An Experimental and Chemical Kinetics Study of the Combustion of Syngas and High Hydrogen Content Fuels

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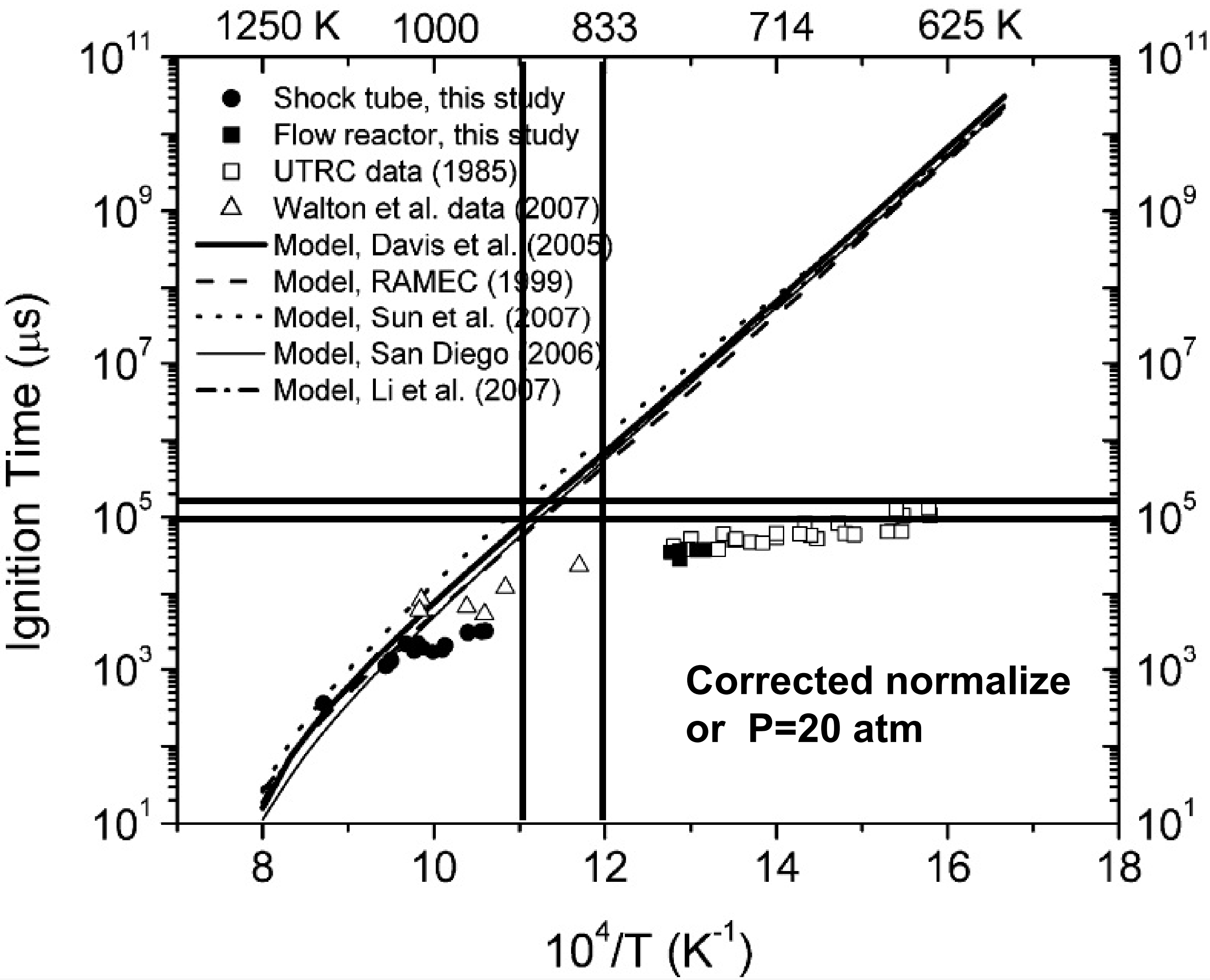
High-Pressure High-Temperature Flow Reactor Studies

Experimental Apparatus for Measuring Ignition Delay

- Shock Tubes
- **Flow Reactors**
  - Most like a premixer in a gas turbine
- Rapid Compression Machines
- Constant volume bombs

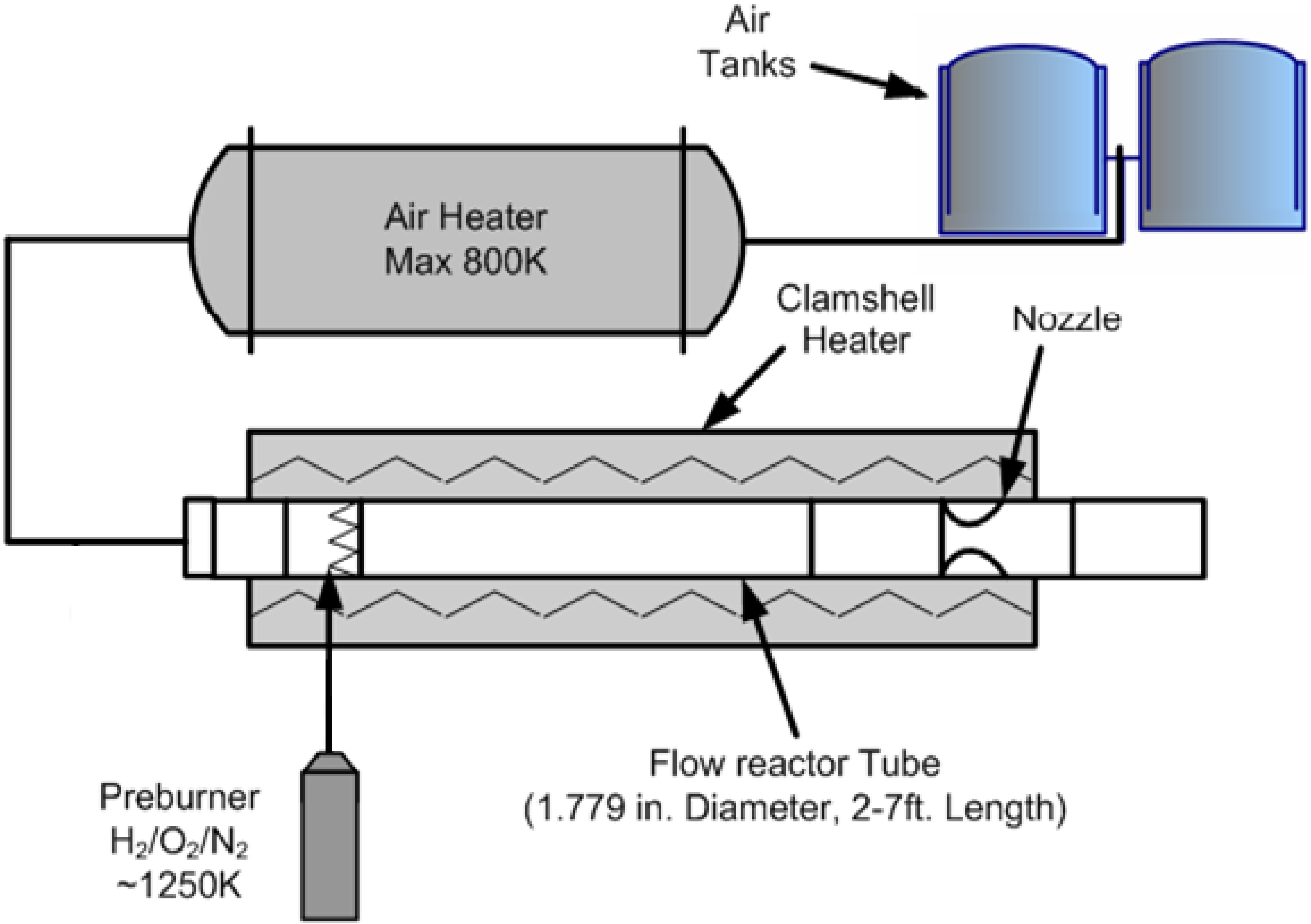
- Literature



Petersen 2007 "New syngas/air ignition data at lower temperature and elevated pressure and comparison to current kinetics models"

Current Experimental Apparatus

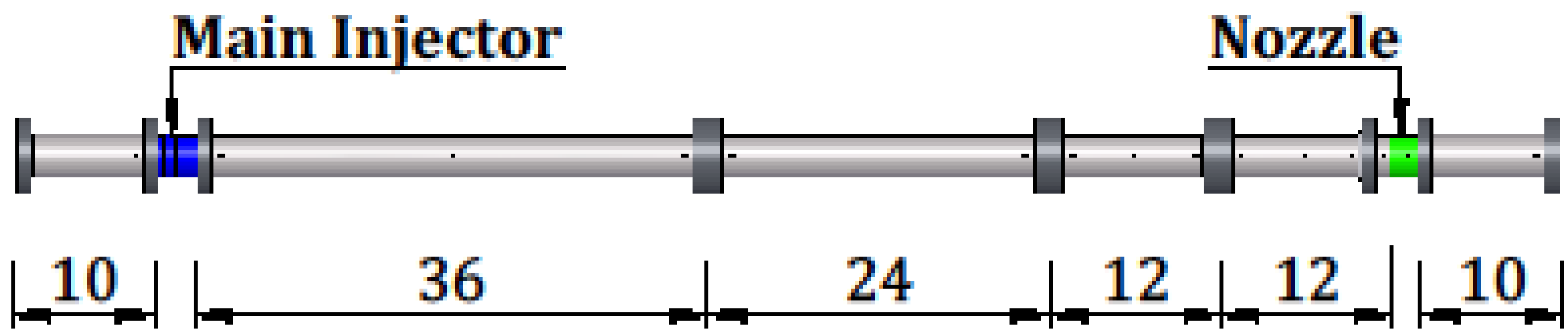
- Flow reactor
- Preburner
- Instrumentation
- Injector
  - Radial
  - Axial


Air
Tanks
Air Heater
Max 800K
Clamshell
Heater
Nozzle
Flow reactor Tube
(1.779 in. Diameter, 2-7ft. Length)
Preburner
$H_2/O_2/N_2$
~1250K

Controlled Variables

- Residence time
  - nozzle
- Composition
  - Fuel flow rate and air flow rate
- Pressure
  - Total mass flow rate
- Temperature
  - Air heater
  - preburner

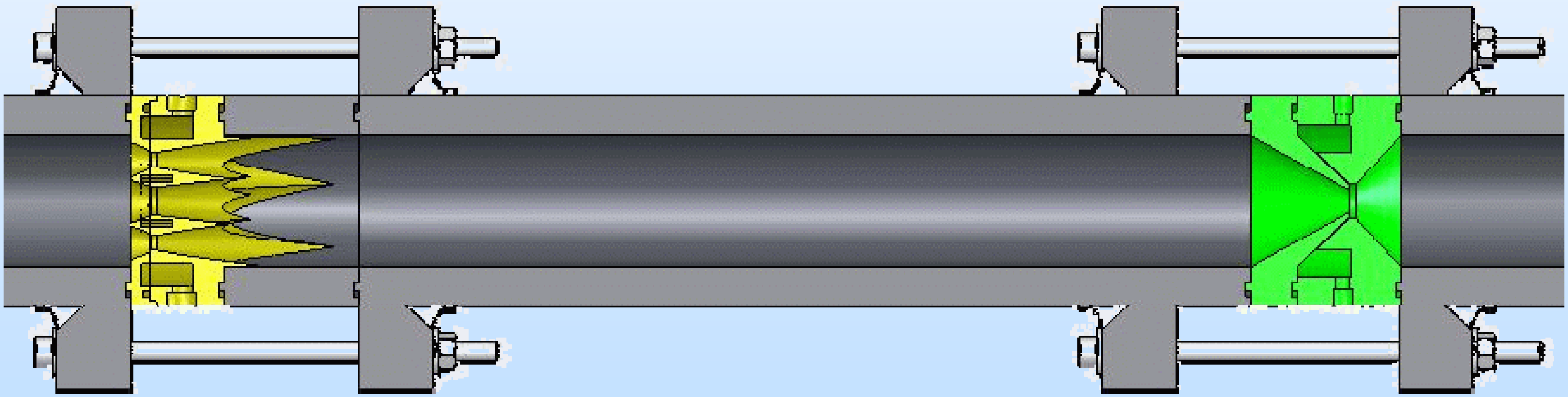
Flow Reactor Test Section



Inner Diameter: 1.779 in
Cold Test Section Length: 84.3 in
Reynolds Number: ~100,000
Total mass flow rate: ~0.2 lbm/s

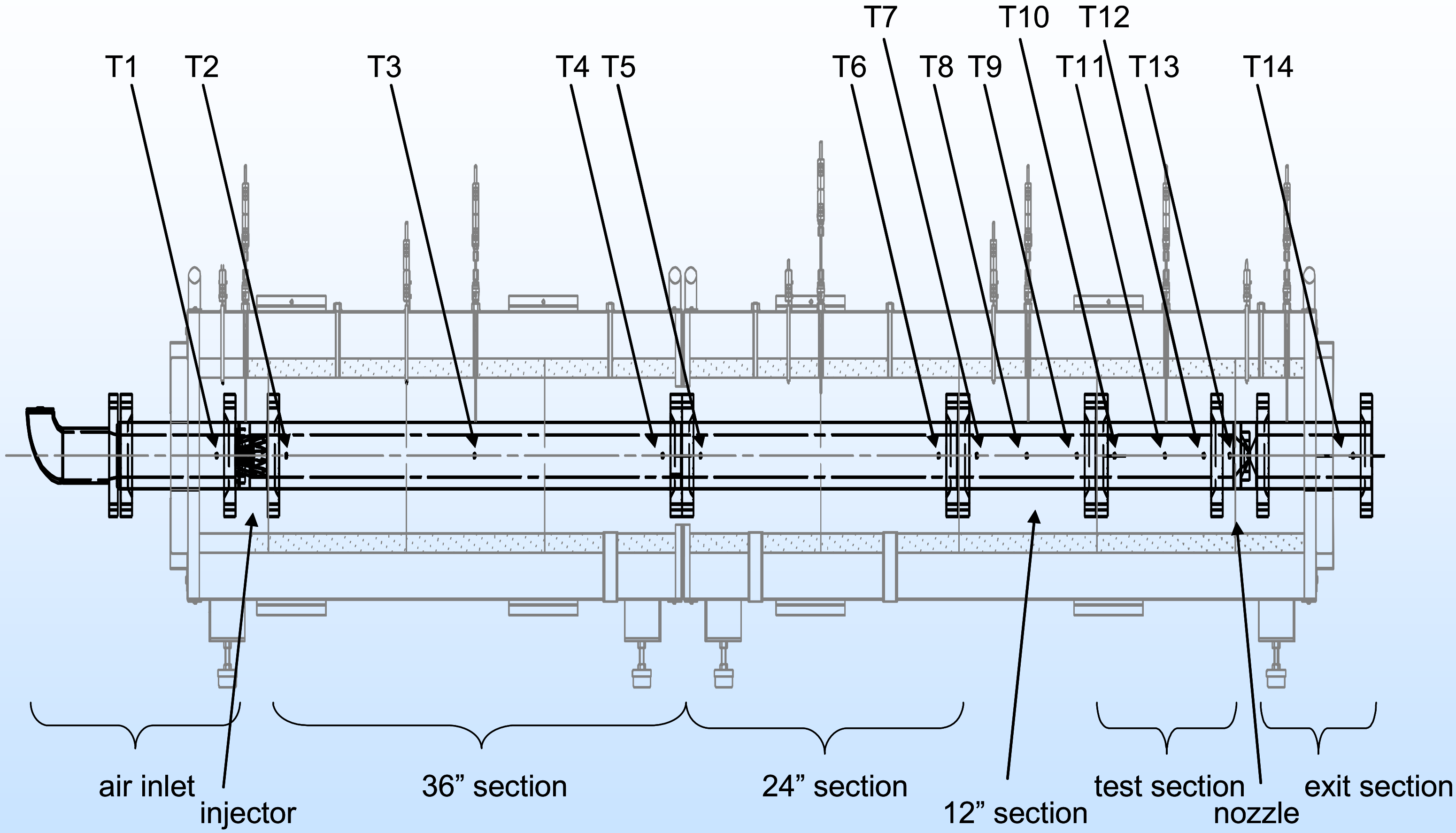
Flow Reactor Design

- Instrumented test section before nozzle
- Sonic nozzle and water quenching to isolate test section from afterburner
- Injector design
  - Venturi design for rapid mixing with minimal recirculation zones
  - 7 venturis with 3 fuel injection holes just upstream of throat
- Re# (Max) = 5×10^{5} to 3×10^{6}



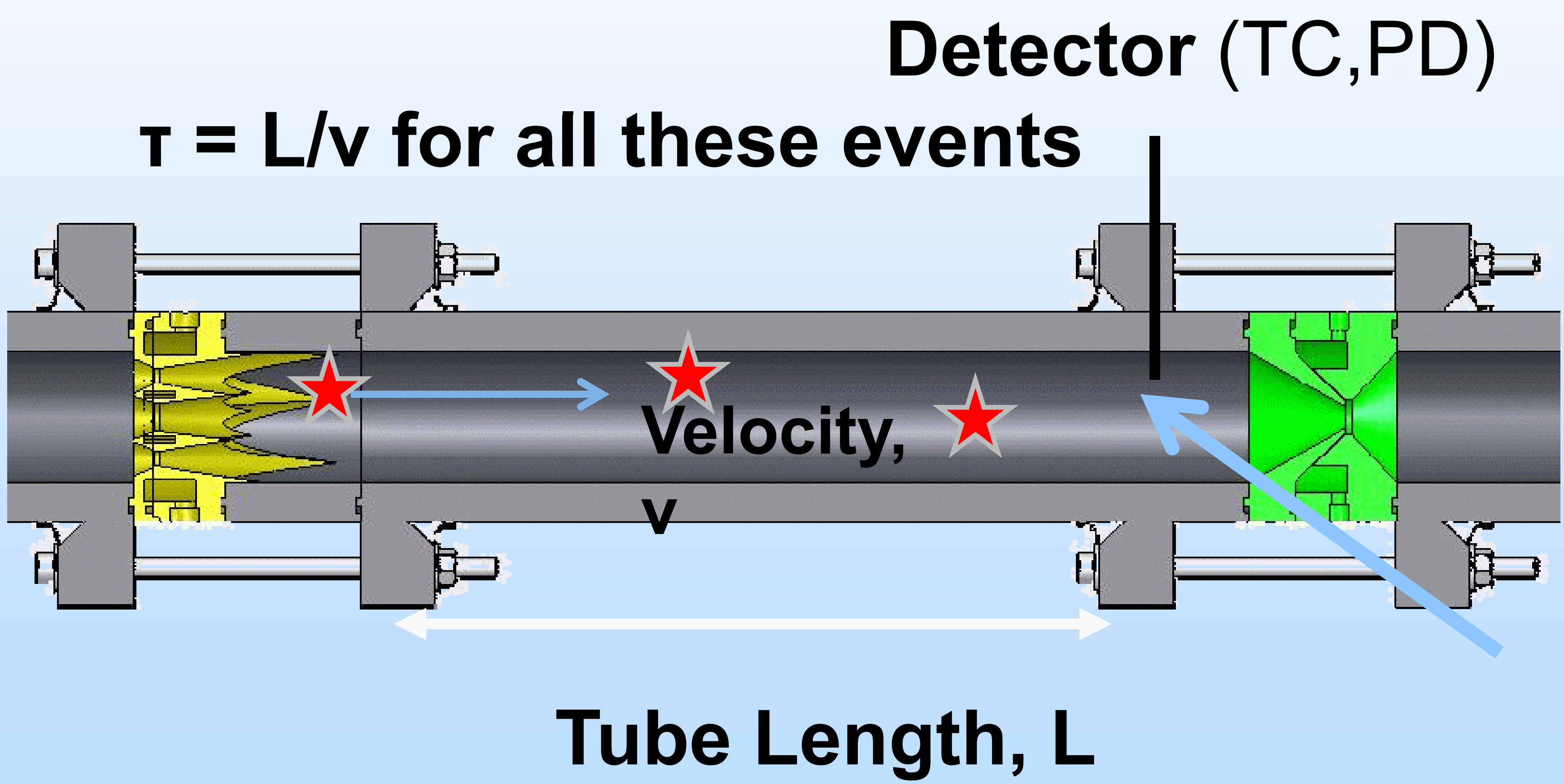
Thermocouple Array

Wall thermocouple positions



Array of thermocouples located 0.2 inches from the wall that provides for detection of the autoignition event in the flow reactor tube

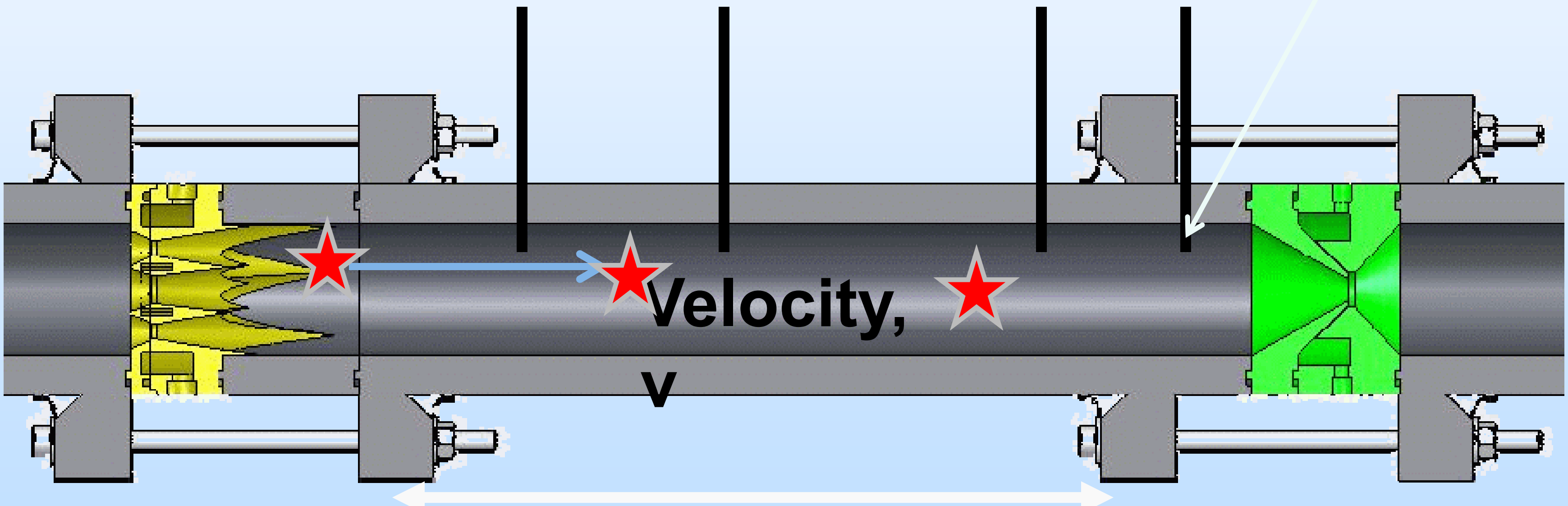
Detection of an Ignition Event

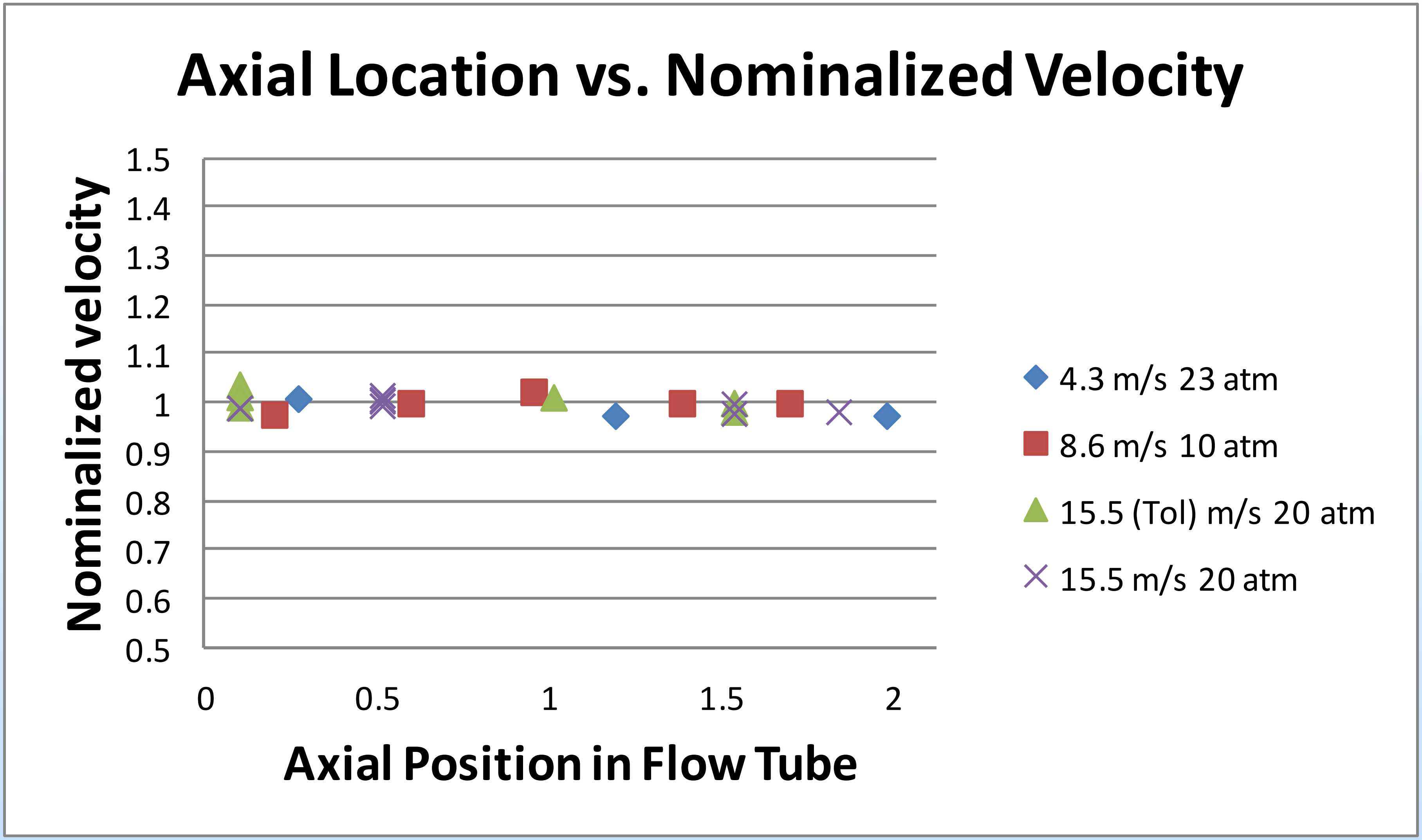


Detection of an Ignition Event

$\tau = L_i$ /v for these events where I = 1,2, and 3

Multiple Detectors (TC,PD)





Axial Location vs. Nominalized Velocity
Nominalized velocity
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0
0.5
1
1.5
2
Axial Position in Flow Tube
4.3 m/s 23 atm
8.6 m/s 10 atm
15.5 (Tol) m/s 20 atm
15.5 m/s 20 atm

Study of H_2-O_2 Autoignition by Beerer and McDonnel

	Pressure (atm)	Equivalence ratio	Ignition Temperature (K)	Residence Time, τ (ms)	Flow Velocity,v (m/s)
1	6.4	0.31	778	451	8.4
2	5.8	0.37	780	178	21.3

$\tau_1/\tau_2 = 2.53$ $\quad$ $v_2/v_1 = 2.54$

D. J. Beerer & V. G. McDonell J. of Engr. Gas Turbine and Power (2008)

Iso-0ctane Autoignition Study
Dr. Michelle Christensen 2012

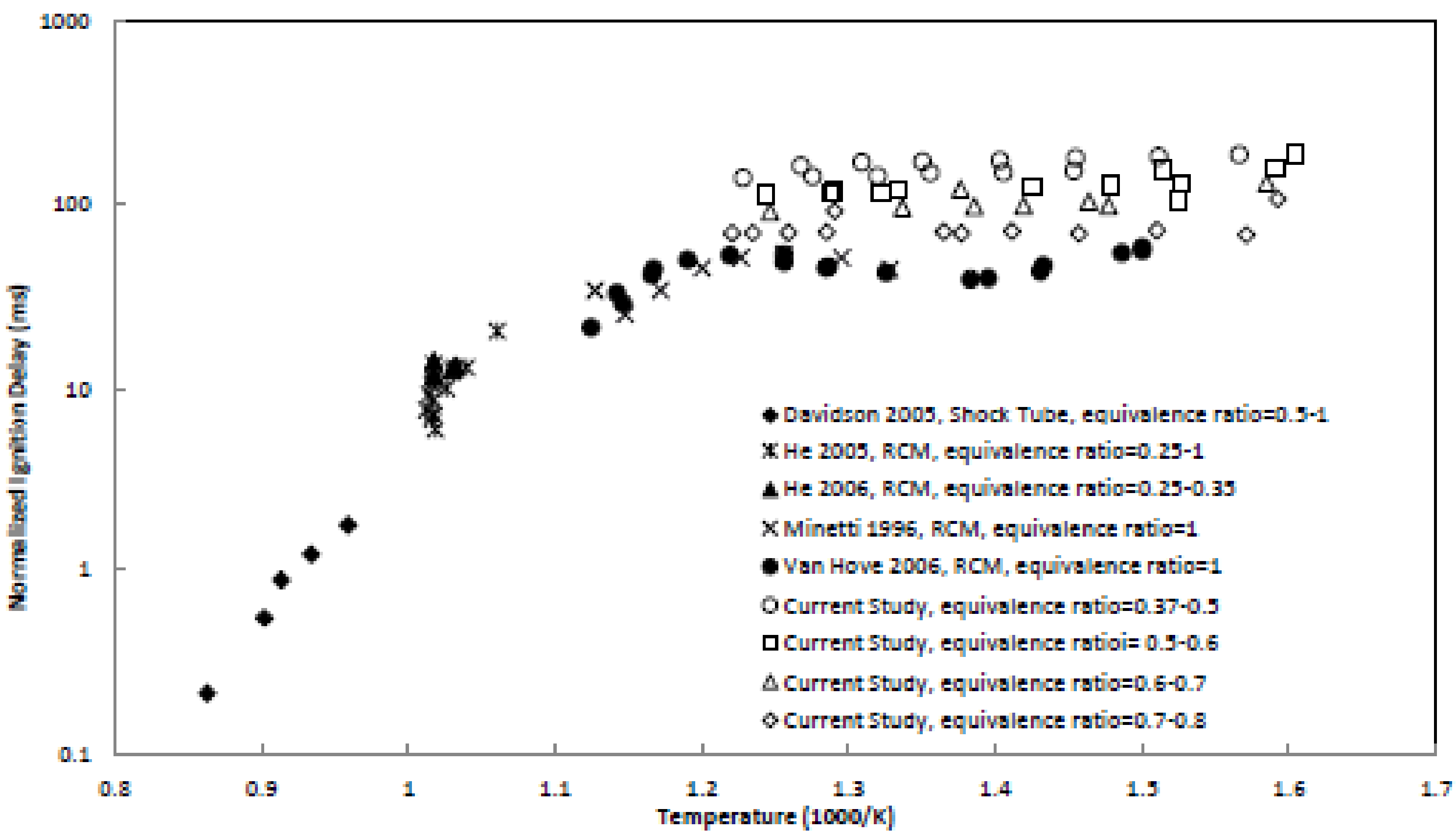


Figure 4-2. Iso-octane autoignition results from shock tubes [51], rapid compression machines [21, 66, 73, 74], and the current flow reactor studies. All data points are from 14-16 atm and have been normalized to 15 atm

Iso-0ctane Autoignition Study Dr. Michelle Christensen 2012

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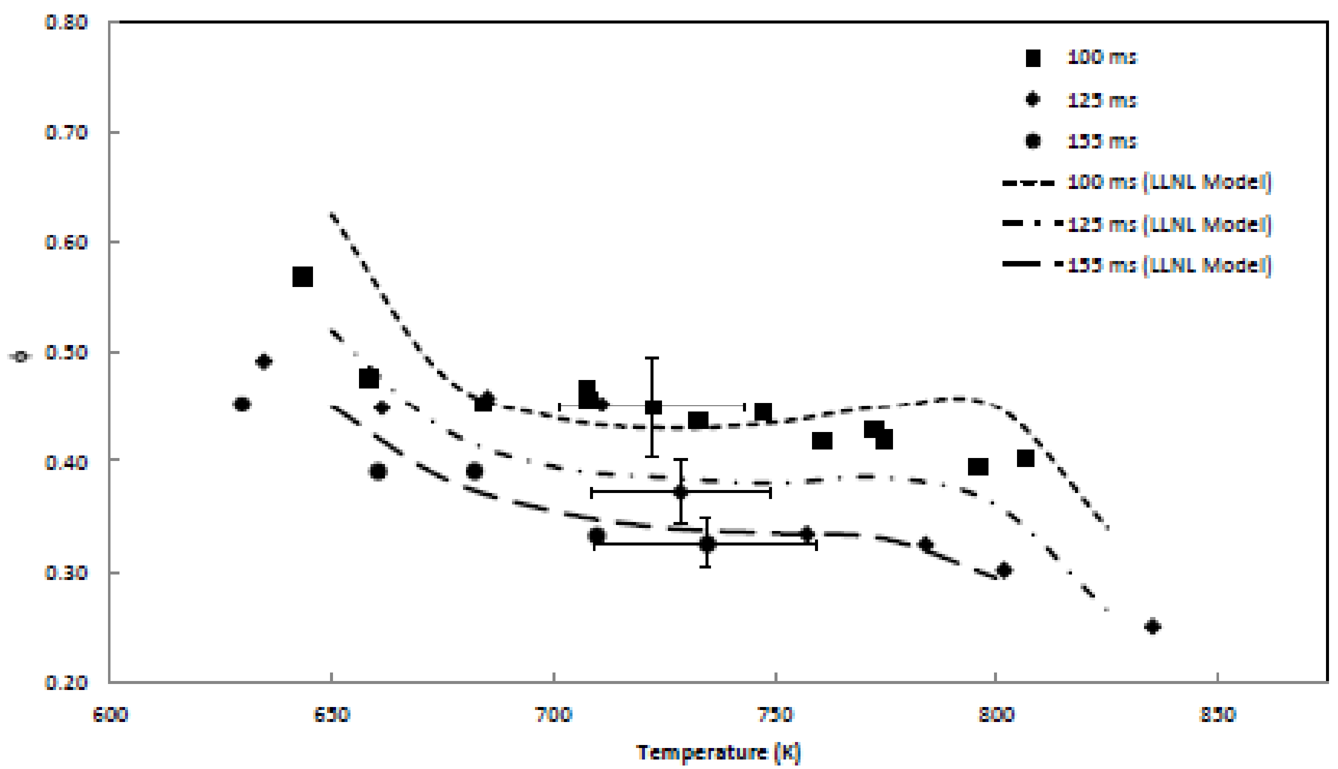
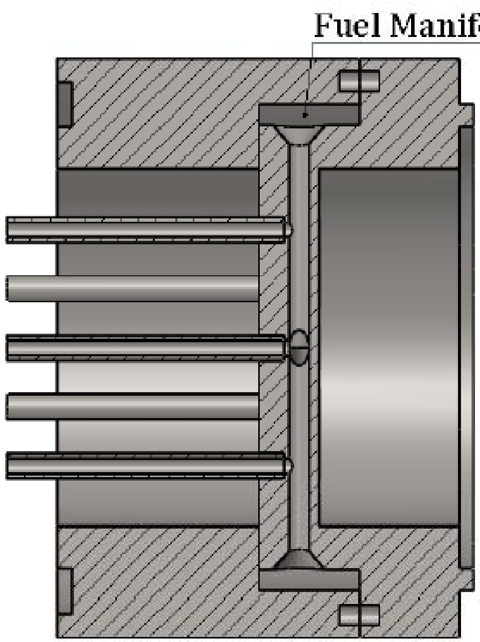
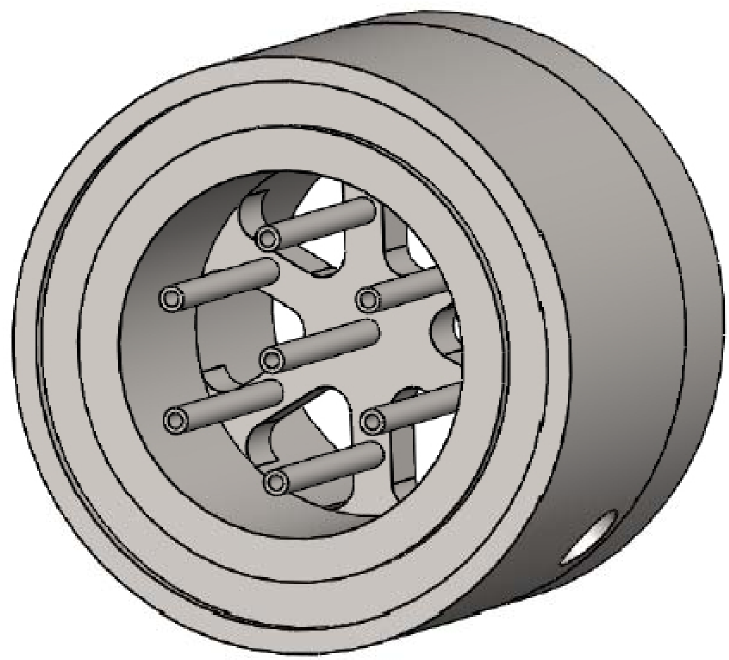


Figure 4-6. Experimental results and model predictions for the threshold equivalence as a function of temperature at 20 atm. Symbols represent experimental results from the current study while lines represent model results using the LLNL mechanism [32].

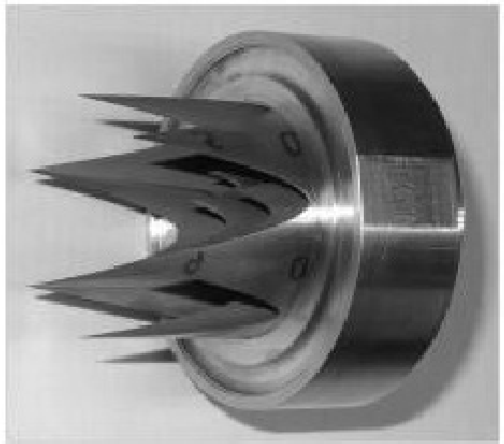
Description of Injectors

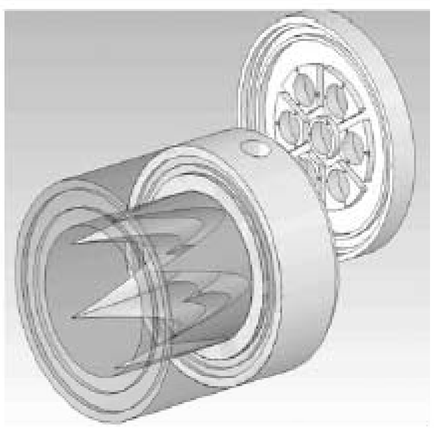
Axial Injector

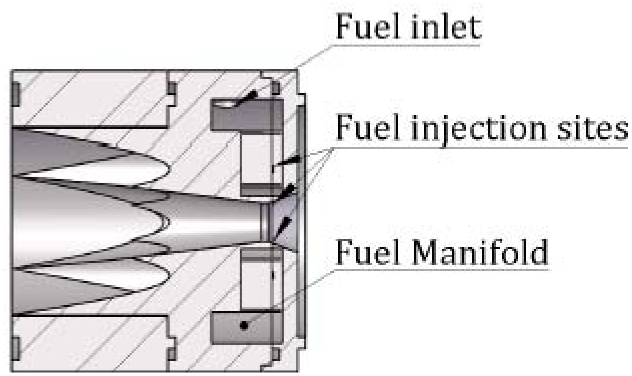


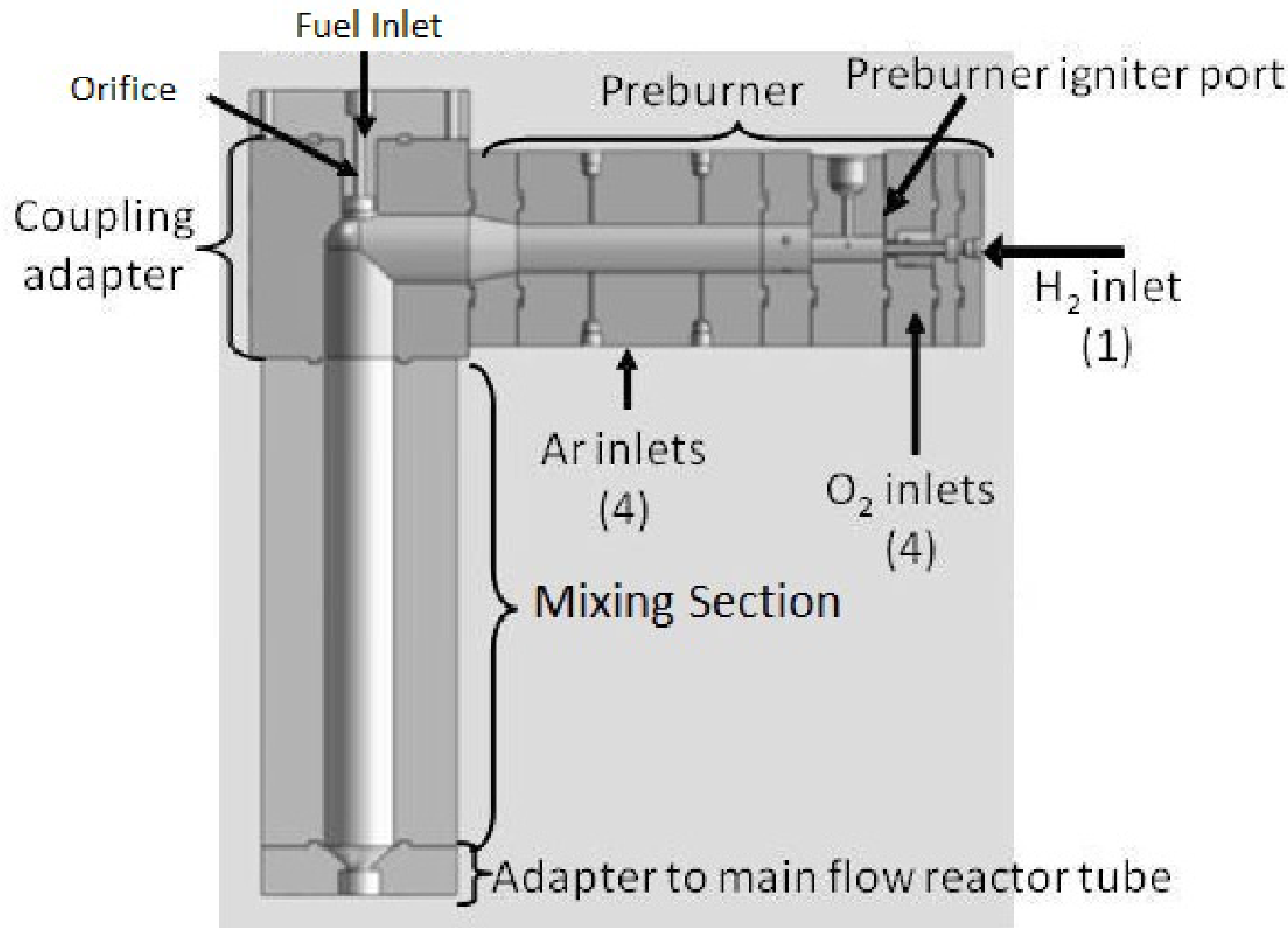


Radial Injector



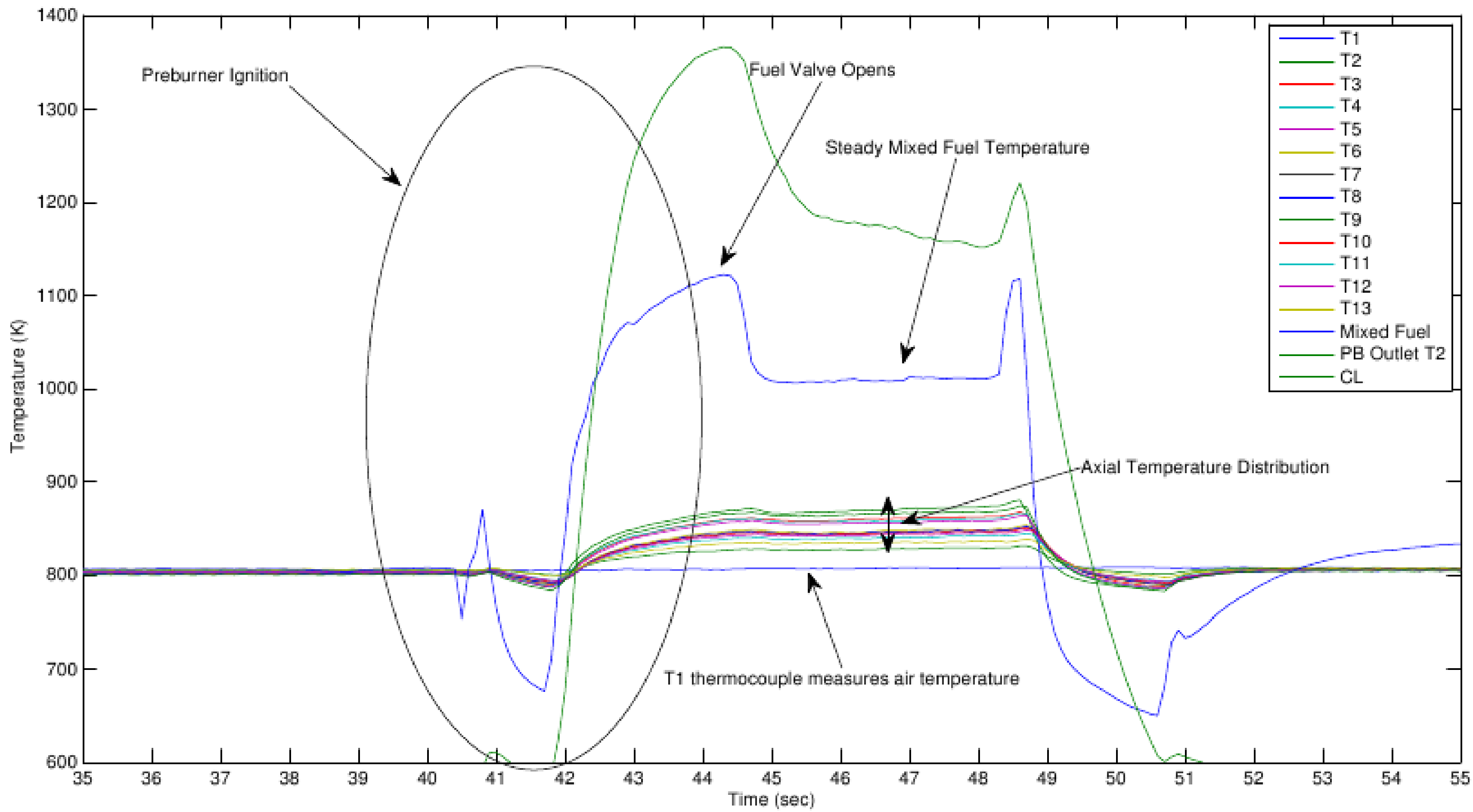





Fuel Inlet
Orifice
Preburner
Preburner igniter port
Coupling adapter
H_2 inlet (1)
Ar inlets (4)
O_2 inlets (4)
Mixing Section
Adapter to main flow reactor tube

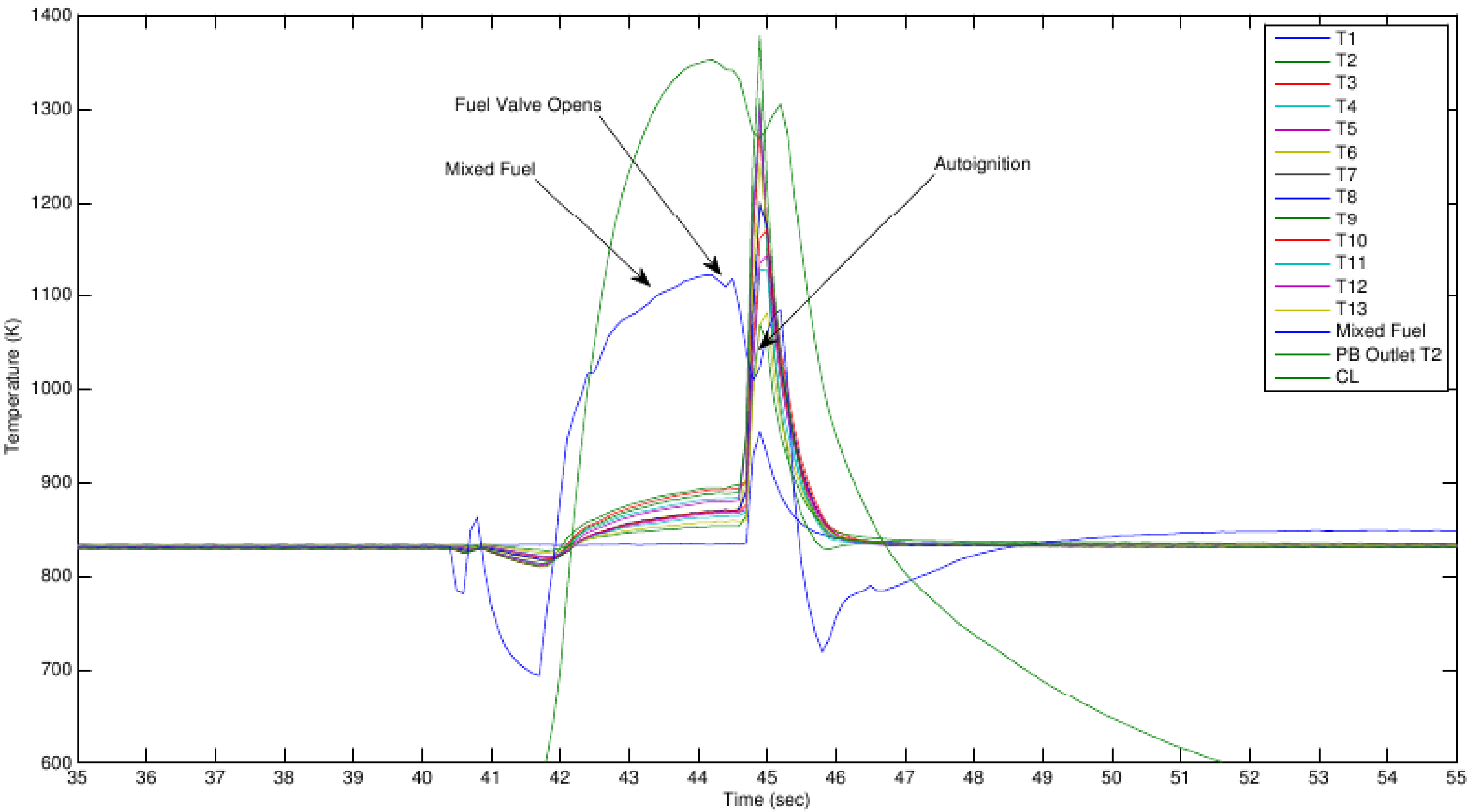
Experimental Method

- Set initial conditions required
  - Pressure, temperature, residence time, equivalence ratio
- Inject fuel using a high speed valve system
- Determine if ignition occurred or did not occur
- Incrementally increase temperature until ignition occurs



Preburner Ignition
Fuel Valve Opens
Steady Mixed Fuel Temperature
Axial Temperature Distribution
T1 thermocouple measures air temperature
Temperature (K)
Time (sec)
T1
T2
T3
T4
T5
T6
T7
T8
T9
T10
T11
T12
T13
Mixed Fuel
PB Outlet T2
CL

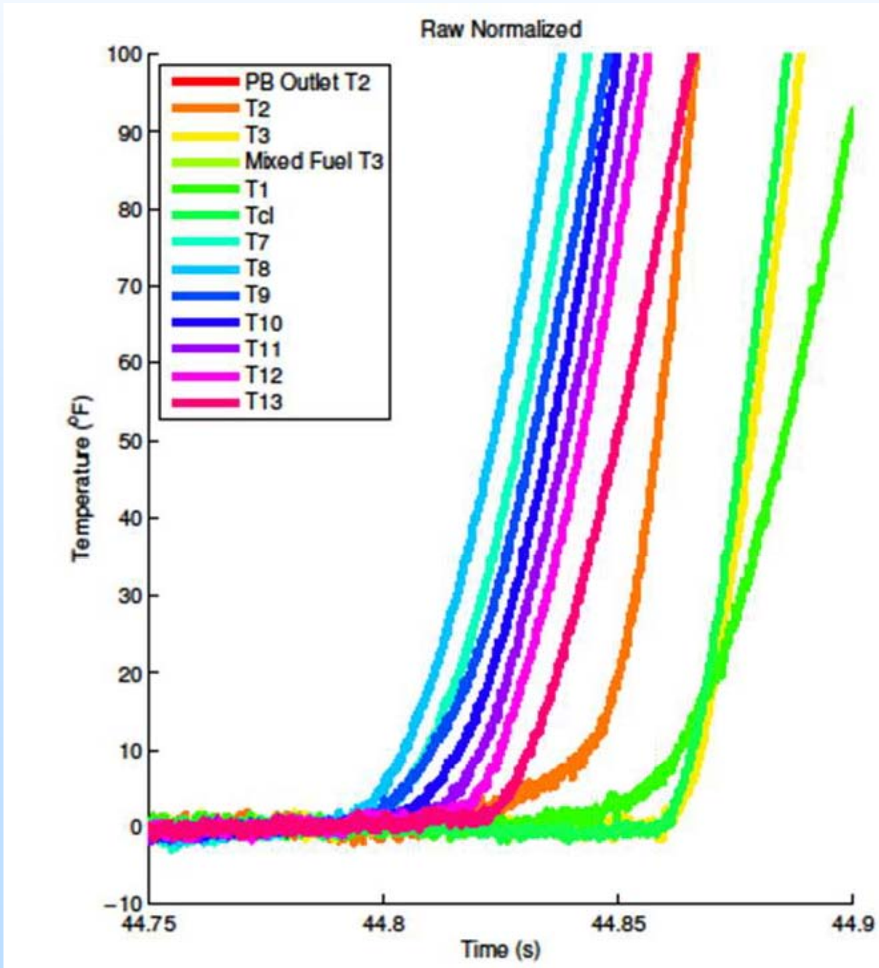
No Ignition

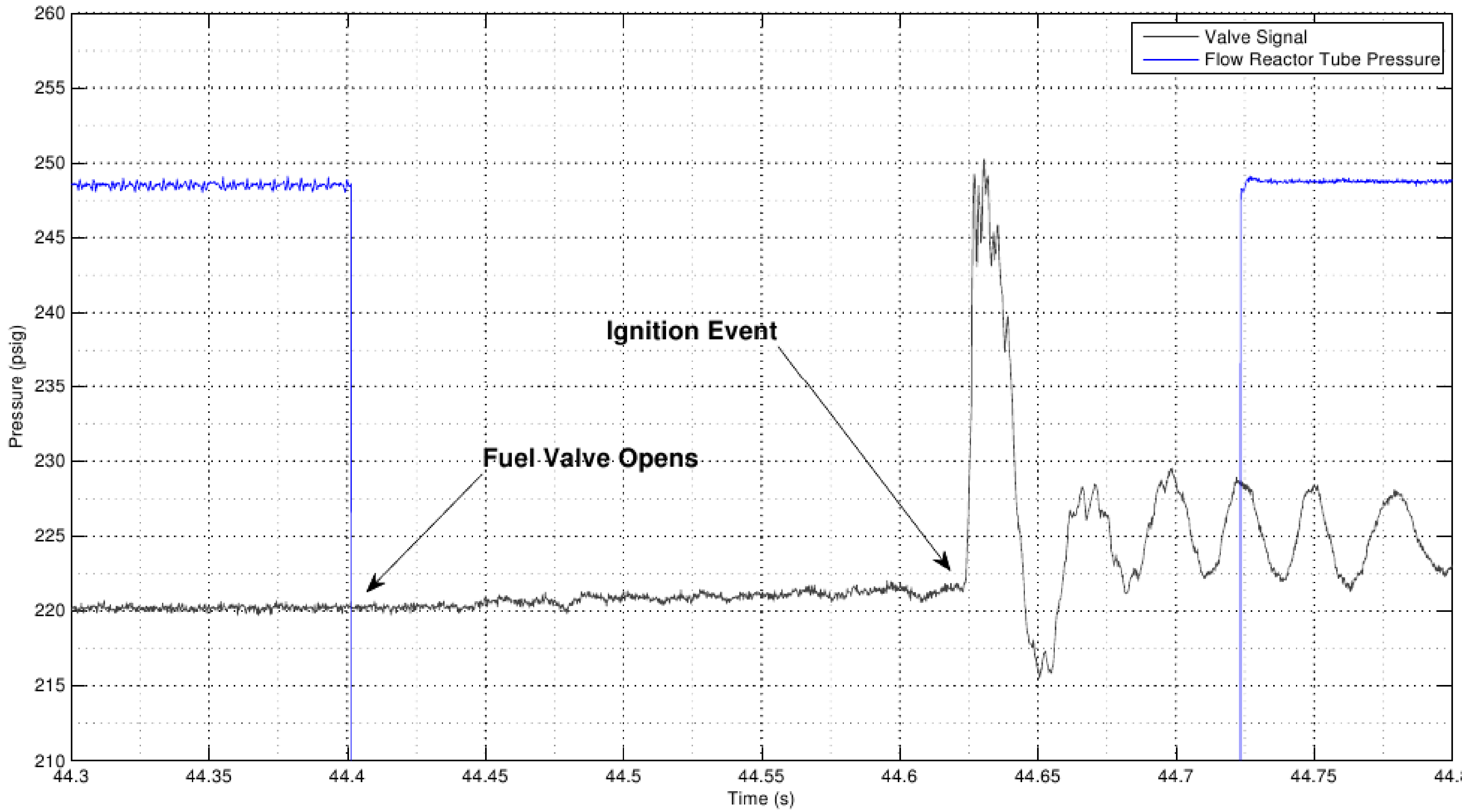

Fuel Valve Opens
Mixed Fuel
Autoignition
T1
T2
T3
T4
T5
T6
T7
T8
T9
T10
T11
T12
T13
Mixed Fuel
PB Outlet T2
CL
Temperature (K)
Time (sec)
1400
1300
1200
1100
1000
900
800
700
600
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55

Ignition

Identifying ignition location

- Location is identified by high speed temperature measurements




Valve Signal
Flow Reactor Tube Pressure
Ignition Event
Fuel Valve Opens
Pressure (psig)
Time (s)
260
255
250
245
240
235
230
225
220
215
210
44.3
44.35
44.4
44.45
44.5
44.55
44.6
44.65
44.7
44.75
44.8

Calculating ignition delay

- L is distance to location of ignition (thermocouple location) from the injection point

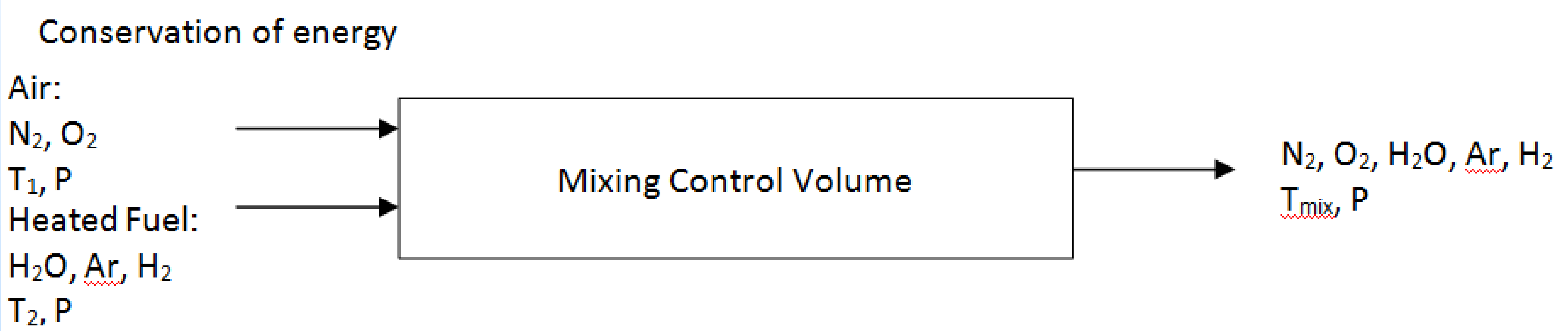
$$\tau_{residence} = \frac{L}{V}$$

$$\rho_{mixture} = \frac{R_{mixture}T}{P}$$

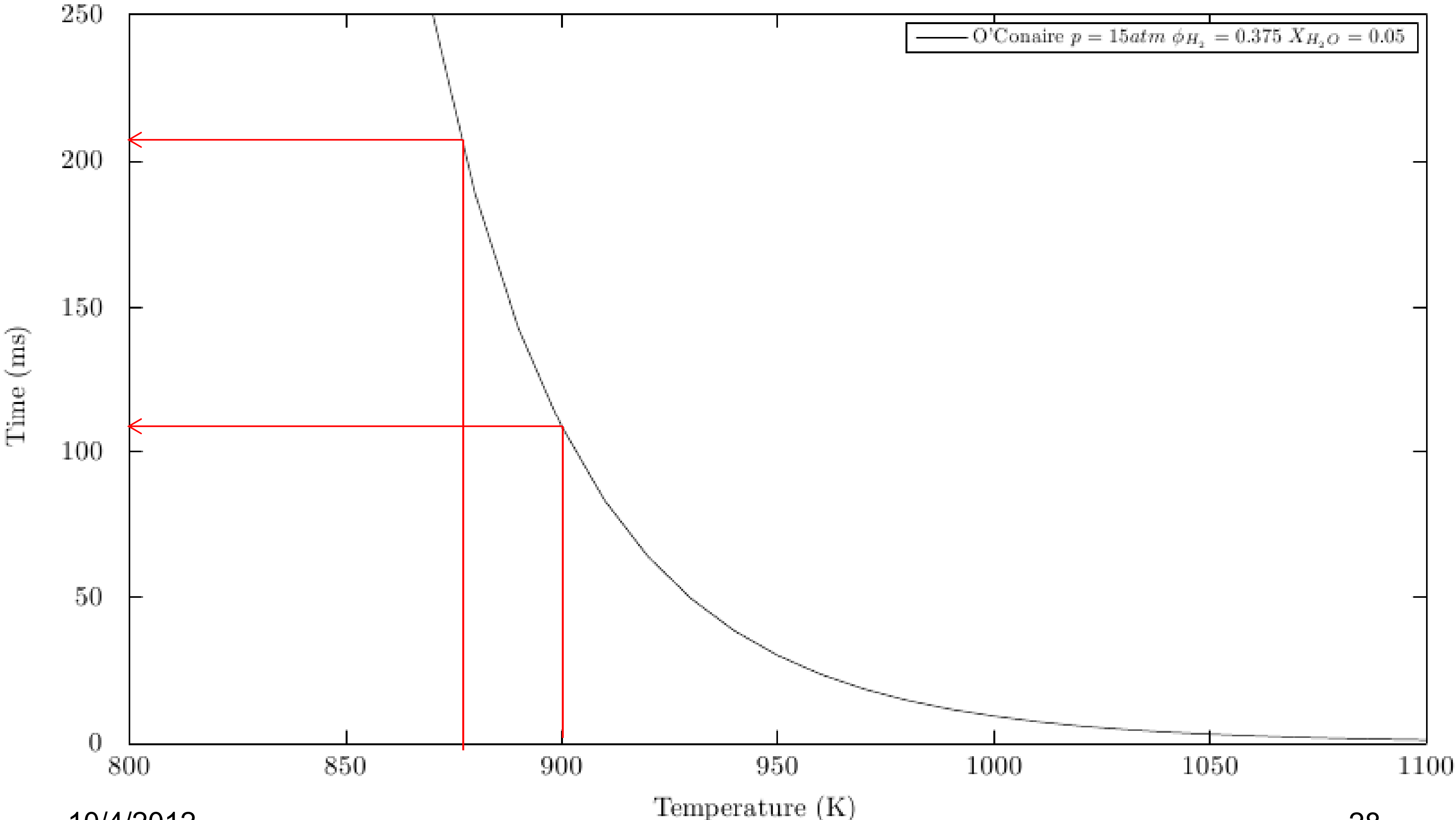
$$V = \frac{\dot{m}_{total}}{\rho_{mixture}A}$$

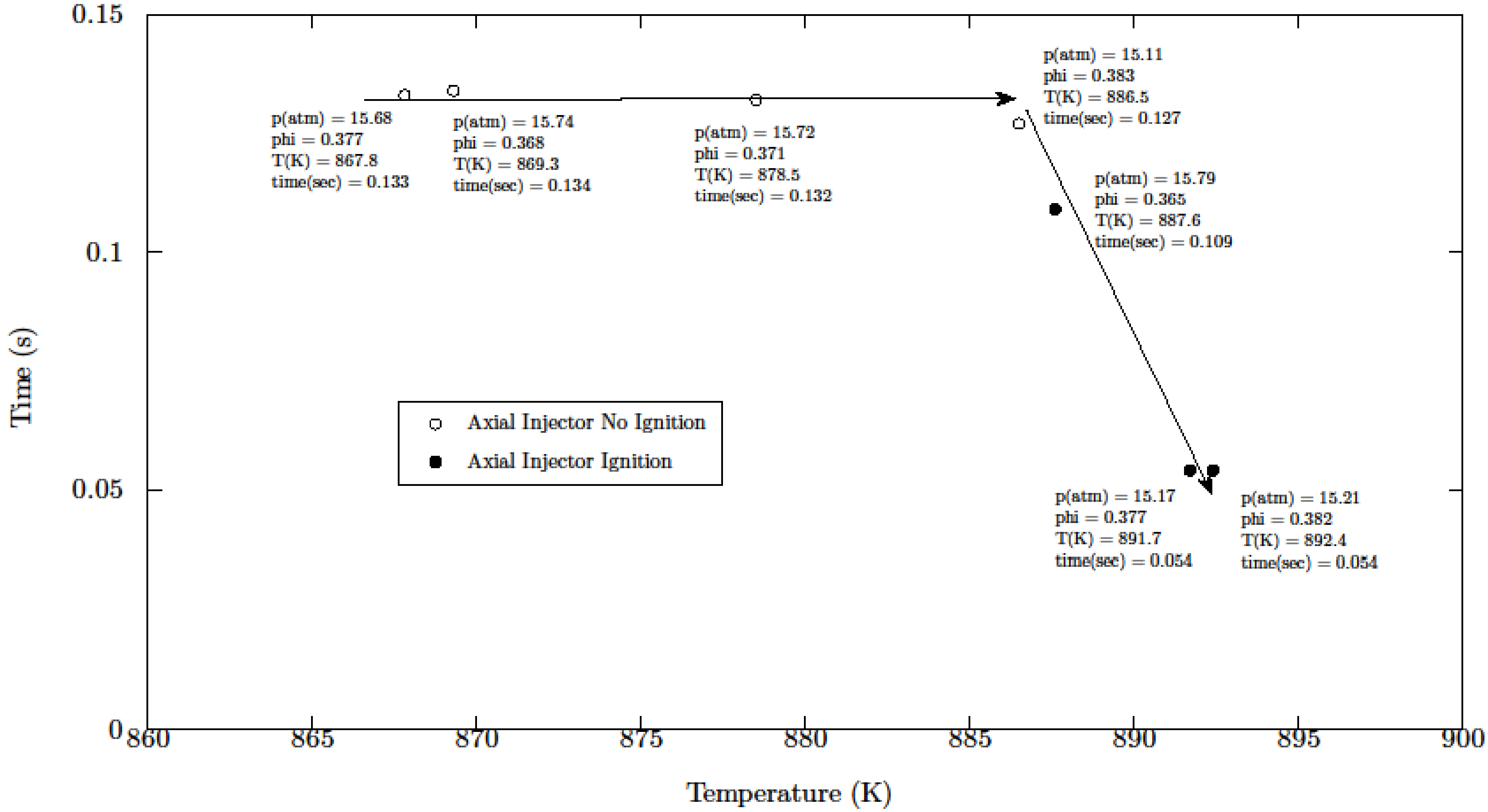
Mixture Temperature

- Calculated by performing energy balance on preburner and air streams



Results

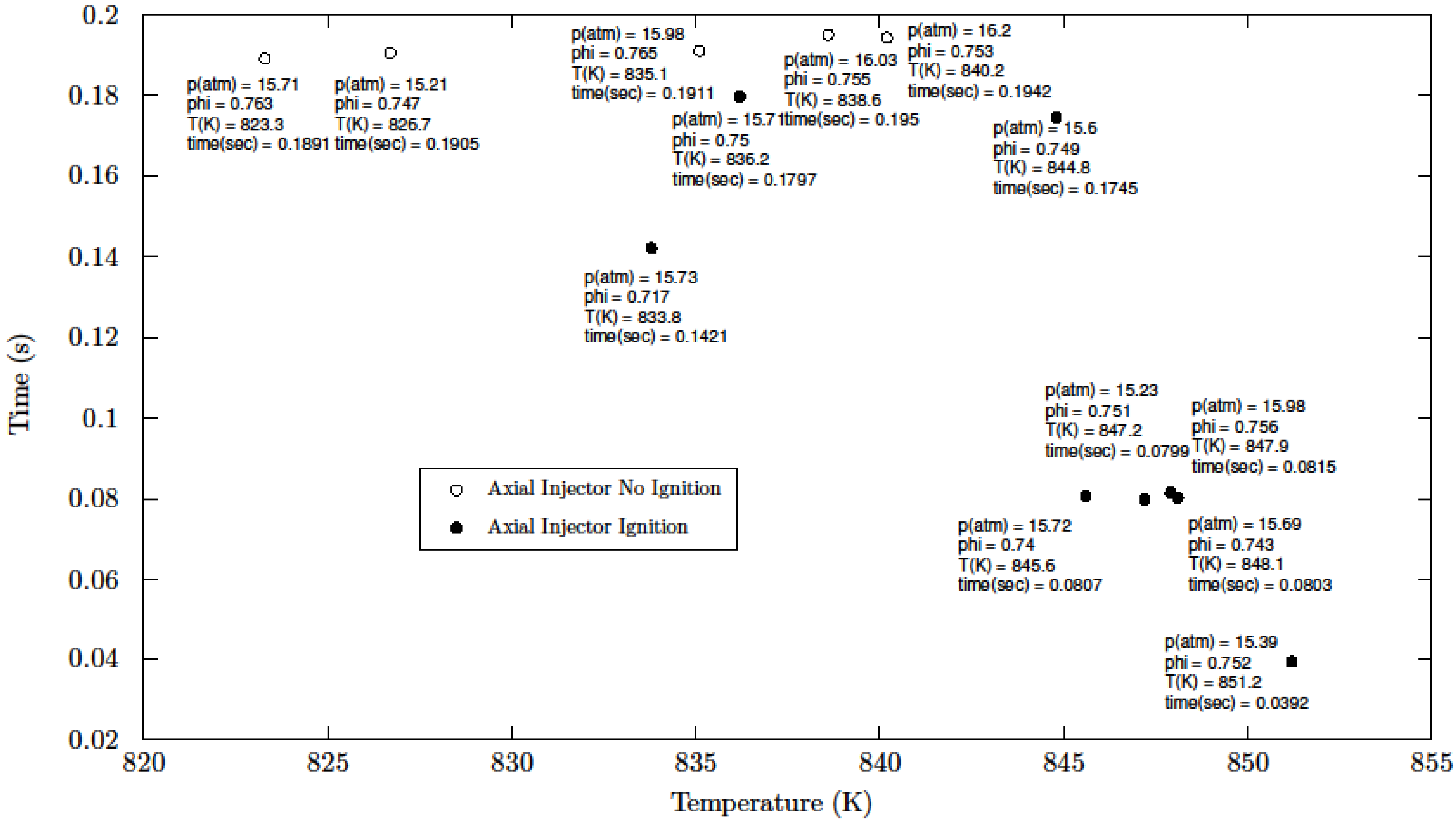

O'Conaire $p = 15atm$ $\phi_{H_2} = 0.375$ $X_{H_2O} = 0.05$
Time (ms)
Temperature (K)
250
200
150
100
50
0
800
850
900
950
1000
1050
1100



Time (s)
Temperature (K)
0.15
0.1
0.05
0
860
865
870
875
880
885
890
895
900
Axial Injector No Ignition
Axial Injector Ignition
p(atm) = 15.68
phi = 0.377
T(K) = 867.8
time(sec) = 0.133
p(atm) = 15.74
phi = 0.368
T(K) = 869.3
time(sec) = 0.134
p(atm) = 15.72
phi = 0.371
T(K) = 878.5
time(sec) = 0.132
p(atm) = 15.11
phi = 0.383
T(K) = 886.5
time(sec) = 0.127
p(atm) = 15.79
phi = 0.365
T(K) = 887.6
time(sec) = 0.109
p(atm) = 15.17
phi = 0.377
T(K) = 891.7
time(sec) = 0.054
p(atm) = 15.21
phi = 0.382
T(K) = 892.4
time(sec) = 0.054

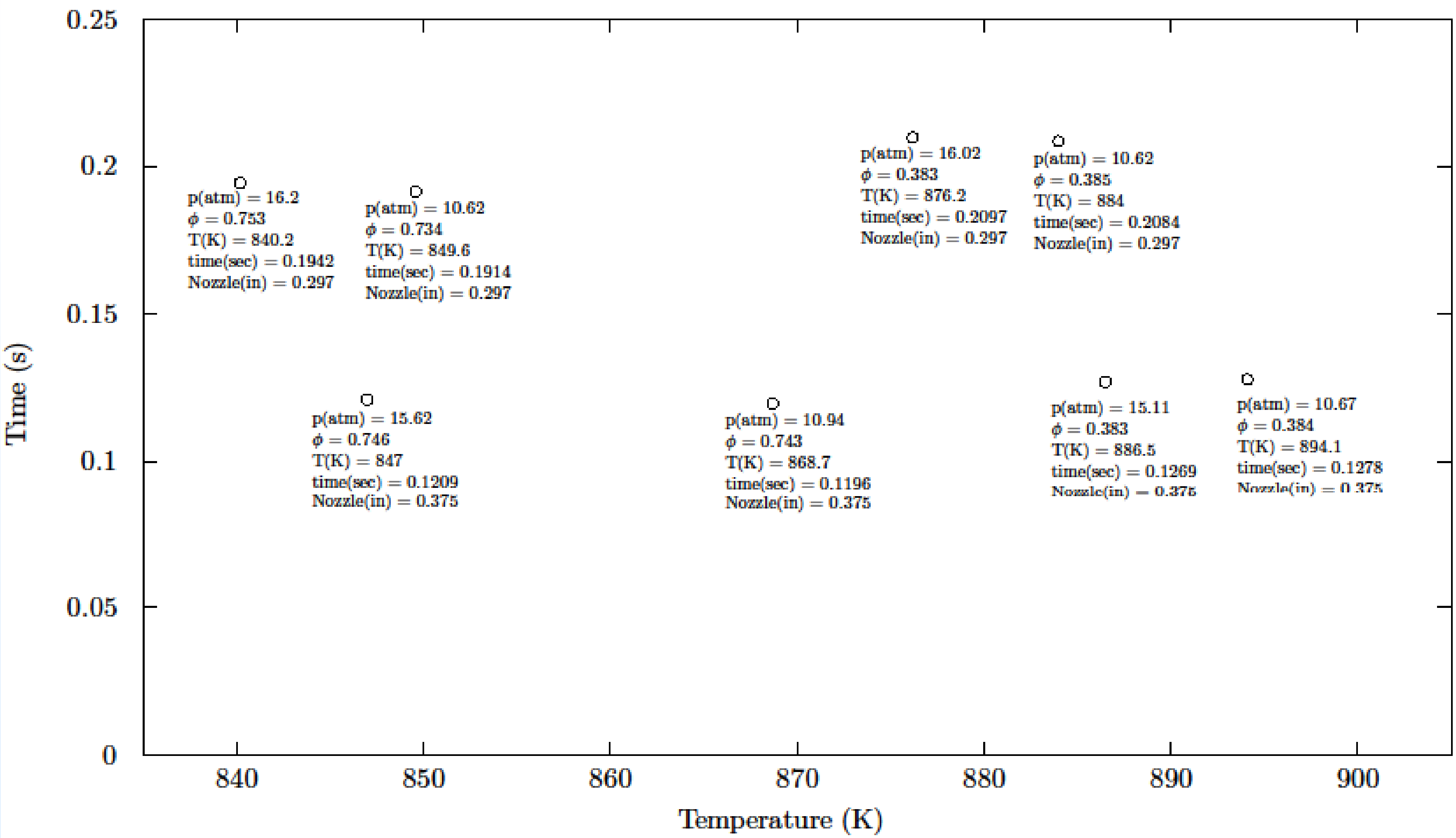
Interpreting Data

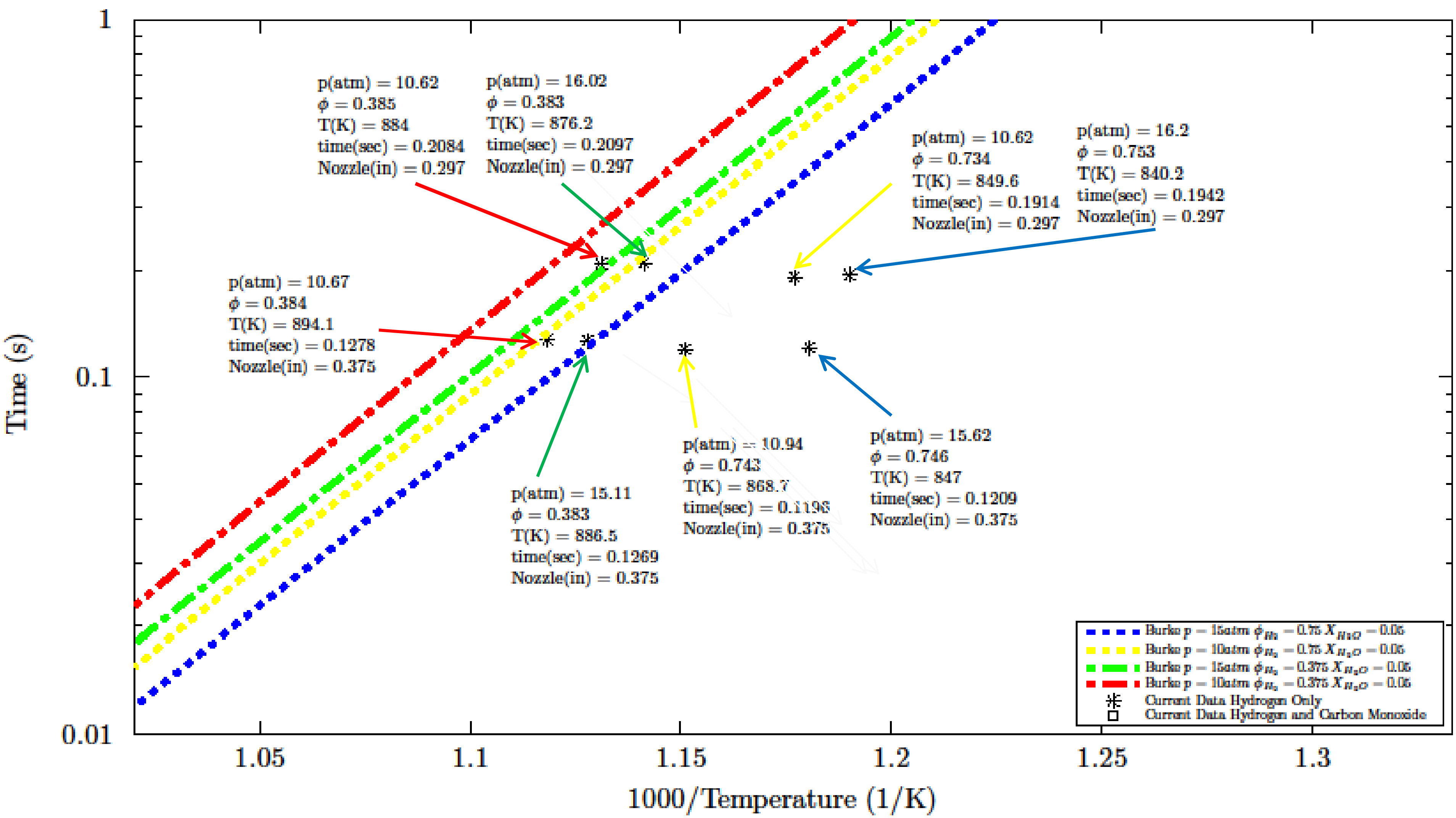
- Use the highest temperature no-ignition experiment for mixture temperature.
  - Can measure fuel and air temperatures reliably
- Use only ignition experiments that occur between thermocouple T9 and T13 when comparing results.
  - Need ignitions that occur near the end of the flow reactor (residence time)



Time (s)
Temperature (K)
Axial Injector No Ignition
Axial Injector Ignition
p(atm) = 15.71
phi = 0.763
T(K) = 823.3
time(sec) = 0.1891
p(atm) = 15.21
phi = 0.747
T(K) = 826.7
time(sec) = 0.1905
p(atm) = 15.98
phi = 0.765
T(K) = 835.1
time(sec) = 0.1911
p(atm) = 15.71
phi = 0.75
T(K) = 836.2
time(sec) = 0.1797
p(atm) = 16.03
phi = 0.755
T(K) = 838.6
time(sec) = 0.195
p(atm) = 16.2
phi = 0.753
T(K) = 840.2
time(sec) = 0.1942
p(atm) = 15.6
phi = 0.749
T(K) = 844.8
time(sec) = 0.1745
p(atm) = 15.73
phi = 0.717
T(K) = 833.8
time(sec) = 0.1421
p(atm) = 15.23
phi = 0.751
T(K) = 847.2
time(sec) = 0.0799
p(atm) = 15.98
phi = 0.756
T(K) = 847.9
time(sec) = 0.0815
p(atm) = 15.72
phi = 0.74
T(K) = 845.6
time(sec) = 0.0807
p(atm) = 15.69
phi = 0.743
T(K) = 848.1
time(sec) = 0.0803
p(atm) = 15.39
phi = 0.752
T(K) = 851.2
time(sec) = 0.0392

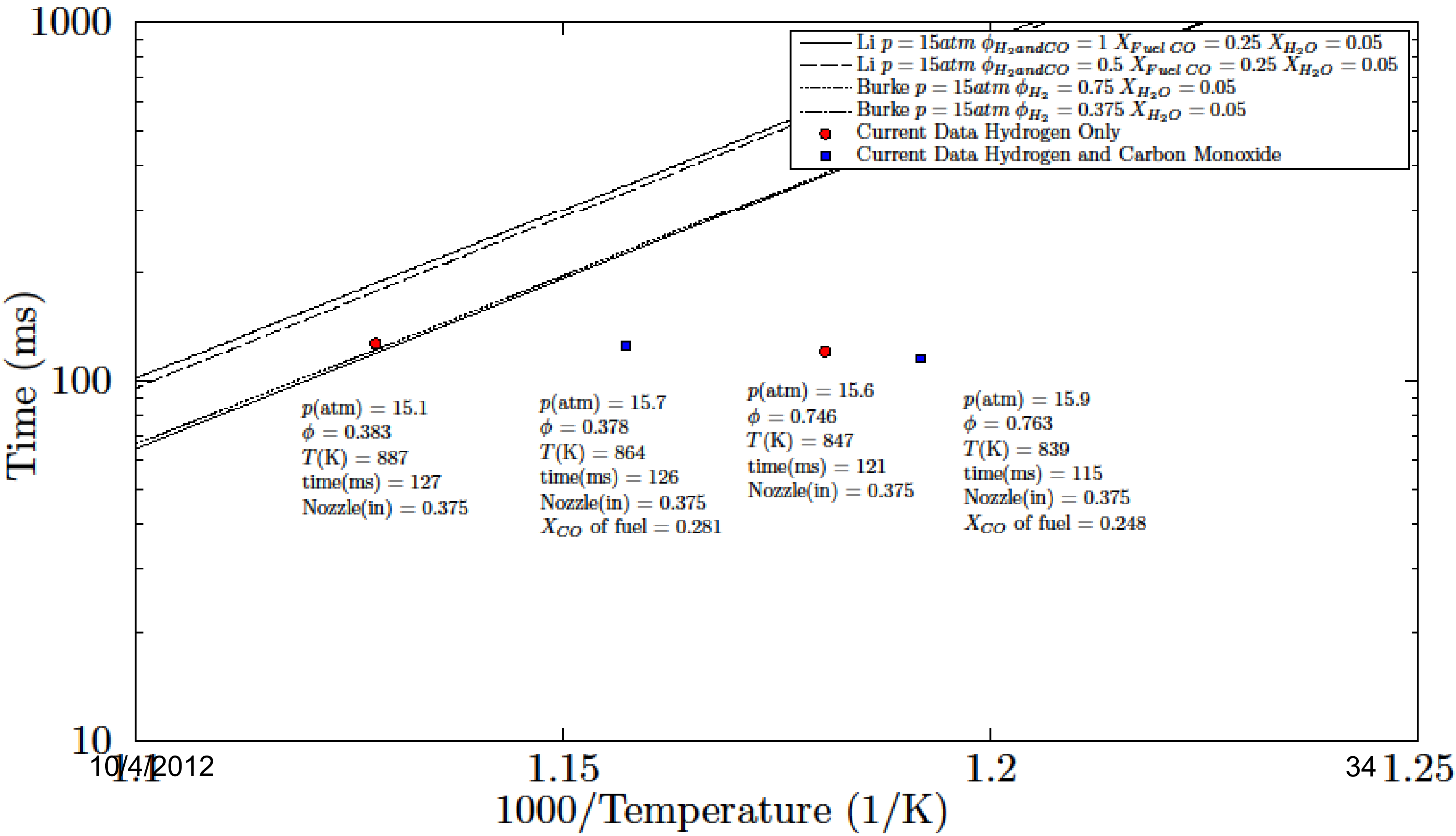
Primary Eight Conditions



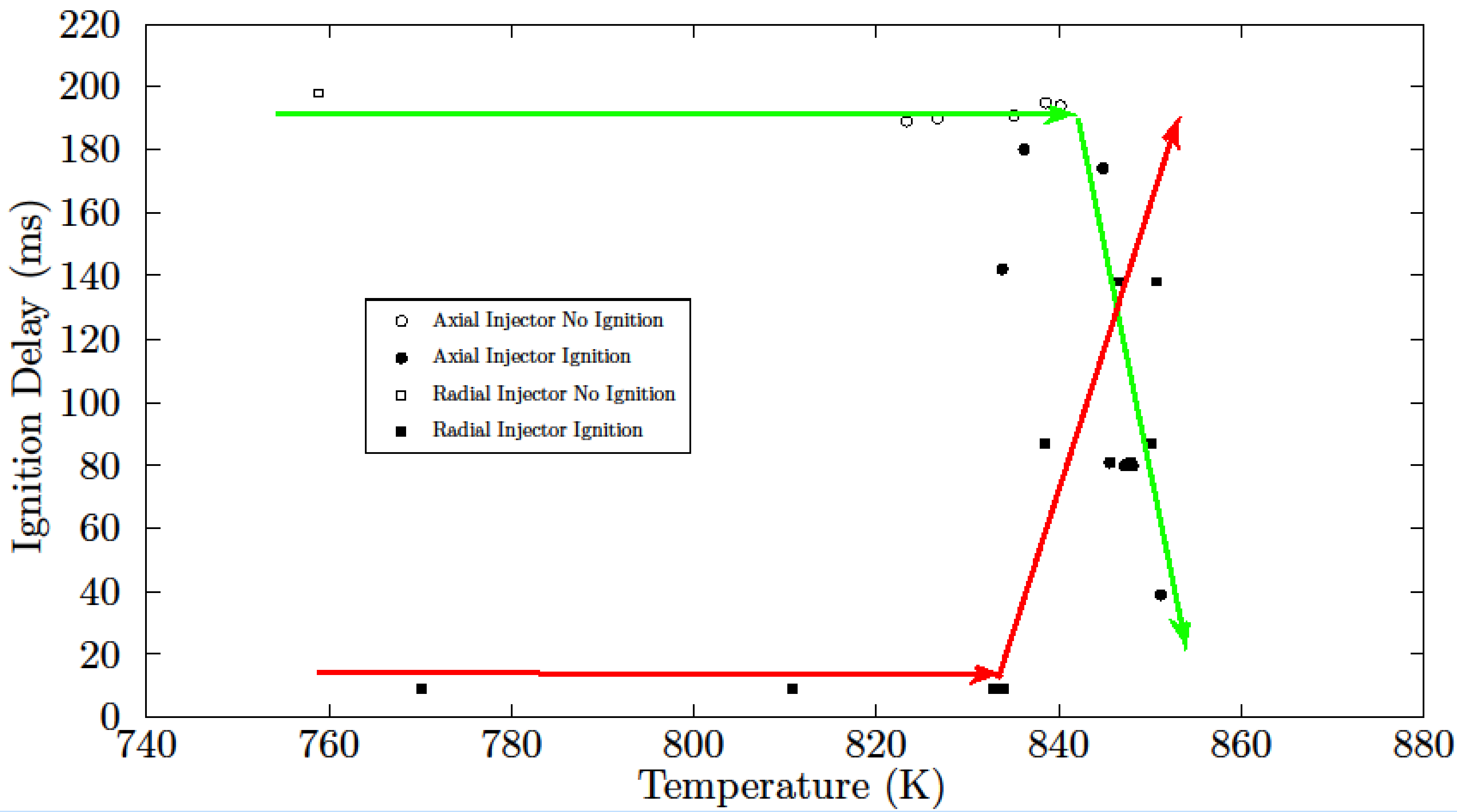


p(atm) = 10.62
ϕ = 0.385
T(K) = 884
time(sec) = 0.2084
Nozzle(in) = 0.297
p(atm) = 16.02
ϕ = 0.383
T(K) = 876.2
time(sec) = 0.2097
Nozzle(in) = 0.297
p(atm) = 10.62
ϕ = 0.734
T(K) = 849.6
time(sec) = 0.1914
Nozzle(in) = 0.297
p(atm) = 16.2
ϕ = 0.753
T(K) = 840.2
time(sec) = 0.1942
Nozzle(in) = 0.297
p(atm) = 10.67
ϕ = 0.384
T(K) = 894.1
time(sec) = 0.1278
Nozzle(in) = 0.375
p(atm) = 15.11
ϕ = 0.383
T(K) = 886.5
time(sec) = 0.1269
Nozzle(in) = 0.375
p(atm) = 10.94
ϕ = 0.743
T(K) = 868.7
time(sec) = 0.1196
Nozzle(in) = 0.375
p(atm) = 15.62
ϕ = 0.746
T(K) = 847
time(sec) = 0.1209
Nozzle(in) = 0.375
Burke p = 15atm ϕ_{H_2} = 0.75 X_{H_2O} = 0.05
Burke p = 10atm ϕ_{H_2} = 0.75 X_{H_2O} = 0.05
Burke p = 15atm ϕ_{H_2} = 0.375 X_{H_2O} = 0.05
Burke p = 10atm ϕ_{H_2} = 0.375 X_{H_2O} = 0.05
Current Data Hydrogen Only
Current Data Hydrogen and Carbon Monoxide
Time (s)
1
0.1
0.01
1.05
1.1
1.15
1.2
1.25
1.3
1000/Temperature (1/K)

Syngas Results

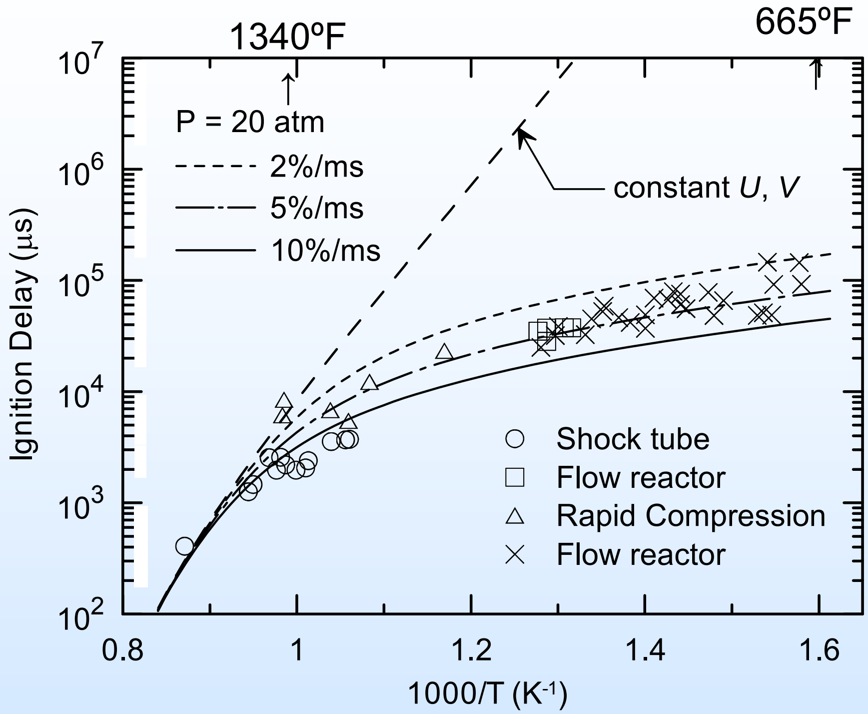


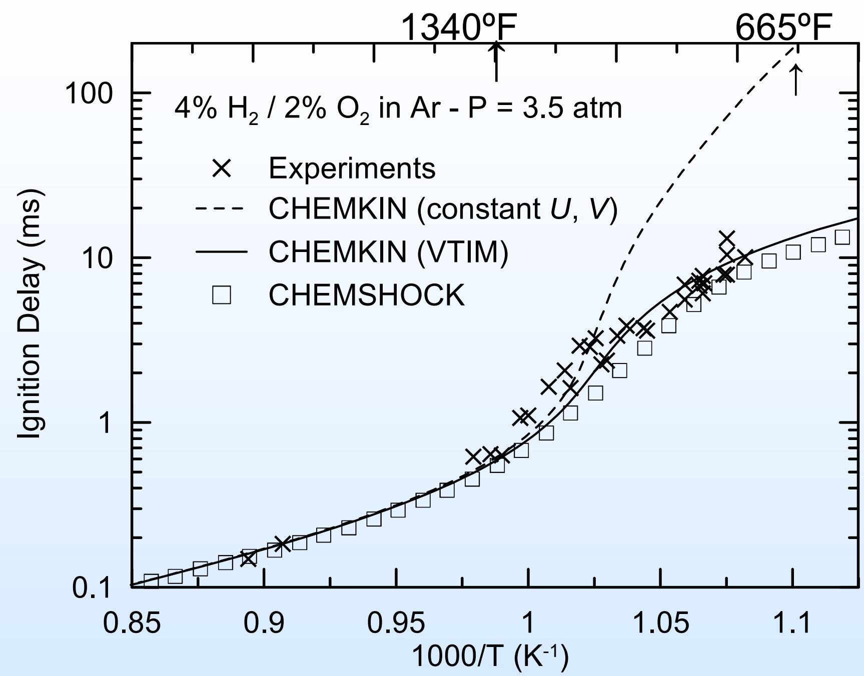
Axial Comparison to Radial Injectors



Additional Comments

Interpreting Experimental Ignition Delay Observations





- **Chemical induction is very important for ignition delay time in the H_2-O_2 system at temperatures below 1000K and is very sensitive to chemical perturbations from any source, e.g., pre-ignition pressure increases (left).**
- **Use of constant U,V constraint to calculate predictions to test models leads of erroneous results andThe volume as a function of time (VTIM) constraint is the proper one to use.**

Conclusions

- These results agree with the homogeneous one-dimensional simulations within a factor of 5.
- Model comparisons were better for the lower equivalence ratio, 0.375, studied than the higher equivalence ratio, 0.750, case.
- The expected trends between results were consistent with expected pressure and equivalence ratio behavior.
- Measurements made using the axial injector indicated that autoignition does not occur below 800 K for the residence time studied. This result is in disagreement with previous work with respect to homogenous chemical kinetic models predictions.

Acknowledgments

I wish to acknowledge:

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Questions?