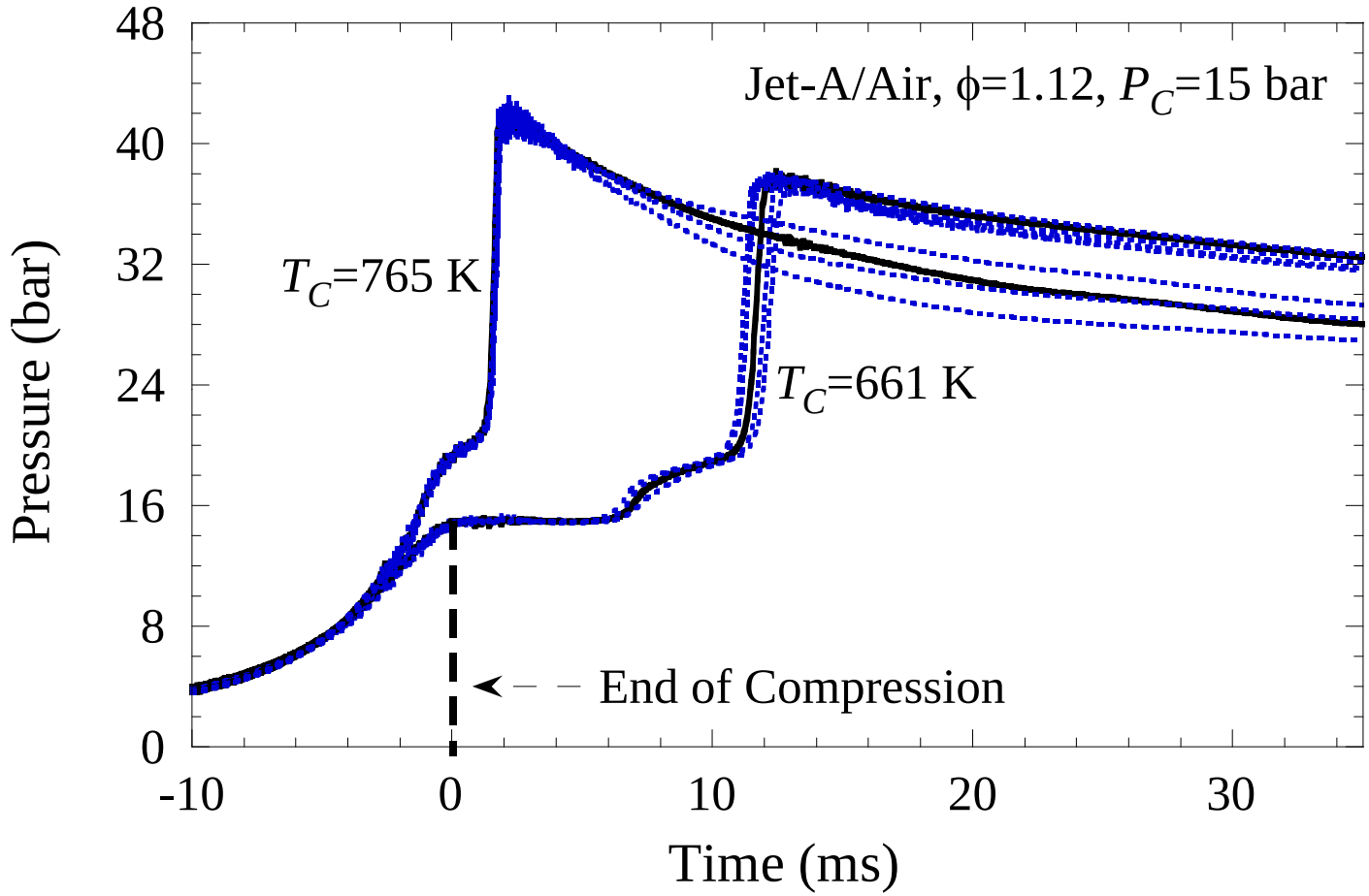
Jet-A Surrogate

COMPONENT	*Mass % in Fuel*	*Mole % in Fuel*
iso-Octane	5.00	6.47
Methyl Cyclohexane	5.00	7.53
m-Xylene	5.00	6.96
Tetradecane	15.00	11.18
Tetralin	5.00	5.59
Dodecane	20.00	17.36
Cyclo-Octane	5.00	6.59
n-Decane	15.00	15.58
Butyl Benzene	5.00	5.51
1,2,4,5-Tertamethylbenzene	5.00	5.51
1-Methylnaphthalene	5.00	5.20
Hexadecane	10.00	6.53

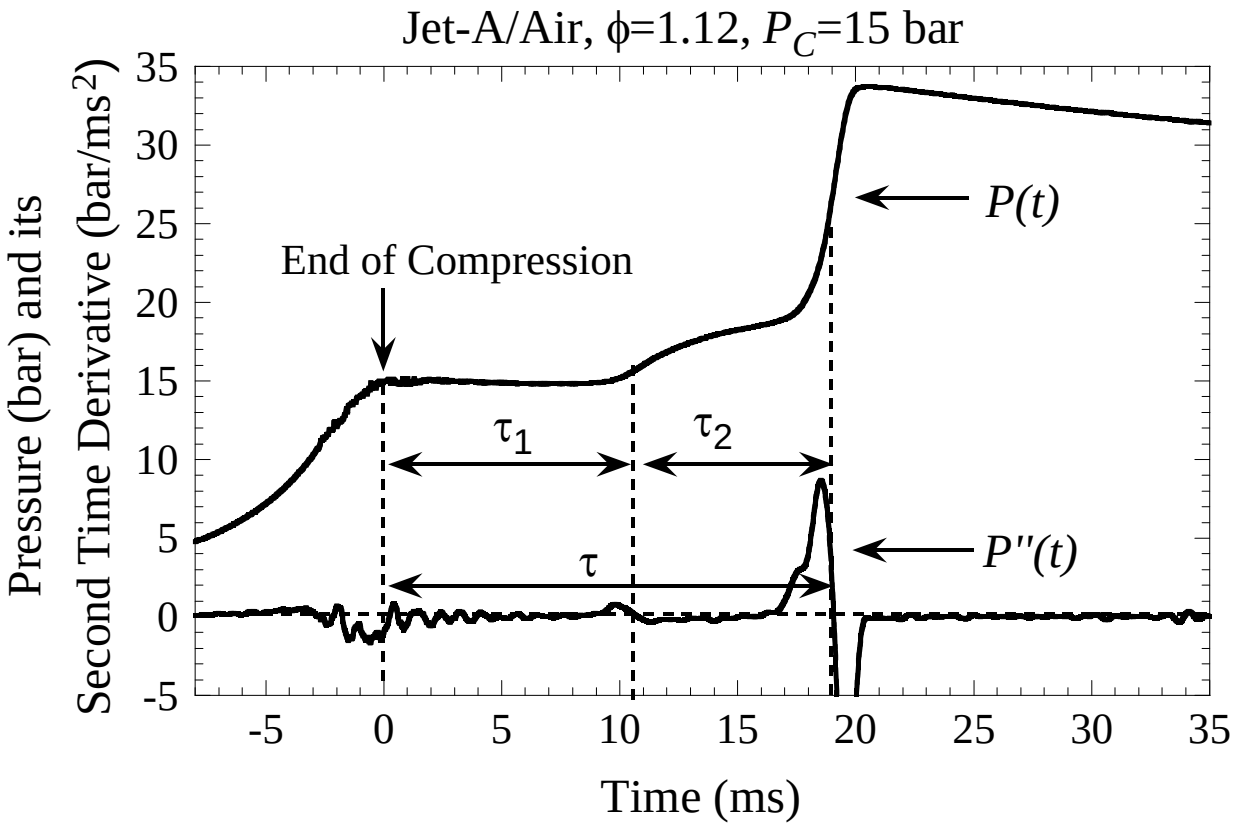
W.D. Schulz, ACS Petroleum Chemistry Division Preprints. 37(2), 383-392, 1991.

Experimental Reproducibility



- Representative trace from at least 4 concordant runs for determining ignition delay.

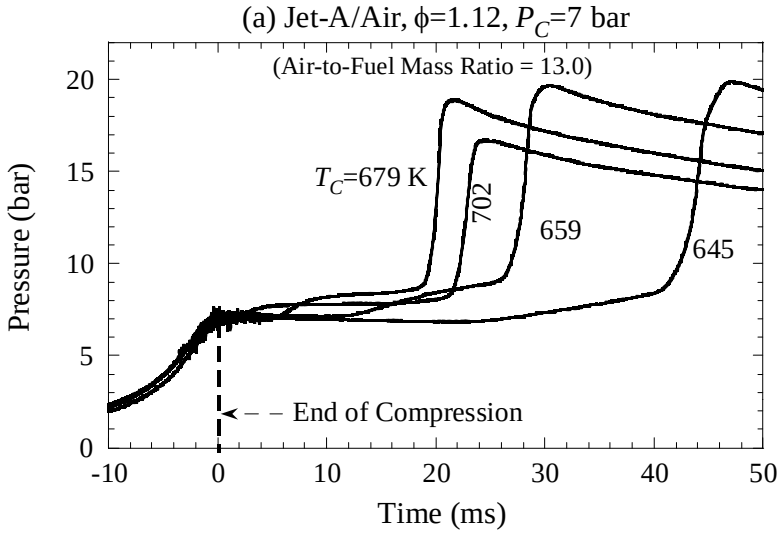
Definition of Ignition Delay

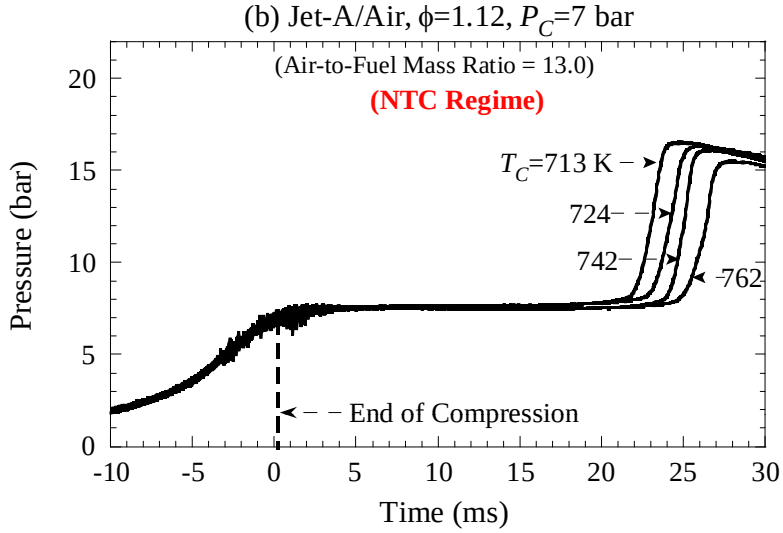


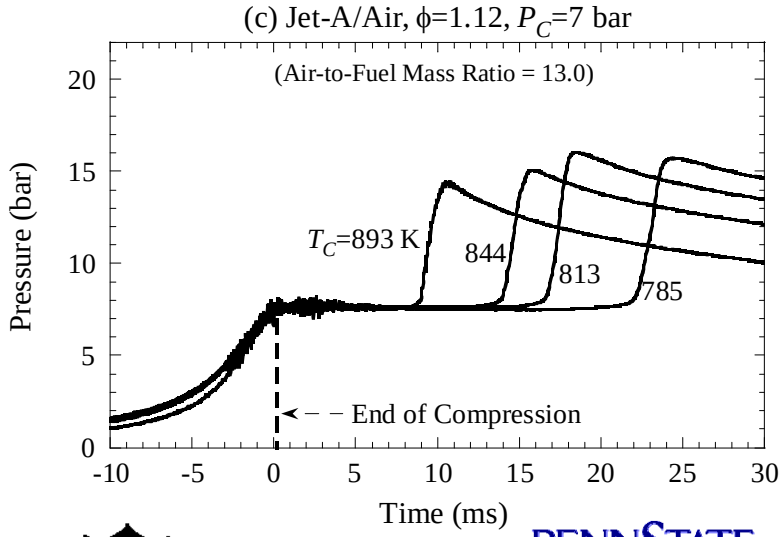
The location of inflection point in the pressure trace identifies the ignition time for both first and second stage.

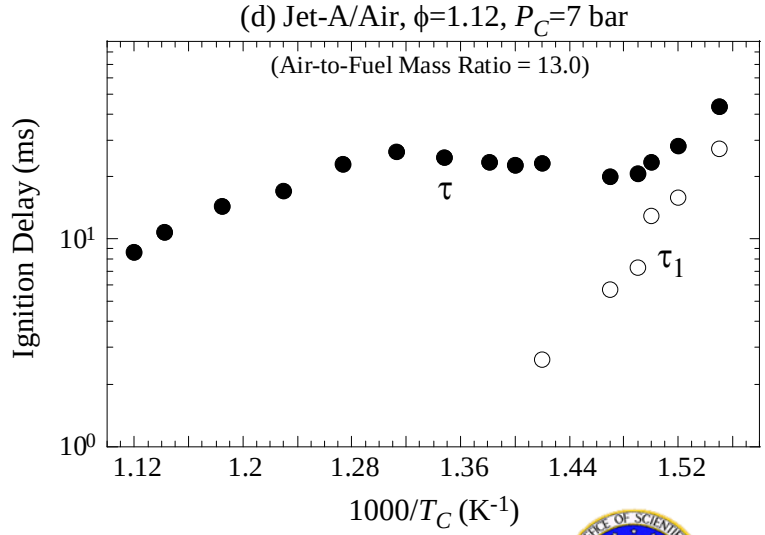
- τ_1 = First stage ignition delay
- τ_2 = Second stage ignition delay

Development of NTC Behavior

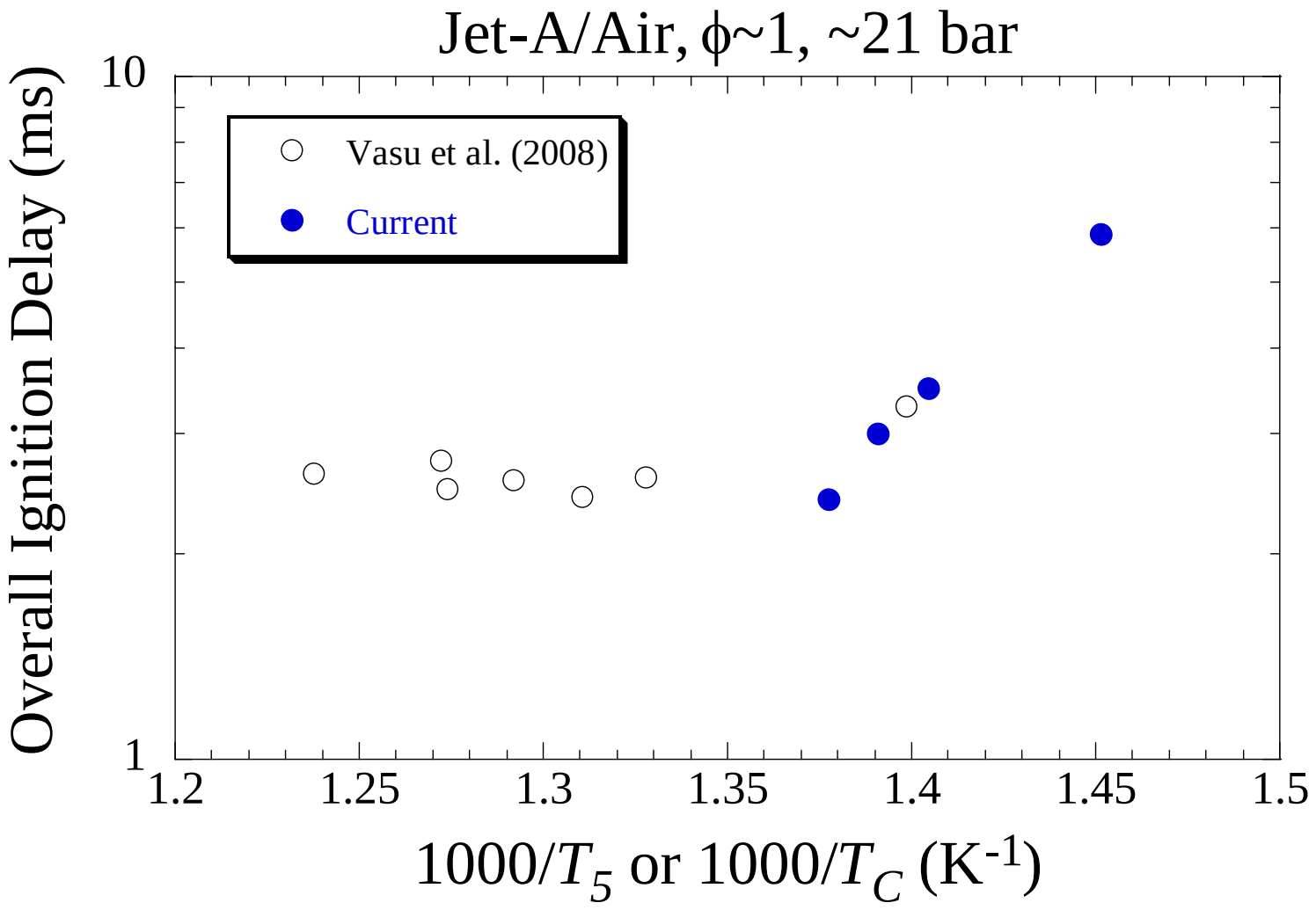




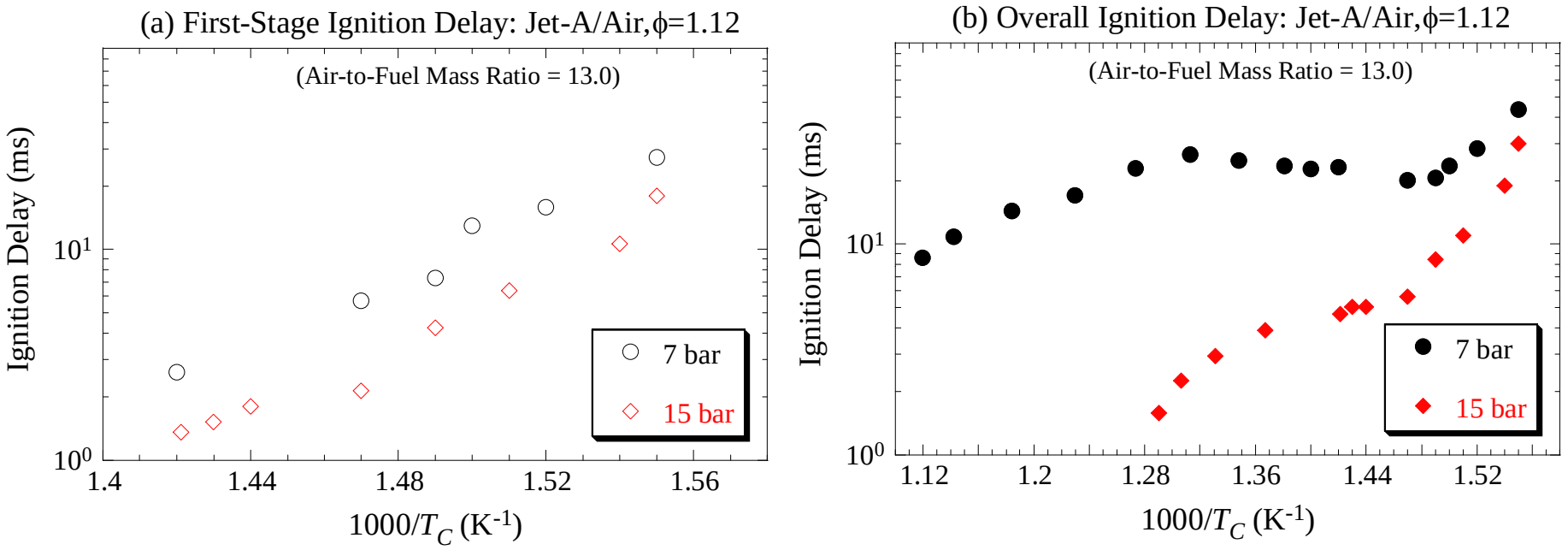




Ignition Delay Comparison

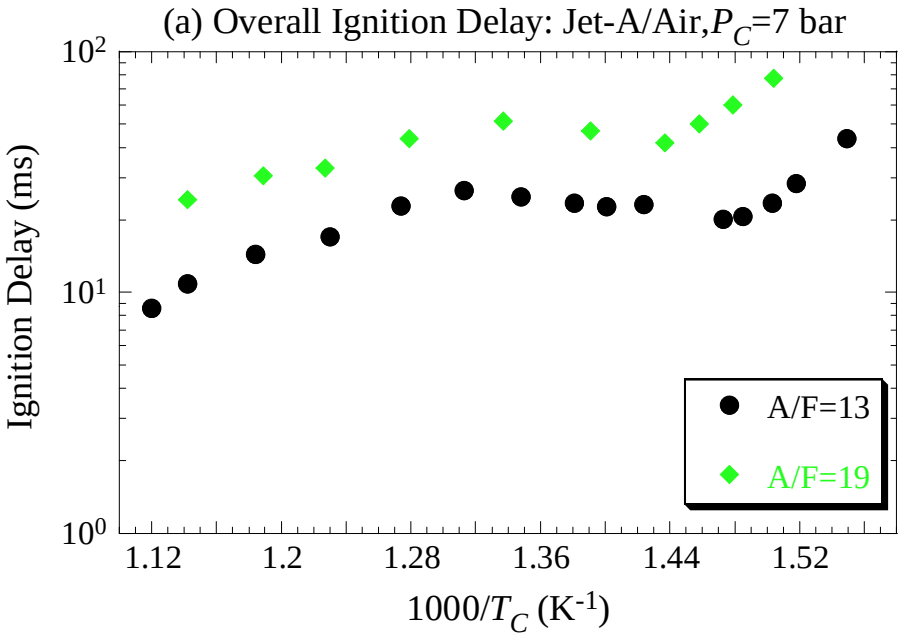


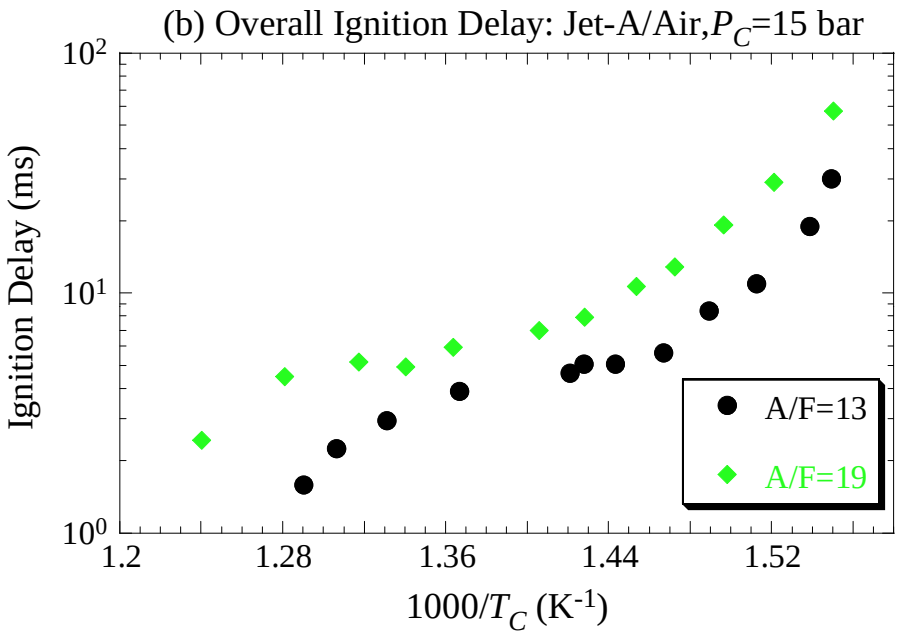
Effect of Pressure



- The first-stage ignition delay is relatively insensitive of pressure

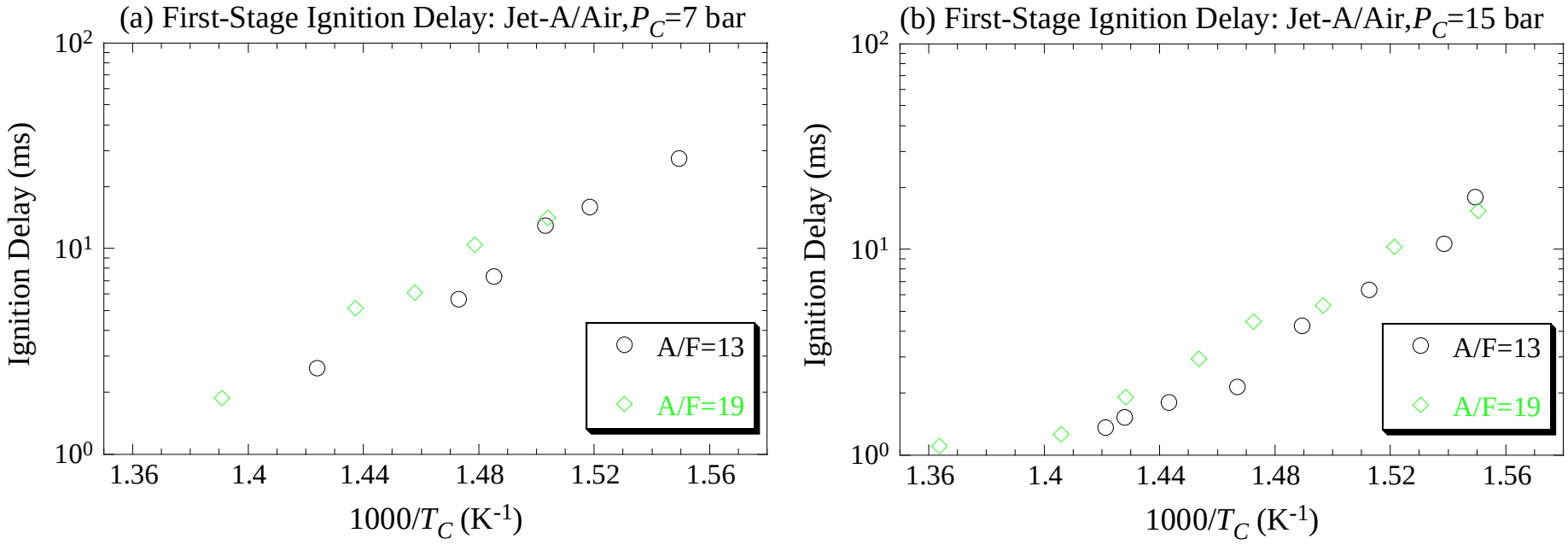
Effect of Equivalence Ratio (1)





- Equivalence ratio has a strong influence on the overall delay.
  - Effect is relatively stronger at lower pressures.

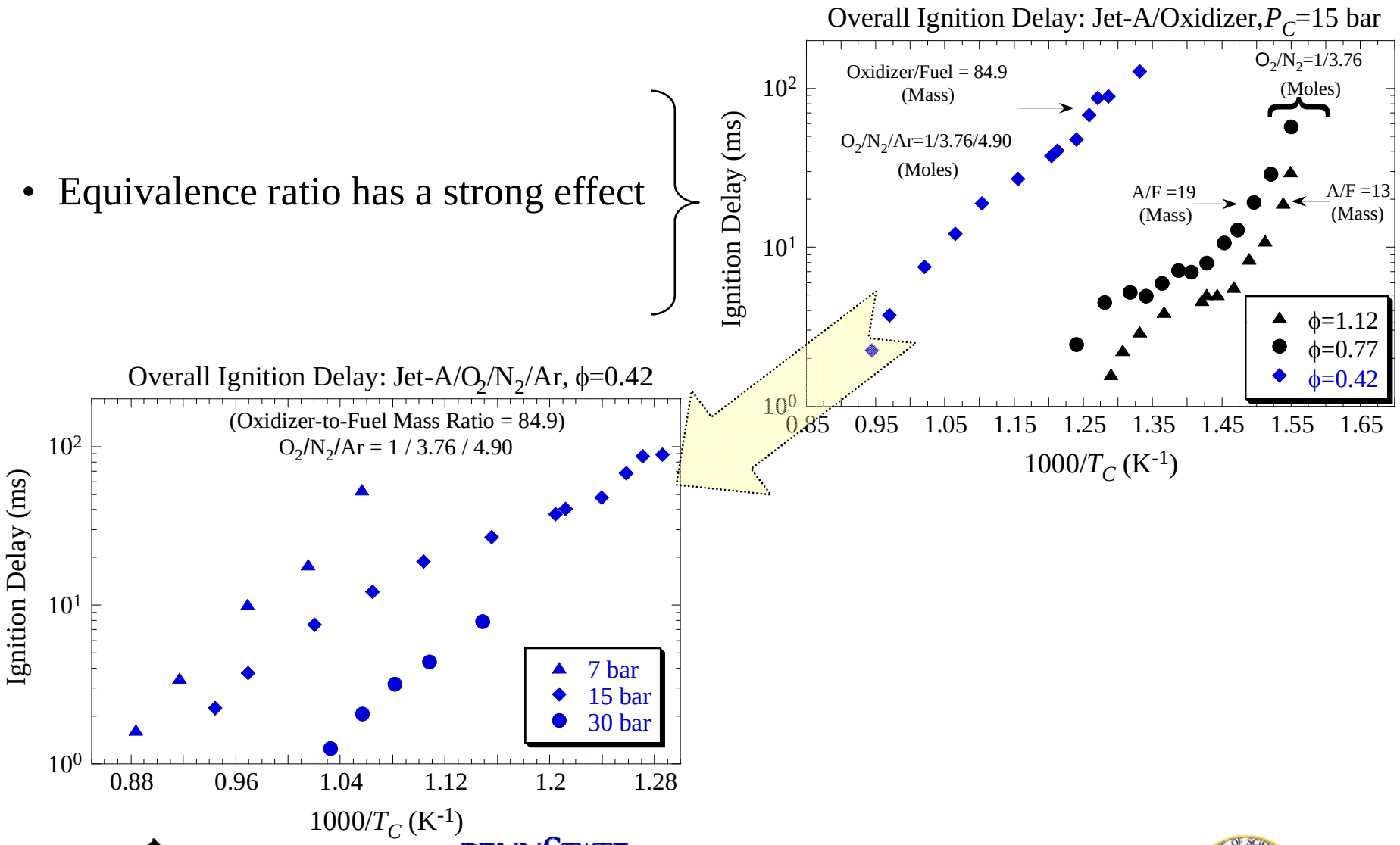
Effect of Equivalence Ratio (2)



- Equivalence ratio has relatively less influence on first-stage delay.
  - The influence of pressure is also limited.

Effects of ϕ and P_C

- Equivalence ratio has a strong effect



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Autoignition of Binary Fuel Blends

Raw pressure traces and heat loss parameters are available at
http://www.mae.case.edu/facilities/cdl/projects/rapidcomp/rapiddatabase

Background

- Hydrocarbon classes differ vastly in reactivity and ignition chemistry.
- It is important to understand the nature of interactions in blended fuels.
- Obtain experimental data for autoignition of neat components and blends under well characterized conditions
  - *iso*-octane *(Alkane)*
  - diisobutylene-1 *(Alkene)*
  - toluene *(Aromatic)*
  - toluene + DIB-1
  - toluene + *iso*-octane

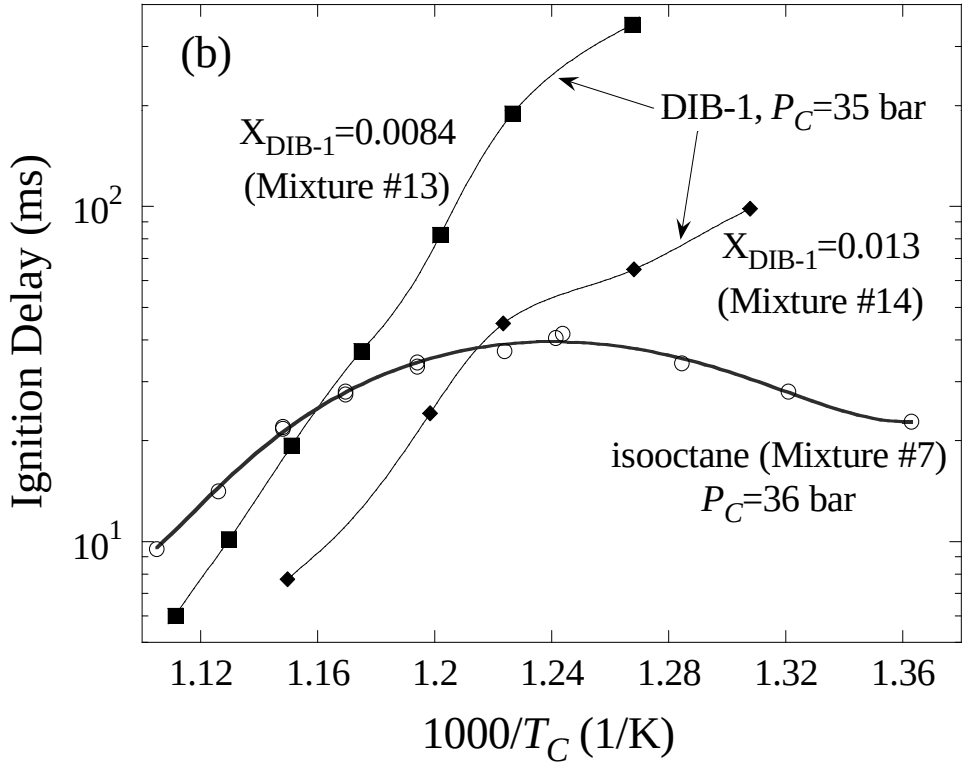
Mixture Composition

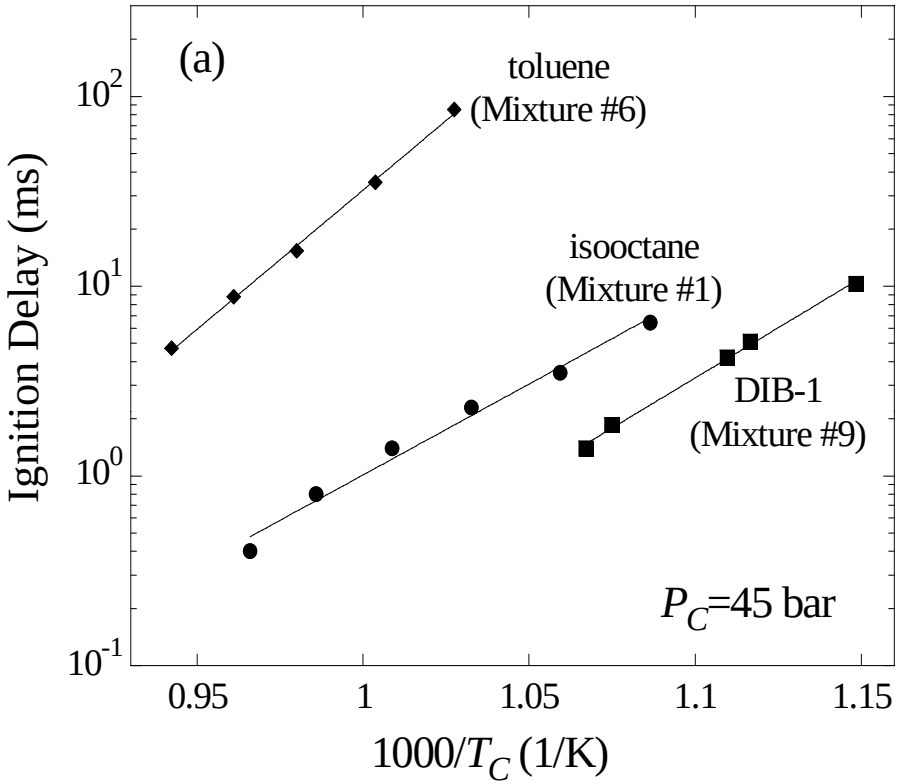
Mixture #	R_I	*iso*-octane	toluene	O_2	N_2	Ar
1	1	0.5	0	8.333	0.000	50.600
2	0.75	0.375	0.125	7.750	2.400	48.784
3	0.5	0.25	0.25	7.166	4.667	47.100
4	0.25	0.125	0.375	6.583	6.990	45.360
5	0.05	0.025	0.475	6.117	8.900	43.917
6	0	0	0.5	6.000	9.323	43.610
7	1	0.5	0	8.333	16.850	33.750
8	0.75	0.375	0.125	7.750	19.183	32.000

Mixture #	R_{DIB-1}	DIB-1	toluene	O_2	N_2	Ar
9	1	0.5	0	8.000	1.343	49.590
10	0.5	0.25	0.25	7.000	5.423	46.510
11	0.05	0.025	0.475	6.100	9.063	43.770
12	0	0	0.5	6.000	9.323	43.610
13	1	0.5	0	8.000	18.300	32.633
14	1	1	0	16.000	7.500	52.660

- R_I (R_{DIB}) is the mole fraction of isooctane in the combined toluene + *iso*-octane (toluene+DIB-1) fuel mixture.
- Total fuel mole fraction is kept constant at 0.0084.
- Mixtures for blends have the same specific heat ratio.

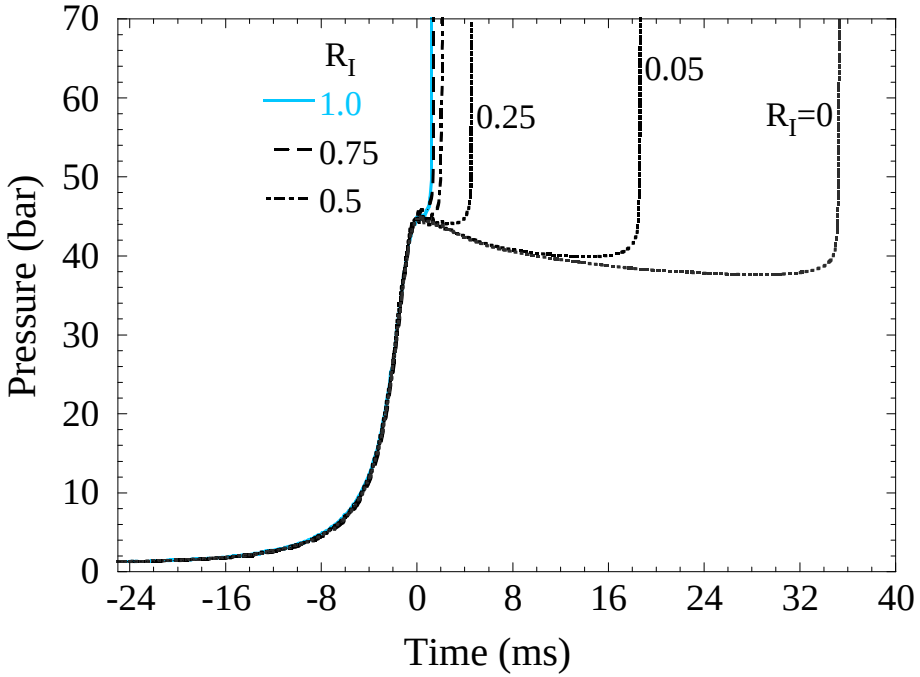
Autoigniton of Neat Components

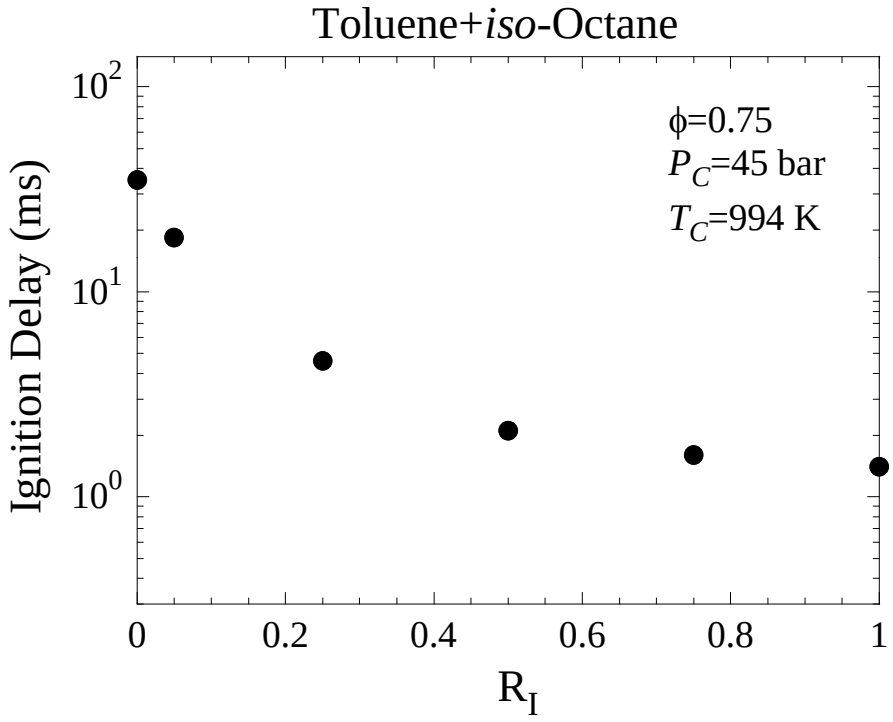




Autoigniton of *iso*-Octane/Toluene Blends

Combined Fuel Mole Fraction=0.0084, Equivalence Ratio=0.75, P_0=930 Torr,
Conditions at TDC: T_C=992–996 K and P_C=45 bar



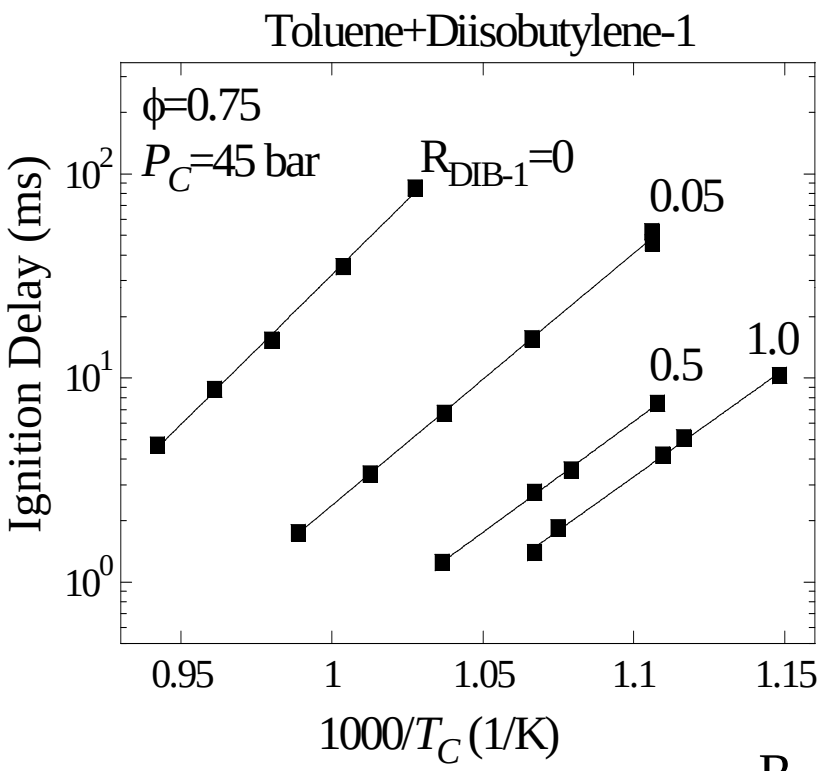


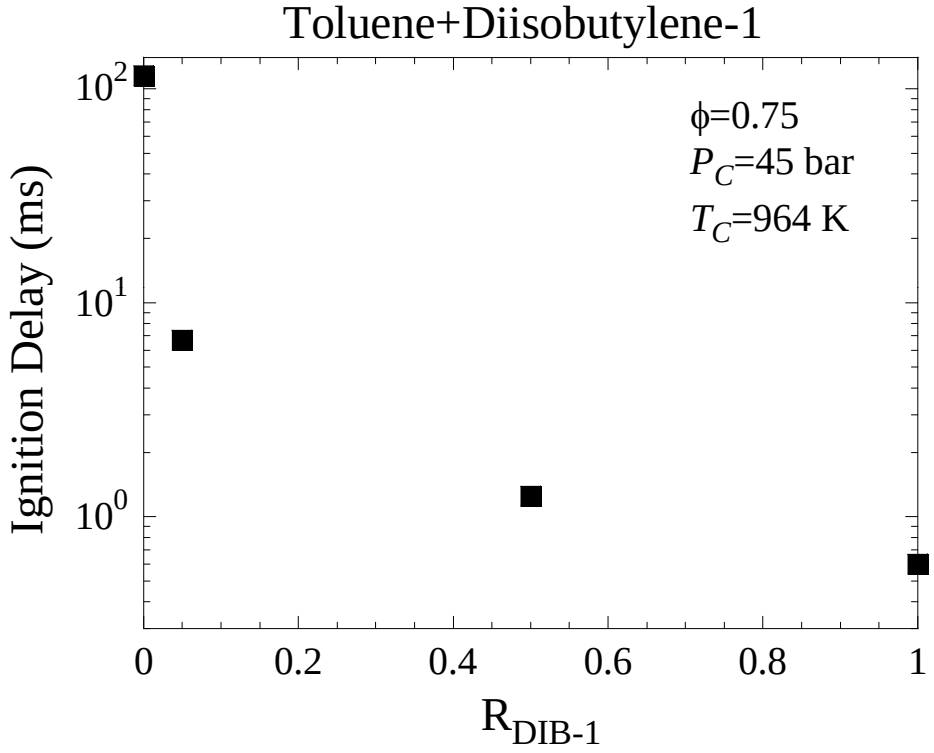
$$R_I = F_I/(F_I+F_T)$$

F_I and F_T are respectively the mole fractions of *iso*-octane and toluene in the fuel mixture.

Autoigniton of DIB-1/Toluene Blends

Combined Fuel Mole Fraction=0.0084, Equivalence Ratio=0.75 and P_C=45 bar





$R_{DIB}=F_{DIB}/(F_{DIB}+F_T)$

F_{DIB} and F_T are respectively the mole fractions of DIB-1 and toluene in the fuel mixture.

Discussion

- The presence of a double bond and its position can significantly alter autoignition characteristics.
  - Overall kinetic behavior of alkenes is a result of competition between the addition reactions to a double bond and the reactions through hydrogen abstraction of alkyl chain.
  - Less pronounced features of NTC behavior for DIB-1 imply that the addition reactions at the double bond dominate over the peroxidation reactions of the alkenyl chain.
- Nonlinear sensitization of toluene by *iso*-octane or DIB-1 similar to that of methane by ethane or propane (Westbrook 1979, 1983).
  - Radicals produced by H atom abstraction from either toluene or methane do not have a decomposition reaction to produce chain branching agents.
  - Early radical generation by small addition of more reactive fuel component accelerates the ignition of the less reactive fuel component.

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Laminar Flame Speeds of Jet-A

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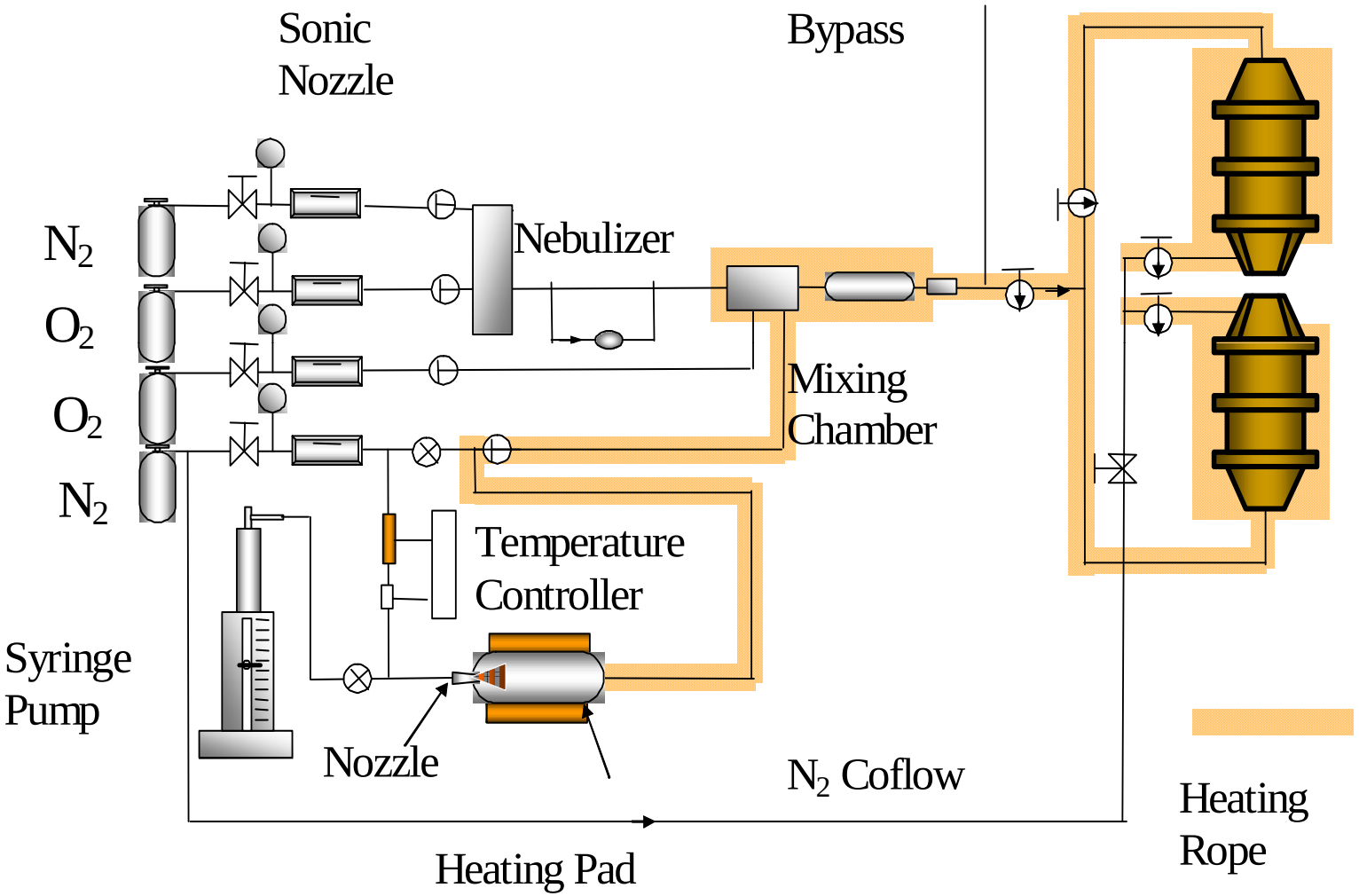
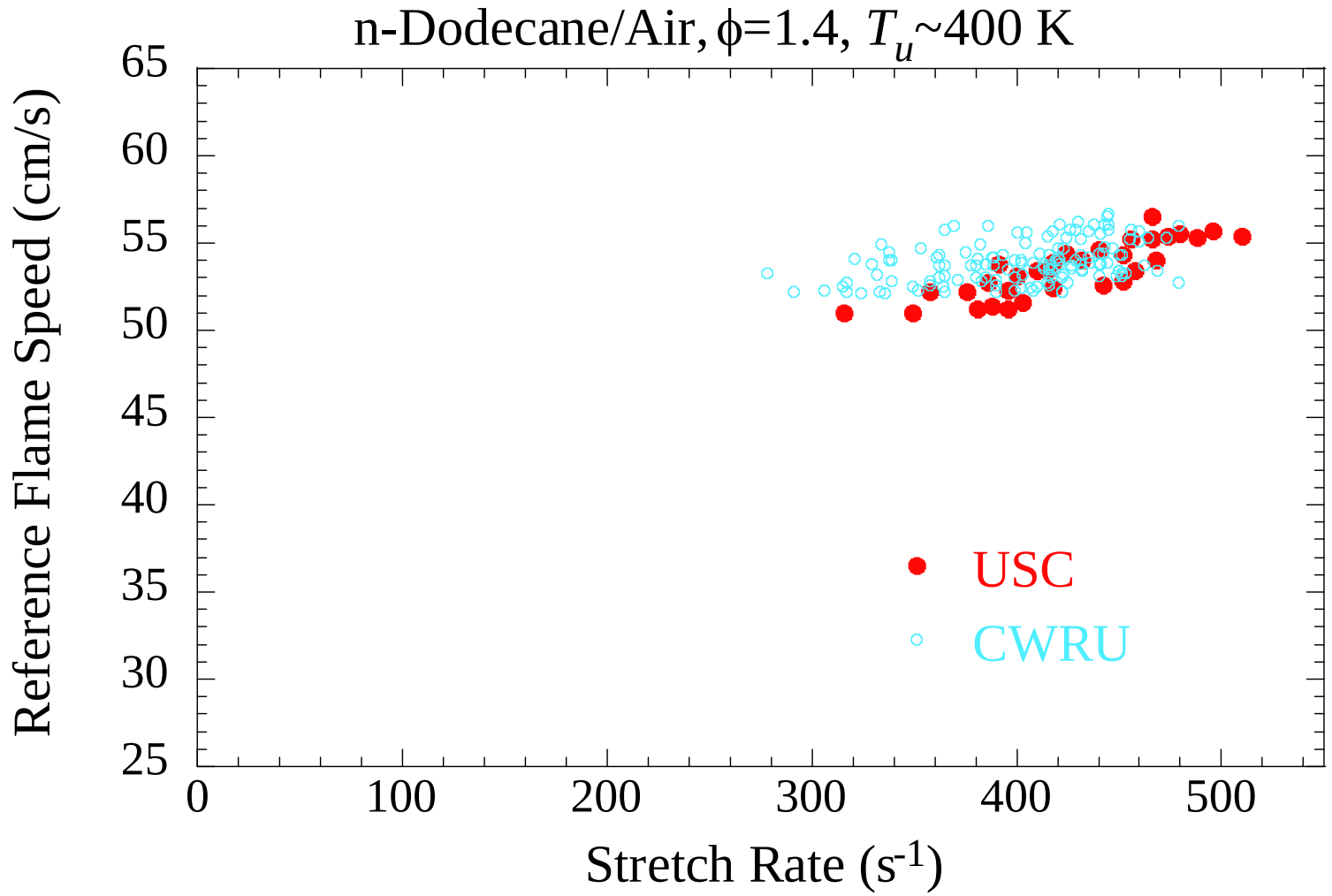
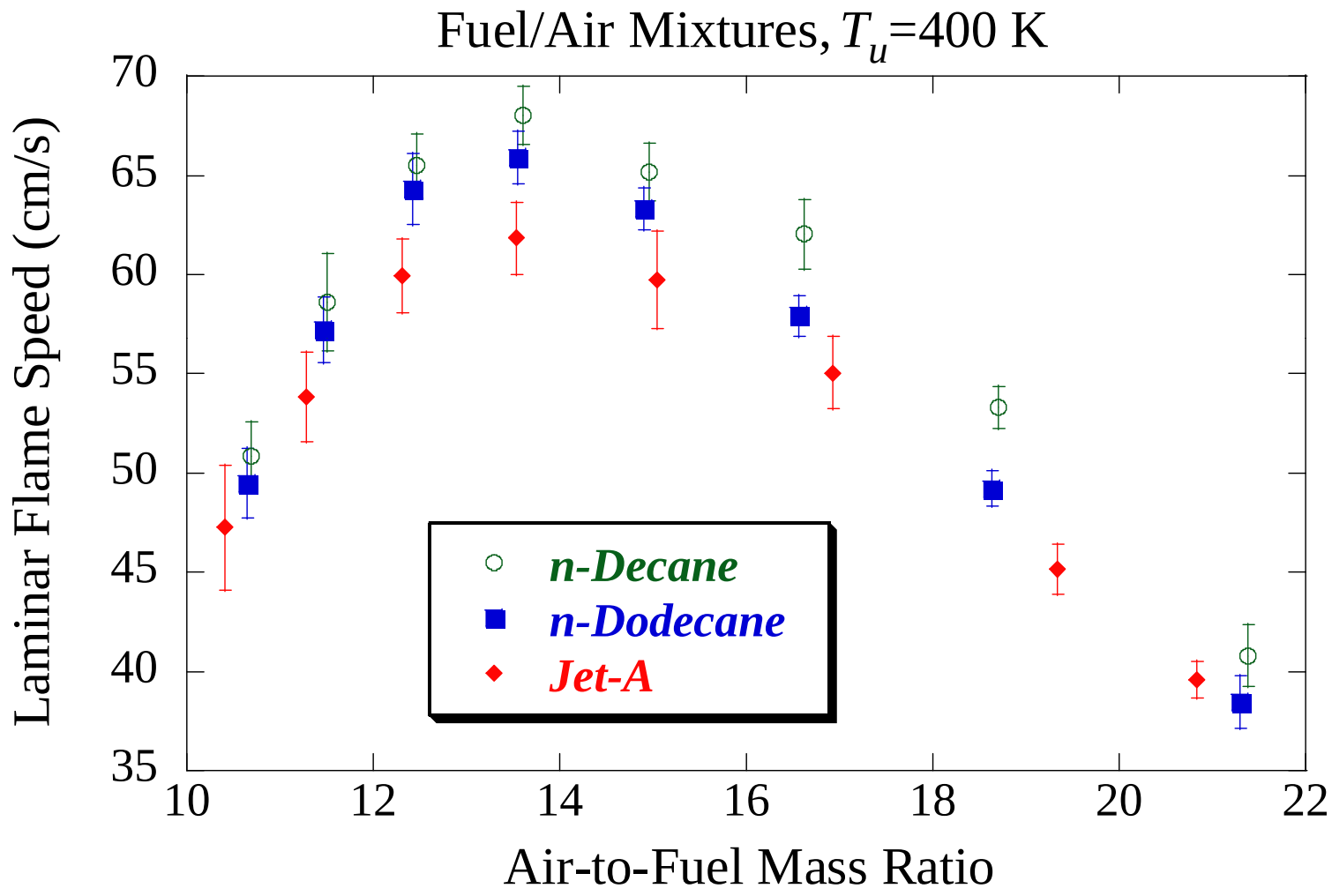
Counterflow Twin-Flame Configuration



Extrapolation



Laminar Flame Speed Results



Future Work

- Acquire autoignition data of neat surrogate components.
  - high priority: *n*-dodecane.
- Acquire autoignition data of binary fuel blends.
  - fuel blends with relatively high Cetane numbers.
  - high priority: *n*-dodecane + MCH; *n*-decane + *iso*-octane.
- Conduct extinction stretch rate measurements of real jet fuels – Jet-A and S-8.
- Complete the setup of a new high-pressure counterflow burner system for flame measurements.

Acknowledgements

- Tim Edwards of AFRL for jet fuel supplies.
- Fred Dryer and Marcos Chaos of Princeton as well as Hai Wang and Xiaoqing You of USC for thermodynamic property calculations.
- CWRU participants –

  Post-Doctoral Research Associates: Kamal Kumar and Gaurav Mittal

  Graduate Students: Bryan Weber and Xin Hui