Autoignition Studies of Syngas and Hydrogen (SGH) Fuels

Penn State University

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SCIES Project 05 - 01- SR117

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Project Awarded (8/1/2005, 42 Month Duration)

Gas Turbine Need

- Current interest in syngas as a fuel for gas turbine power generation applications requires knowledge of a wide range of syngas combustion properties.
- Given the widespread use of lean premixed combustion to control NOx emissions understanding the autoignition properties of syngas is critical.
- Syngas autoignition studies must address:
  - the wide compositional variation of syngas.
  - the need for data at high pressures (e.g. 30 atm)

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Project Objectives

- Parametrically determine the autoignition delay time for CO/H2 mixtures as function of CO concentration, equivalence ratio, pressure and temperature.
- Determine effect of water concentration on autoignition using mixtures of CO/H2/H2O.
- Measurements will be obtained for operating pressures up to 3.0 MPa (30 atm) and 950 K (1250°F) and typical air mass flow rates of 0.5 kg/s (1 lbm/s).

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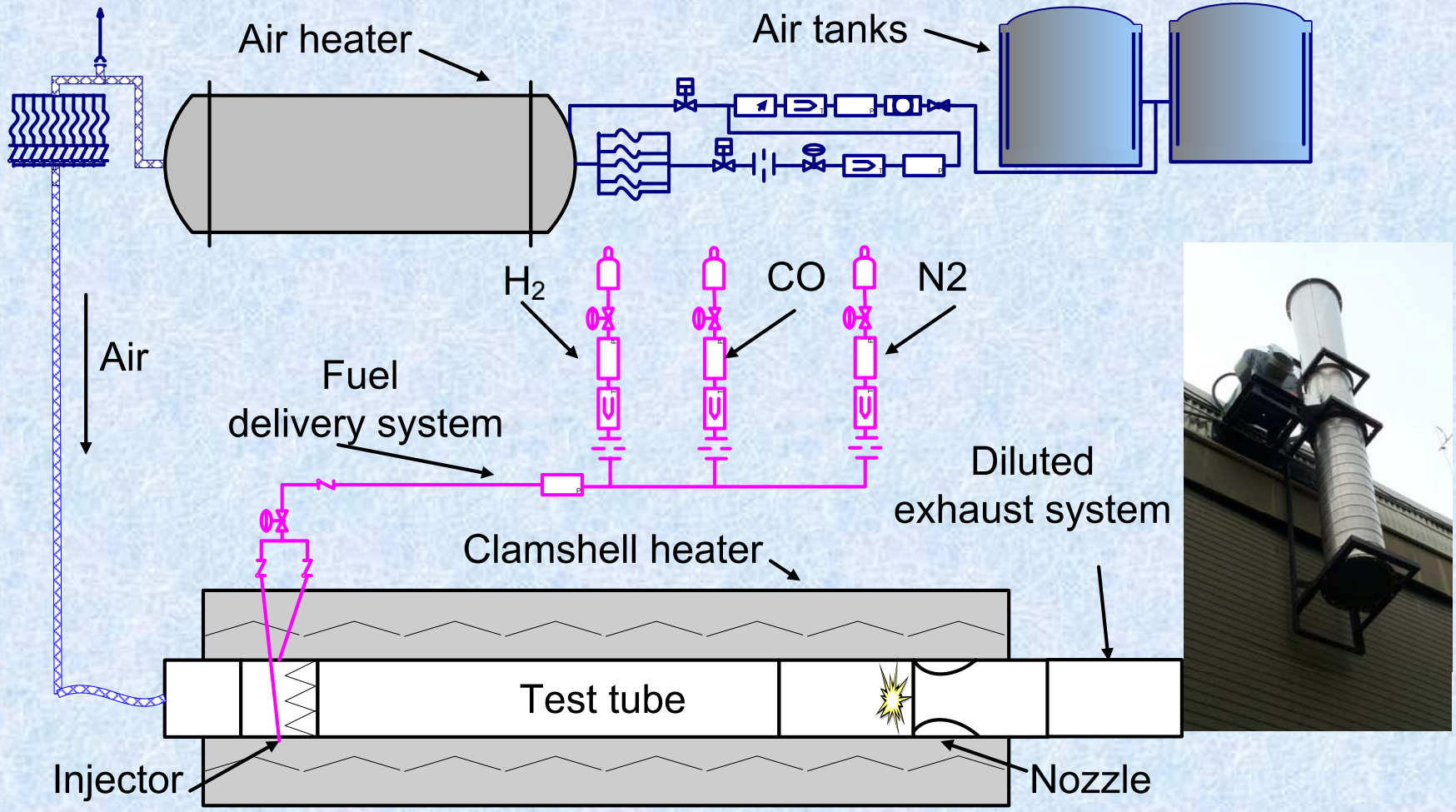
Overall Result

Results for both H2 and H2/CO show similar behavior in terms of the high variability of the measured autoignition time.

Experimental Setup

Simplified Schematic of the High-Pressure Flow Reactor



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Experimental Approach

Fuel composition	Equivalence Ratio	Pressure Range	Temperature Range
H_2 to $CO+3H_2$	$0.3 < \phi < 1$	10 to 30 atm (147 to 440 psi)	Mixture temperature: 590K to 800K (600°F to 980°F)

Tube Dimensions	Nominal Chamber Velocity	Air Flow rate	Fuel Flow rate
Diameter = 46 mm (1.8 in.) Length = 0.3 to 2.1 m (1 to 7 ft)	10 m/s, 20 m/s, 30 m/s, 40 m/s	0.05 to 0.6 kg/s of air	0.003 to 0.016 kg/s of H_2 0 to 0.06 kg/s of CO

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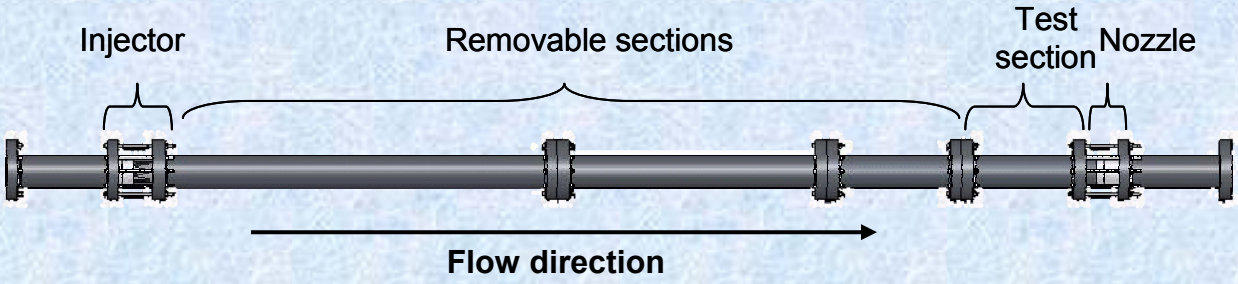
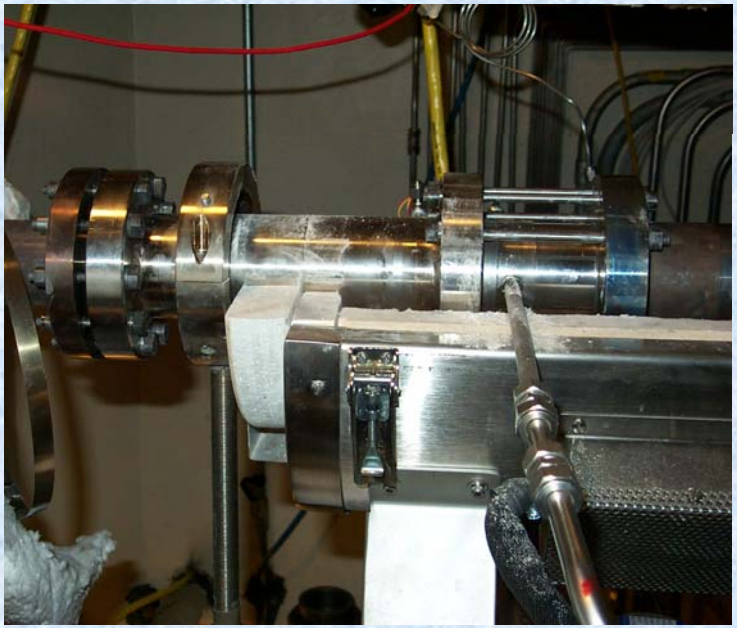
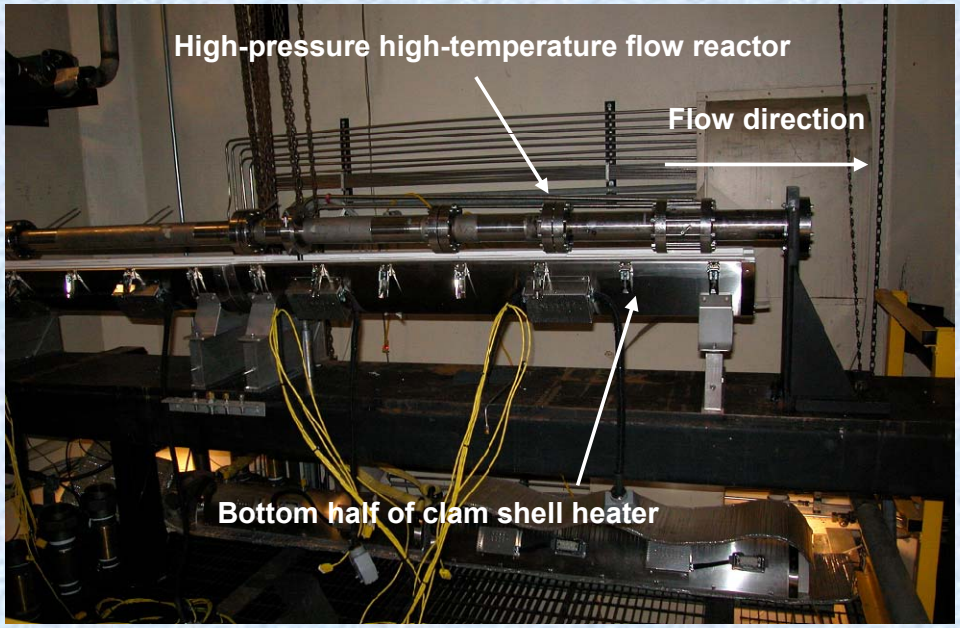
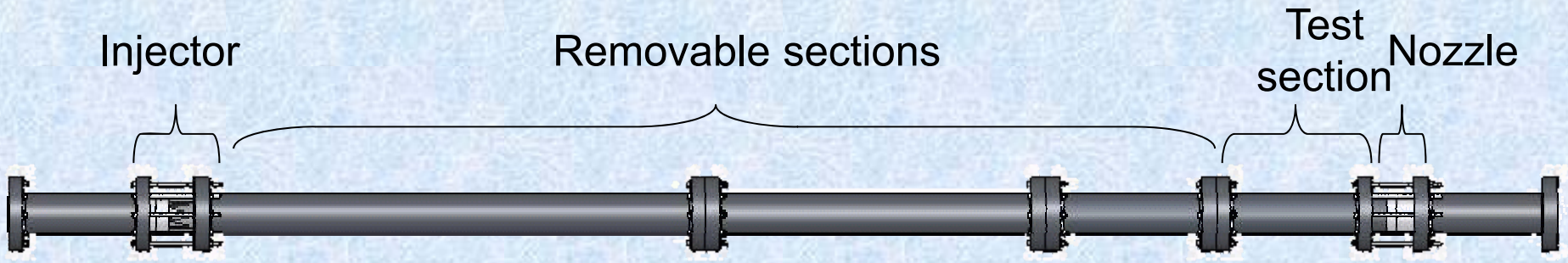
Pictures of High-Pressure Flow Reactor







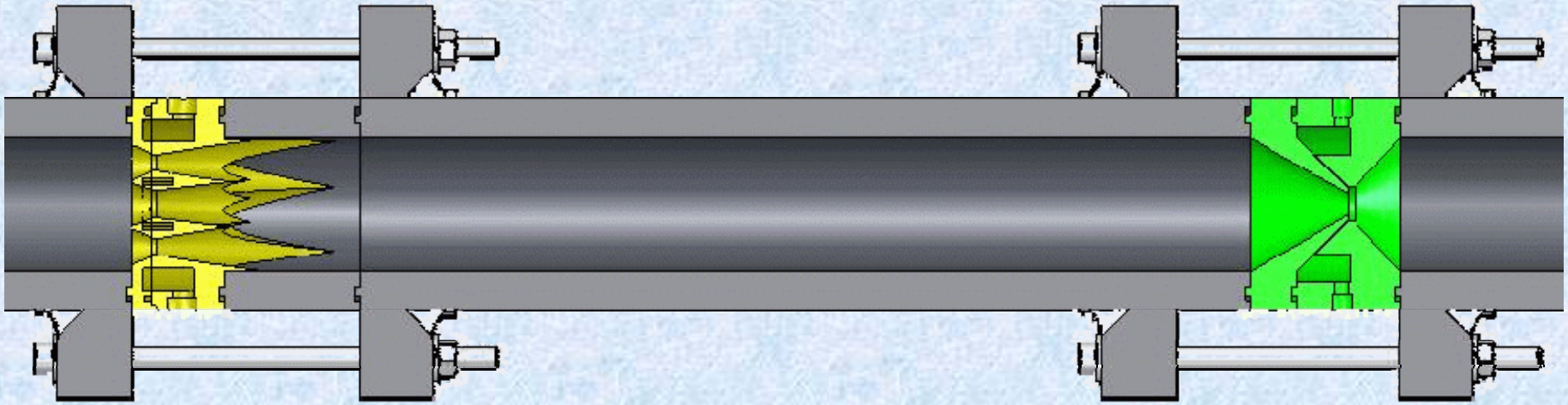
Flow Reactor Design



- **Modular design to vary flow reactor length if necessary**
- **310ss for strength at high pressure and better oxidation and corrosion resistance at high temperature**
- **Metallic (inconel) c-rings for sealing**

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# = 5×10^5 to 3×10^6**



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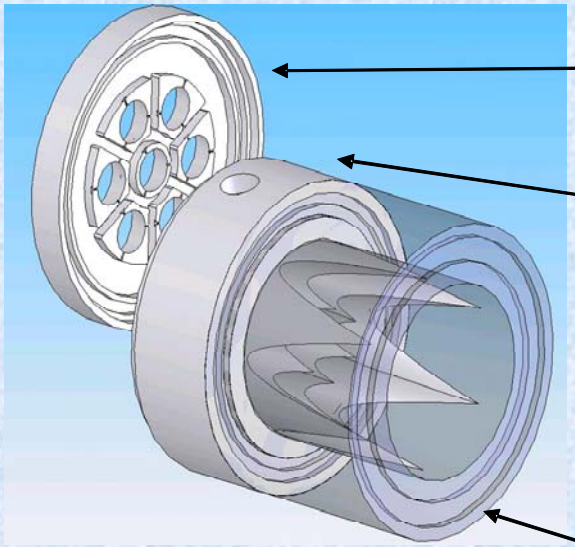
Injector Design Concept and Resulting Hardware



Back piece (injection holes

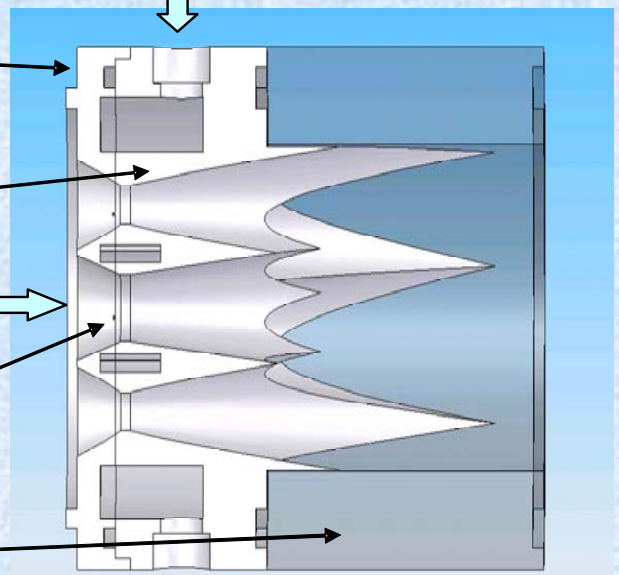
Back piece

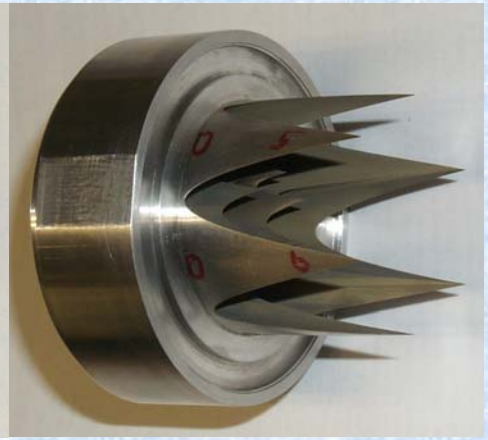
Air (7 places)

Fuel injection (21 places)

Tube wall

Fuel inlet (2 places)





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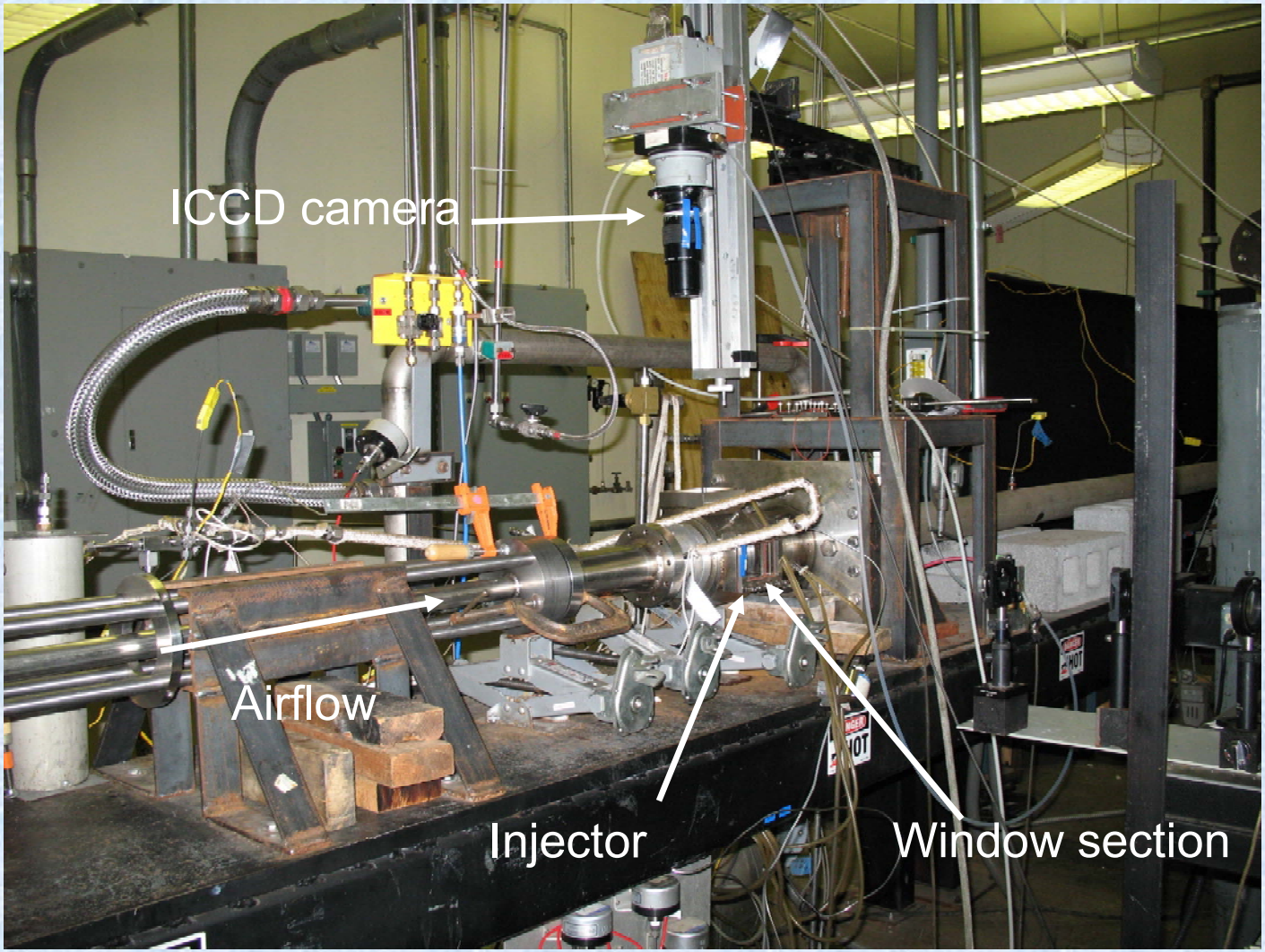
Acetone PLIF Set-up



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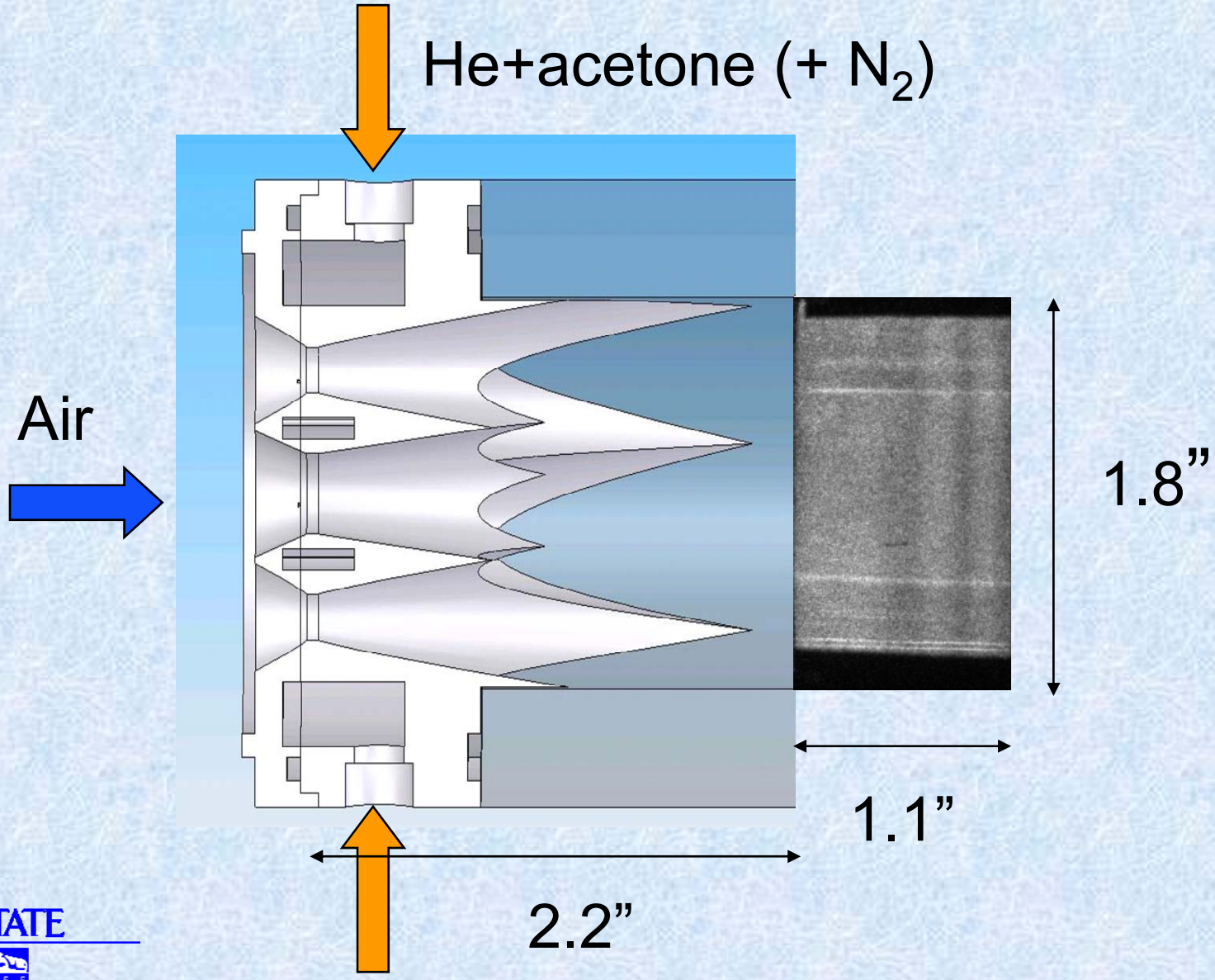
Field of View for Acetone PLIF Measurements



Acetone PLIF Testing of Injectors

- Test done at atmospheric pressure, T=200ºF for air and fuel simulant.
- Fuel simulant: helium+acetone+N_2
- Acetone concentration: 1% by volume of total flow
- Laser ≈ 40 mJ/pulse
- 100 images per run

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Test Conditions for Acetone PLIF Measurements

- **Match momentum flux ratio: $\rho_{fuel}V^2_{fuel}/\ \rho_{air}V^2_{air}$ between simulated conditions and actual conditions**
- **Maintain 1% (by volume) acetone concentration in chamber**
- **When possible matched velocity ratio between simulated conditions and actual conditions**
  - Requires matching $\rho_{fuel}/\ \rho_{air}$, which is not possible for all fuel cases.

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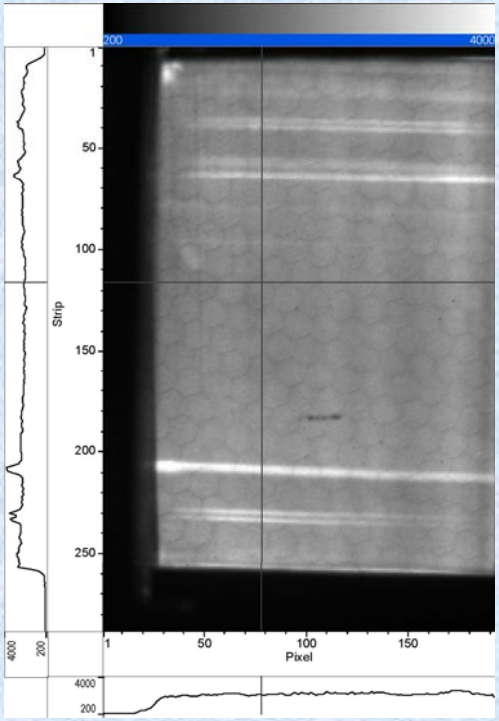
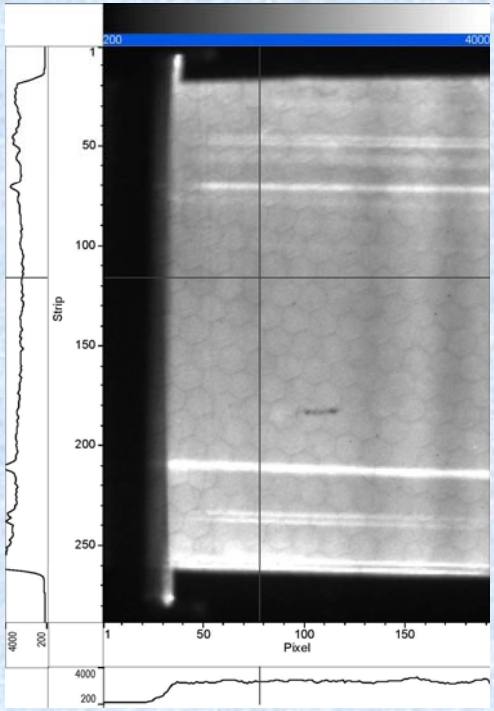
Average Intensity

- Average over 100 images for injector 4
- a) Totally mixed flow (acetone injected far upstream of injector), b) Momentum flux ratio of 90, c) momentum flux ratio of 9 (only case showing non-uniformity)
- Average images do not always differentiate between well and poorly mixed cases

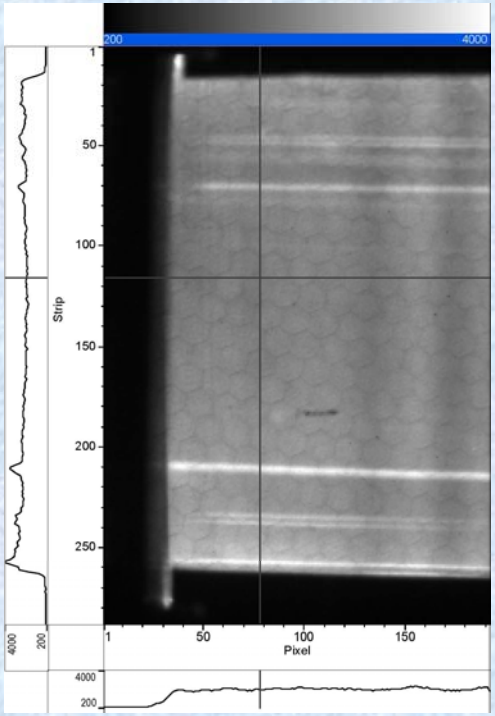
a



b



c



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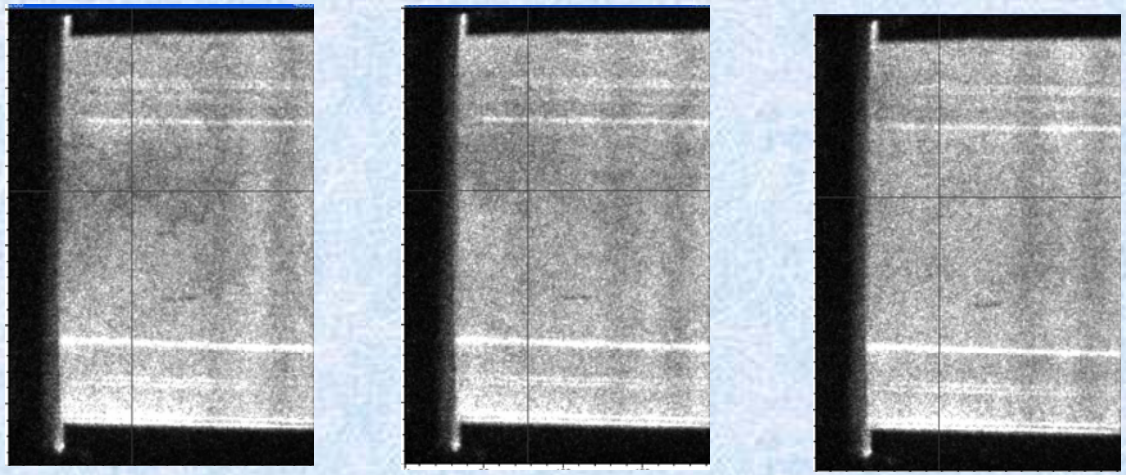
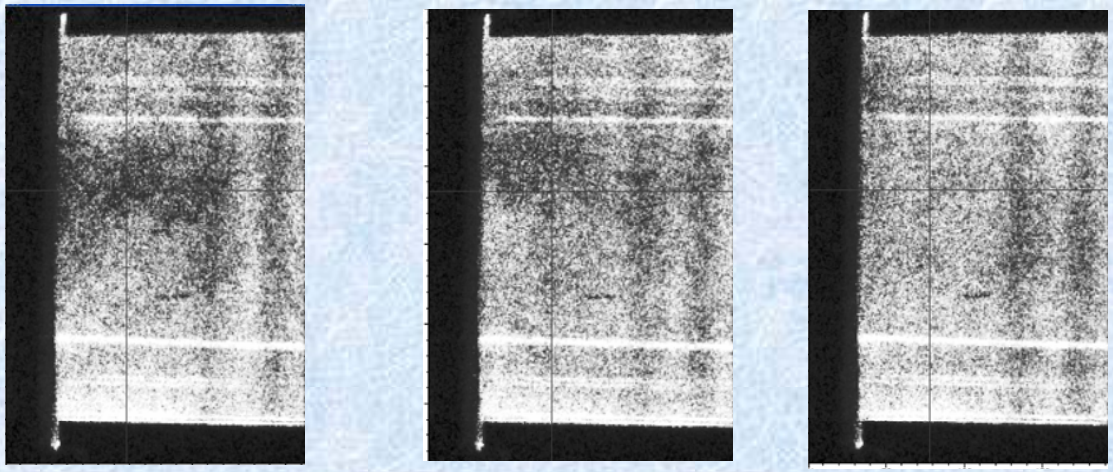
Instantaneous Images

- Sample 3 images from momentum flux ratio of 9 for injector 4 (previous case c)

- Linear intensity scale



- Enhanced contrast scale



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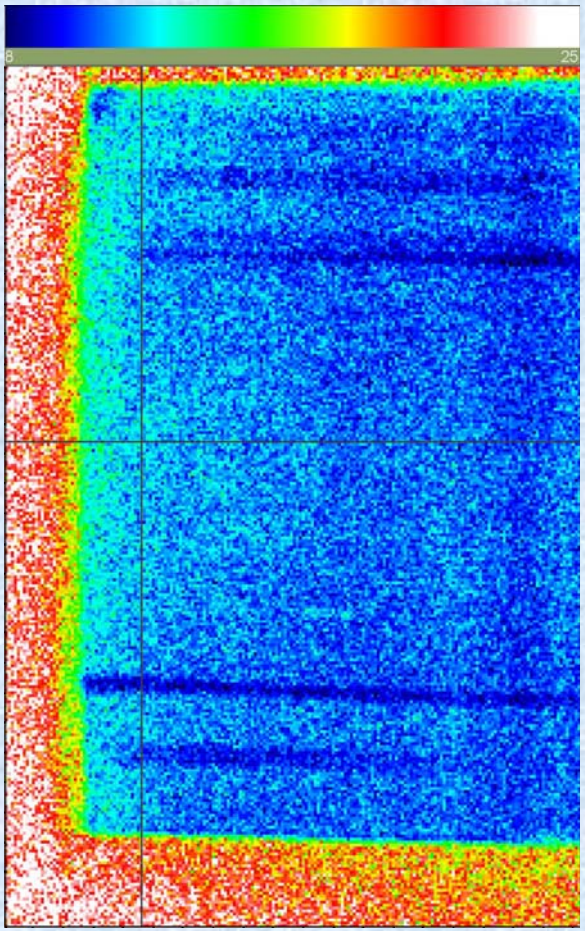
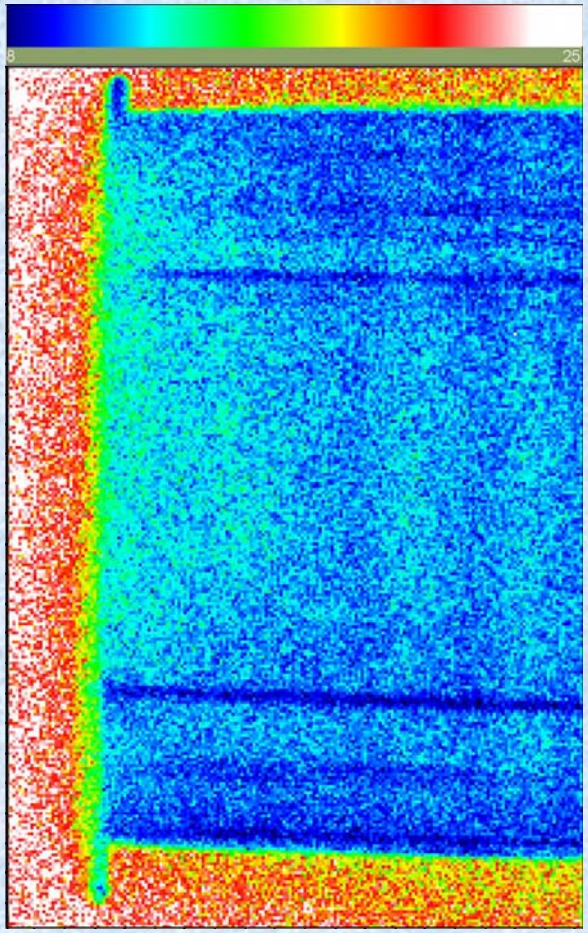
% RMS Variation in Acetone Concentration

Scale: 8 to 25%

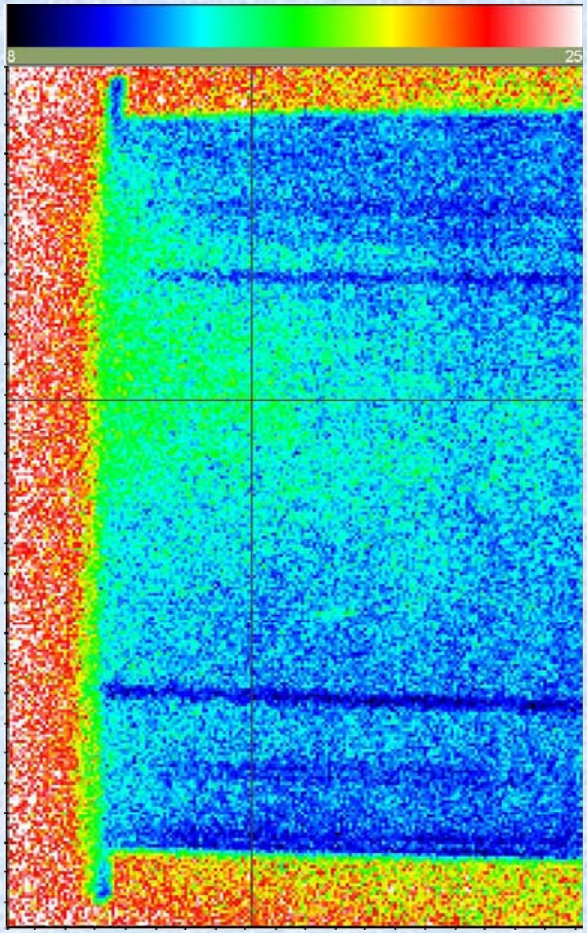
fully mixed



momentum flux ratio 33



momentum flux ratio 9



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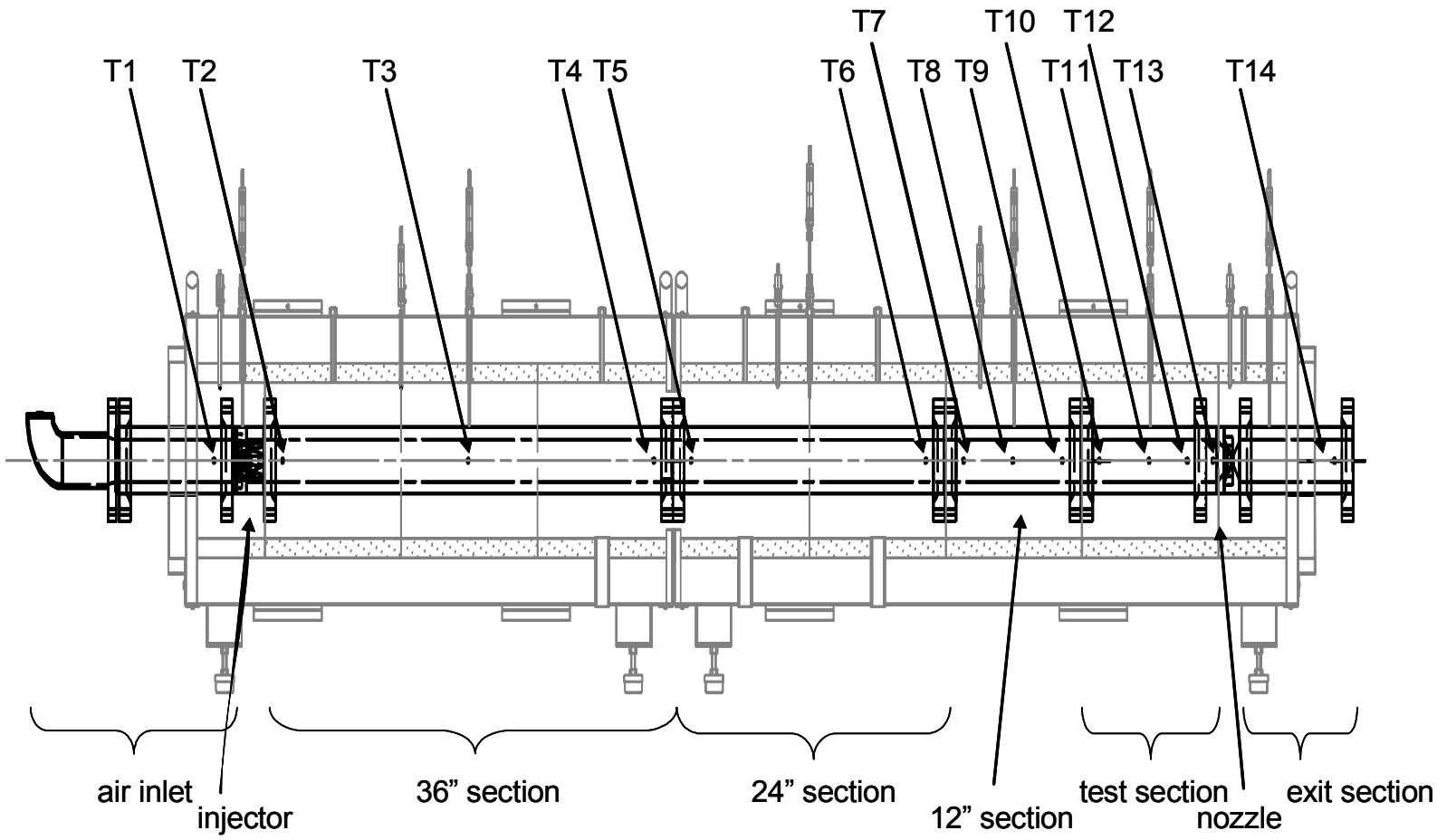
Wall Thermocouple Positions

Wall thermocouple positions



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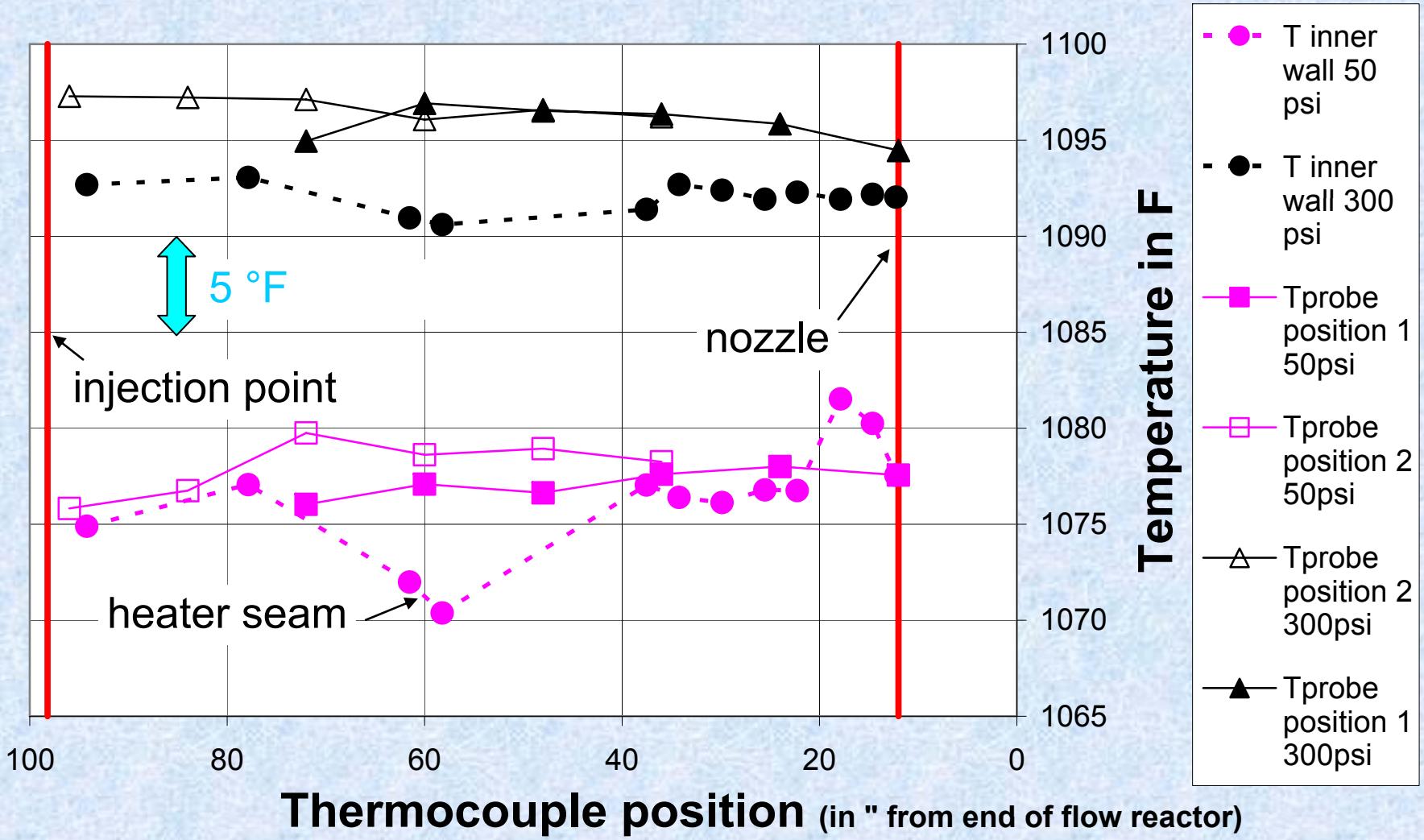
Detailed Probe Measurements



- **Heater outlet temperature: 1100F Clamshell heaters : 1100F**
- **2 flow rates: 0.15 lb/s (50 psi), 0.8 lb/s (300 psi)**
- **No nozzle water**

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Experimental Method

- Start at a set nominal chamber velocity, pressure, fuel composition and equivalence ratio
  - The size of the exit nozzle sets the chamber velocity and the pressure is a function of the flow rate and equivalence ratio
- Ramp temperature up until autoignition occurs just upstream of nozzle
- Record autoignition characteristics
- Change equivalence ratio, pressure, fuel composition
- Change chamber velocity

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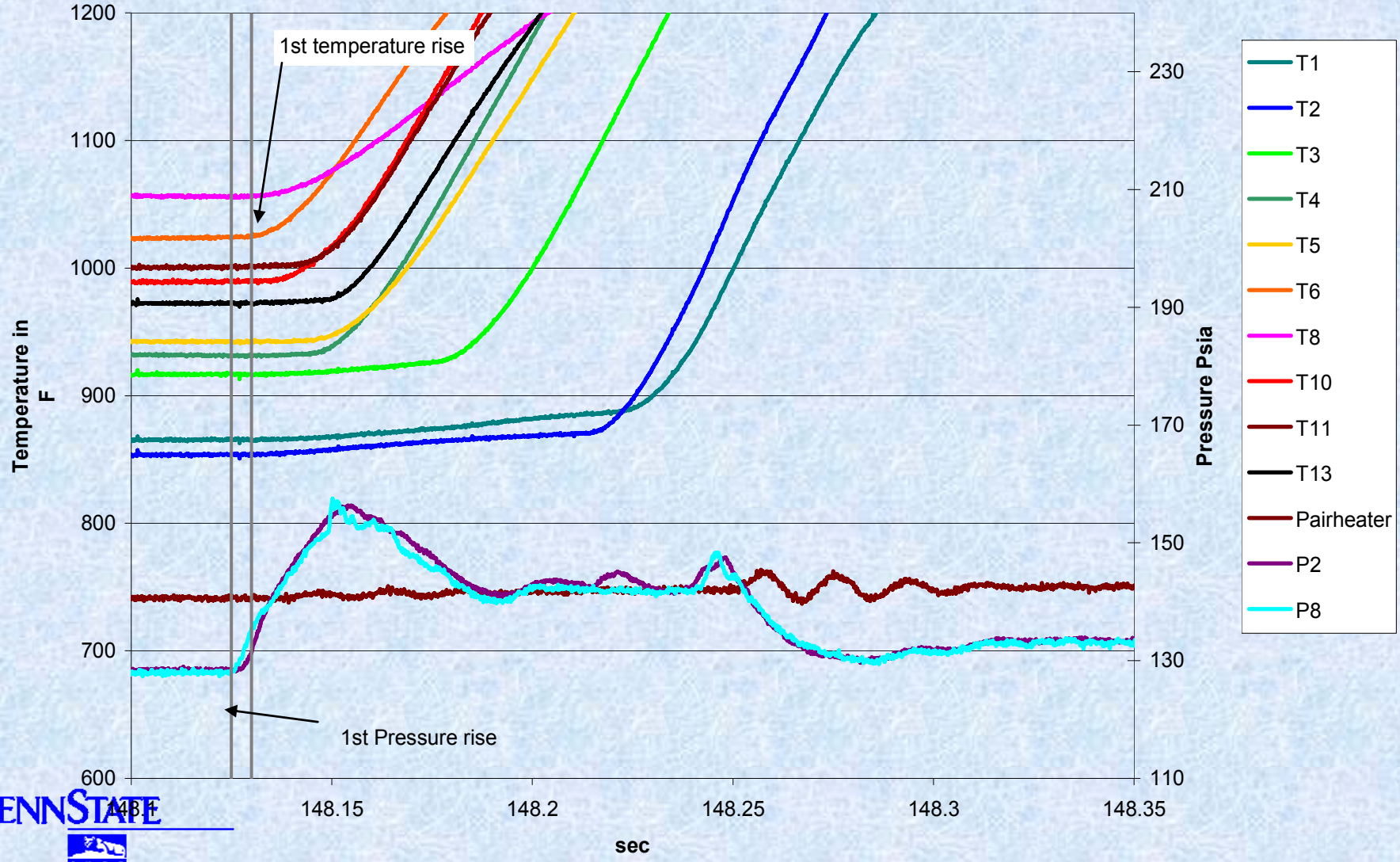
Results

Example Thermocouple Measurements



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Variations in Autoignition Measurements (1)

- There are observations of ignition near the injector face as the air temperature is increased from its starting value.
- More specifically such ignition events occur in the region between the injector face and first downstream thermocouple (T2), that is 10.1 cm (3.98 in.) downstream of the injector face.

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Variations in Autoignition Measurements (2)

- When autoignition does occur in the flow reactor tube downstream of the injector, the location of the event varies in terms of the position in the flow reactor tube for similar conditions
- Finally, often under similar operating conditions no autoignition was observed.
- For cases where autoignition occurred in the flow reactor tube, the resulting autoignition results are similar to autoignition times observed by other researchers.

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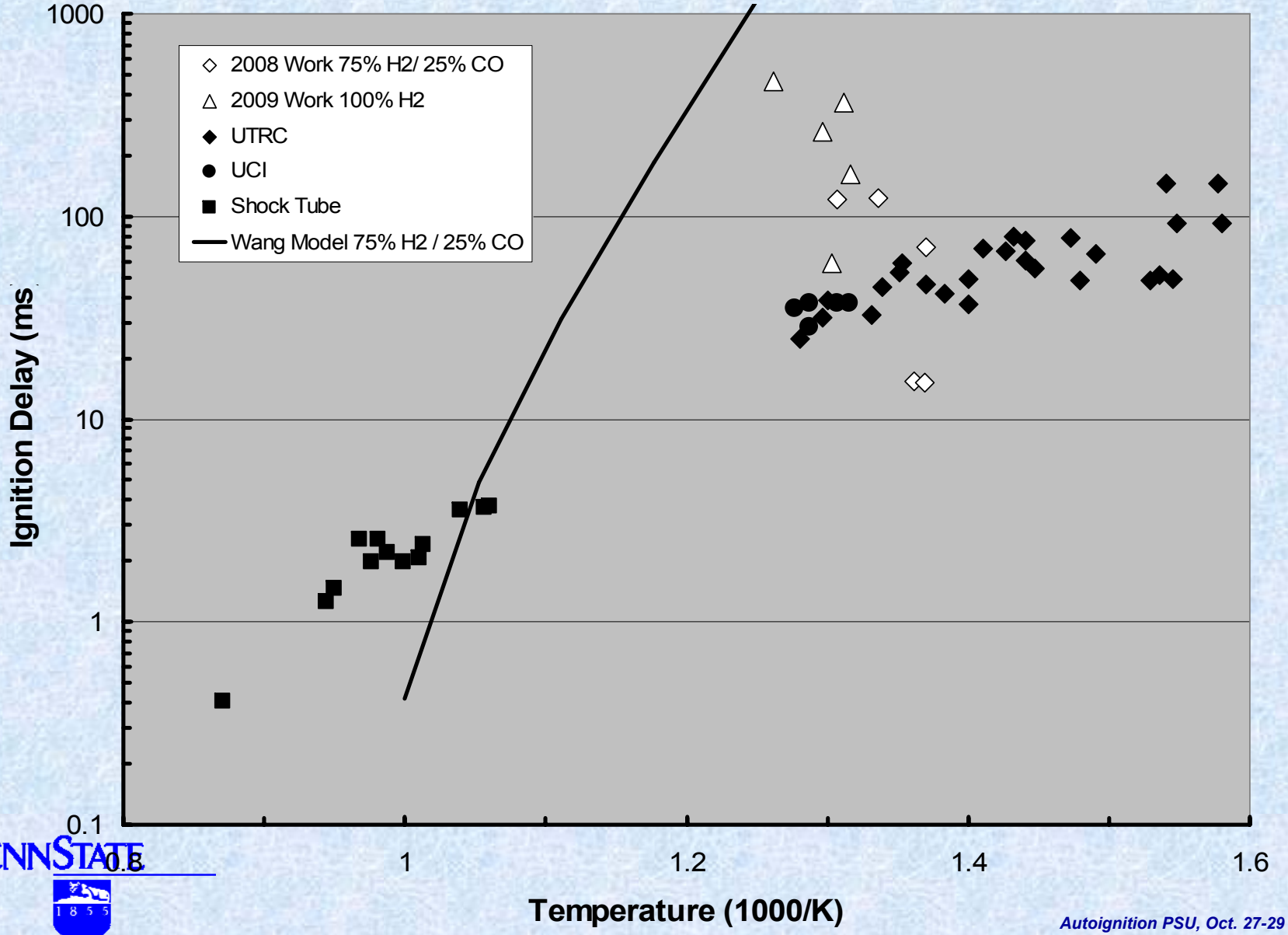
Plot of the Results for the Autoignition Time for Cases Where Ignition Occurred in the Reactor Tube



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Tabulated Data

	ϕ	% H_2 in Fuel	P (atm.)	T (K) at ign. Loc	velocity (m/s)	t (ms)	t_{adj} (ms) to 20 atm
2008 Work (75% H_2/25% CO)	0.98	74.3	9.6	748.2	8.9	258.0	123.2
	0.98	74.0	9.8	734.4	8.7	31.2	15.3
	0.99	73.9	9.7	730.2	8.7	31.2	15.1
	0.97	73.7	10.2	764.9	8.4	236.4	121.1
	0.98	73.2	10.0	730.1	8.4	142.3	70.9
2009 Work (100% H_2)	0.51	100	23.3	792.5	4.3	396.0	461.1
	0.52	100	23.0	759.6	4.3	139.4	160.4
	0.51	100	22.7	762.5	4.3	323.1	366.3
	0.47	100	24.7	767.3	4.2	48.0	59.1
	0.51	100	23.9	771.2	4.4	217.6	259.6

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Comparisons

75%H2/25%CO

- T_{ign}: 730-765K
- P: 9.6 – 10.2 atm
- τ : 31-258 ms
- V= 8.4 – 8.9 m/s

100% H2

- T_{ign}: 760-792K
- P: 22.7 – 24.7 atm
- τ : 59-461 ms
- V= 4.2 - 4.4 m/s

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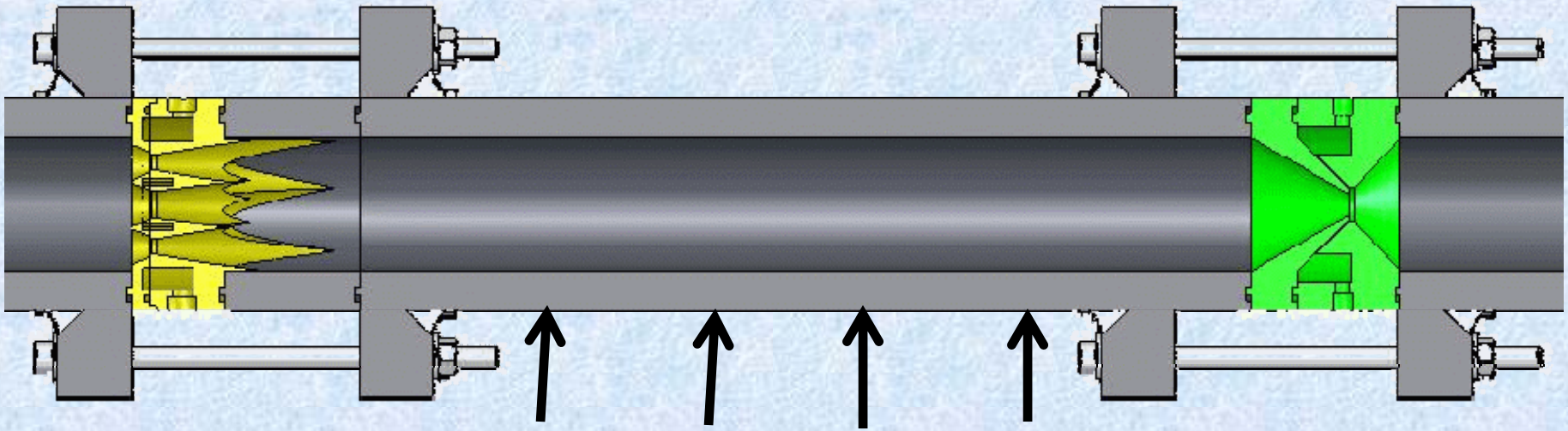
Notional Schematic

$$\tau = L/v$$



Hypothetical Ignition Locations

Related Work in Flow Reactors

Autoignition of H_2: φ = 0.2-0.6; T_{mix} = 700-800K; P =5-7 atm

Beerer and McDonell J. Engr. Gas Turb. and Power, 130 (2008)

- **"Full ignition (temperature rise of several hundred degrees) only occurred at higher temperatures but was rather sporadic, occurring only roughly one-half the time within the time scale of the experiment."**
- **Examples:**
  - **At residence time of 180 ms ignition was seen as low as 750K, however for another run with the same residence time at 795 K, ignition did not occur.**
  - **For a residence of 400 ms where ignition should occur at a lower temperature, ignition was not observed until 780K.**

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Beerer and McDonell J. Engr. Gas Turb. and Power, 130 (2008)

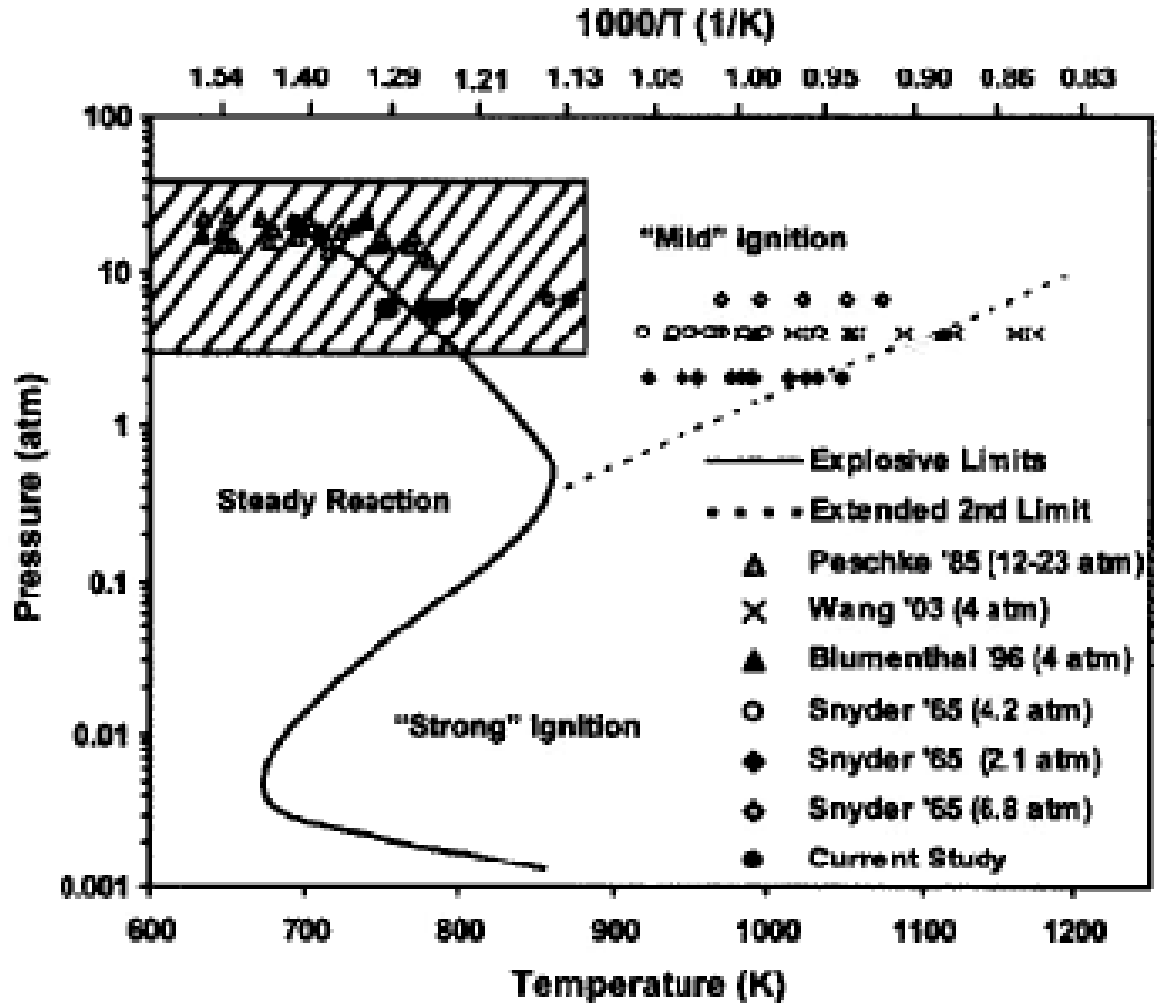

Fig. 8 Hydrogen-oxygen explosion limit chart with experimental test conditions identified. The shaded region represents typical gas turbine combustor inlet temperatures and pressures.

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Earlier Ignition Studies of Hydrogen and Hydrocarbons Using Shock Tubes

- V. V. Voevodsky and R. I. Soloukhin, 10th Symposium (International) on Combustion, 279-283 (1965)
- J. W. Meyer and A. K. Oppenheim, 13th Symposium (International) on Combustion, 1153-1164 (1971)
- D.J. Vermeer et al. Combust. Flame, 18, 327-336 (1972)
- R. K. Cheng and A. K. Oppenheim, Combust. Flame 58, 125-139 (1984)
- K. Feiweger et al. Combust. Flame, 109, 599-619 (1997)
- Huang et al., Combust. Flame, 136 25-42 (2004)

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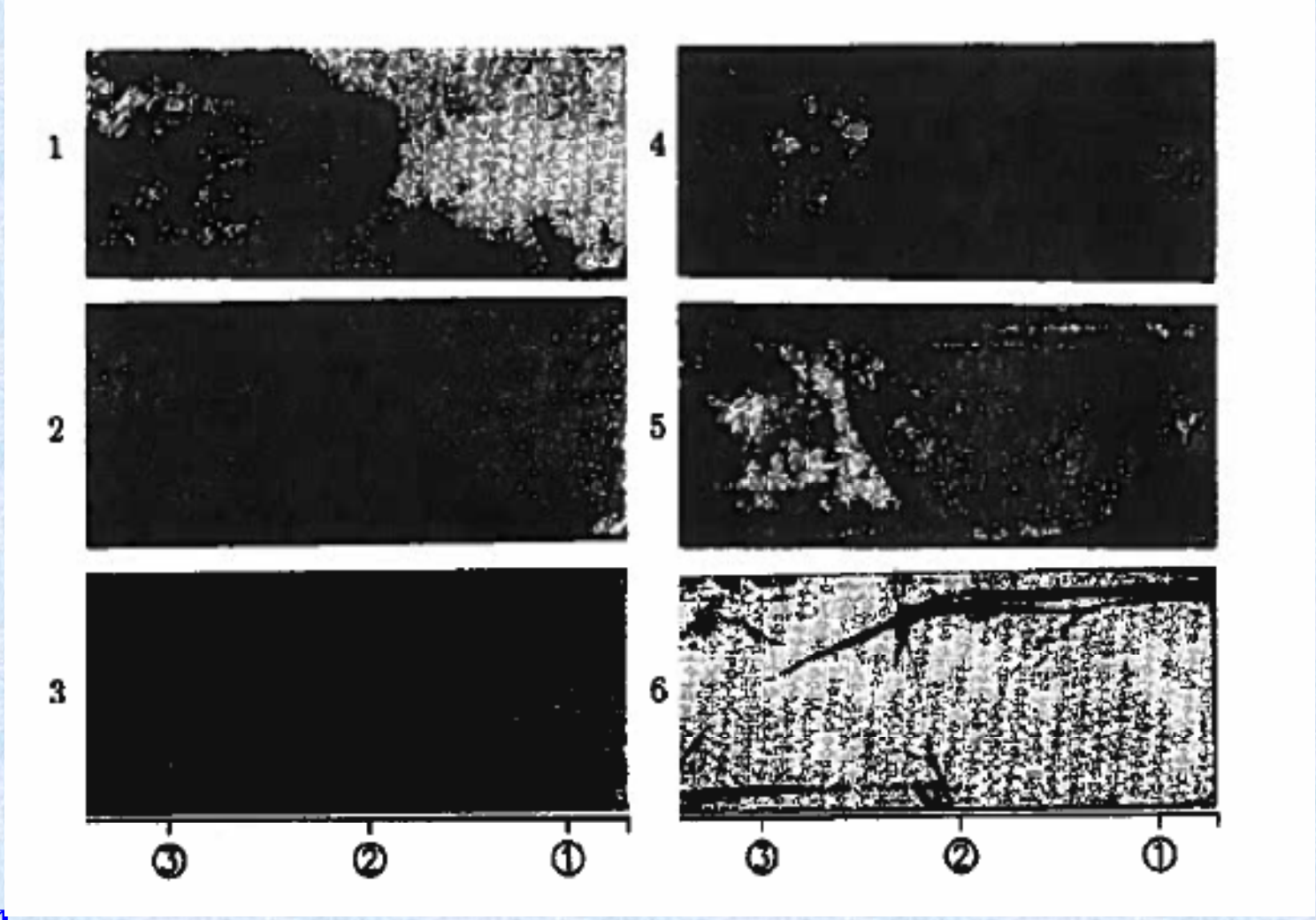
Fieweger et al., Combust. Flame, 109, 599-619
Iso-octane; T=1028K, P=13.5 bar; Φ=1

Δt=10 μs



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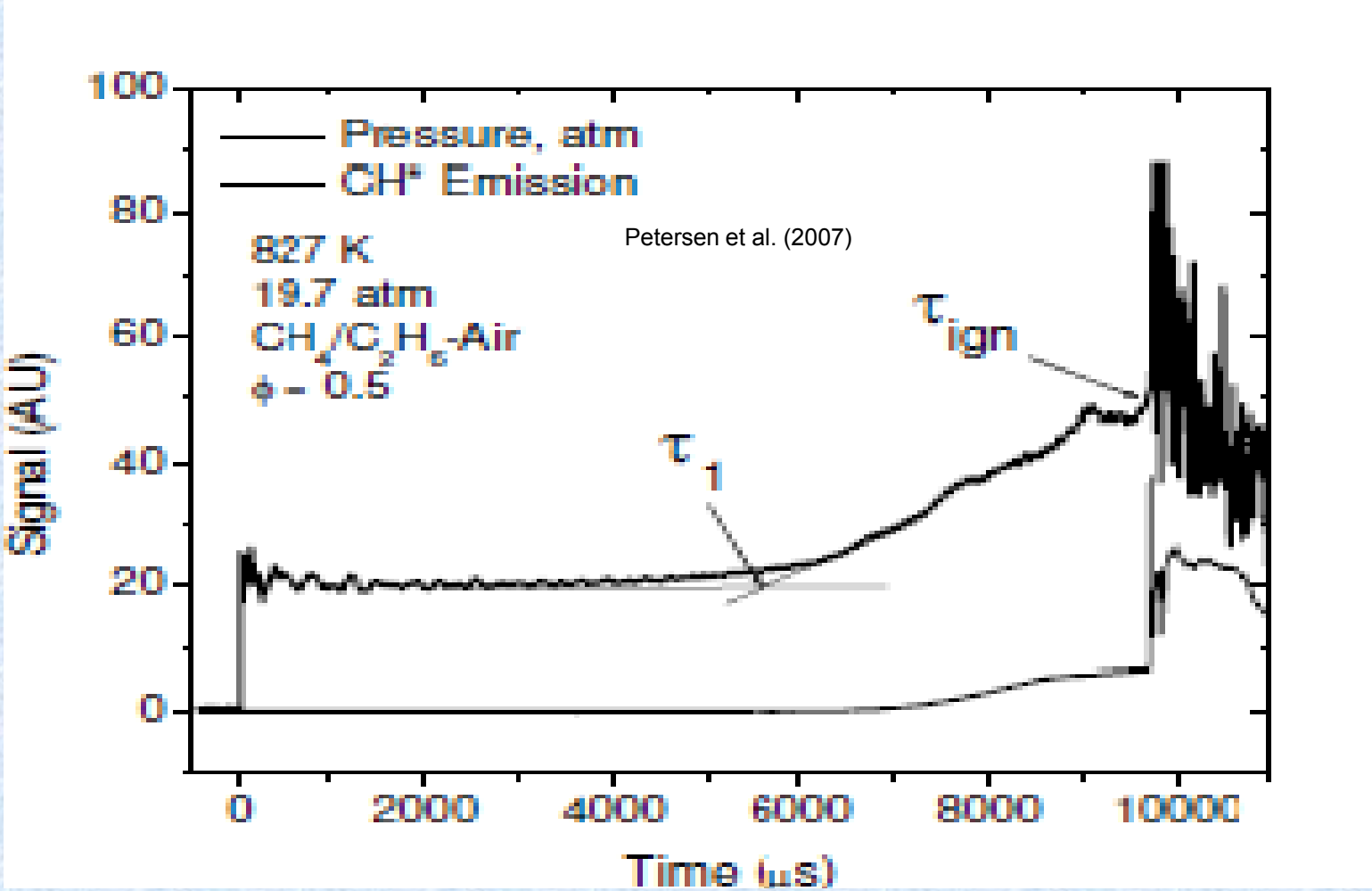
Recent Developments in the Analysis of Shock Tube Data for High P/Low T Conditions



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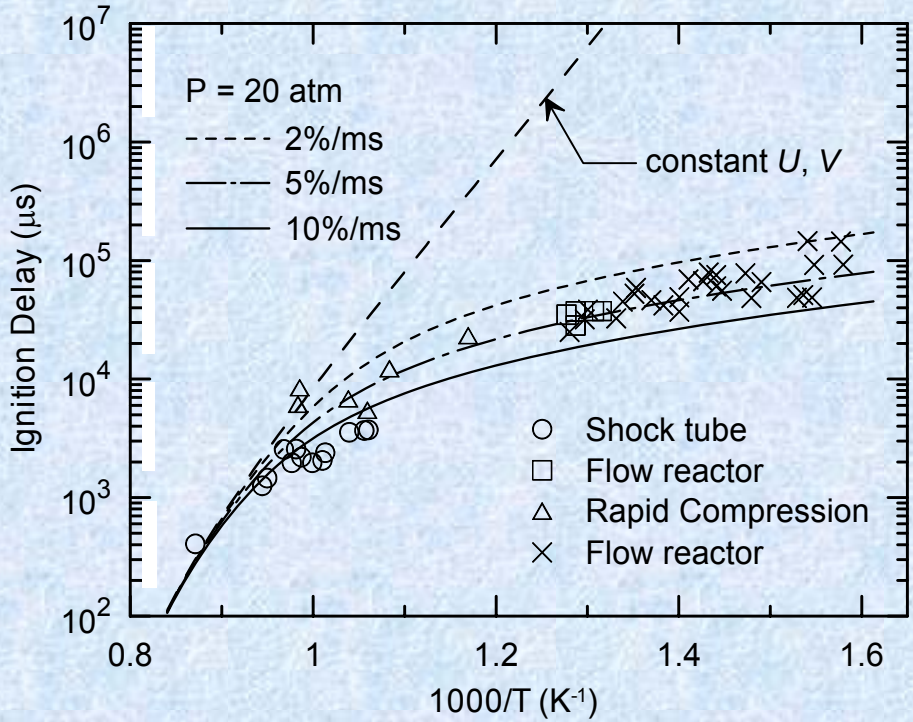
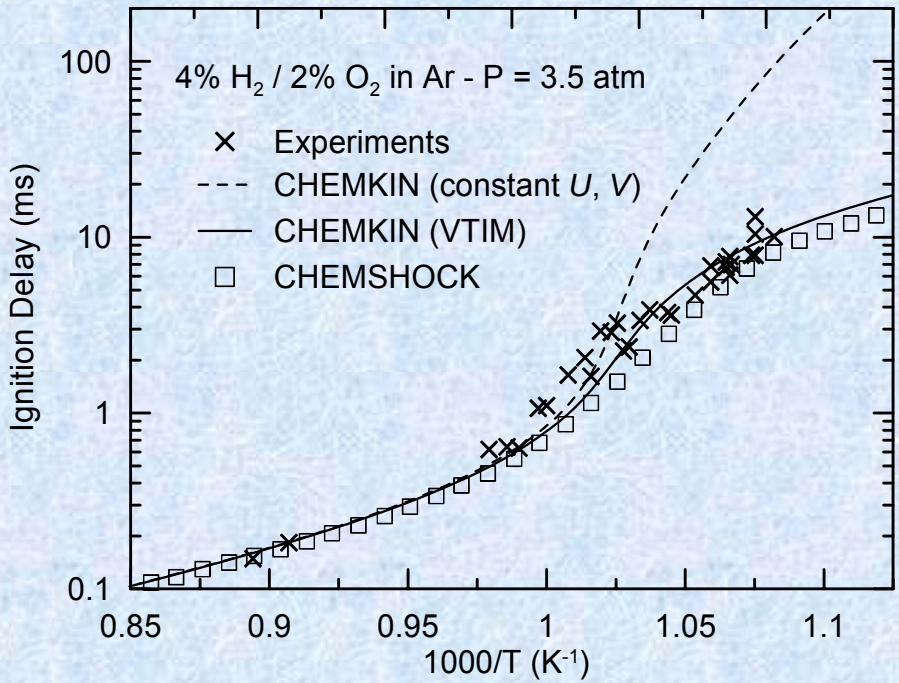
Interpreting Experimental Ignition Delay Observations





- Chemical ignition delay is composed of chemical induction time and post induction reaction. The chemical induction time results in the pressure rise observed in the shock tube experiments, which invalidates the use of a constant U,V assumption.
- Modifying the analysis to take into account the effects introduced by this chemical induction time can be treated using “volume as a function of time” approach, which brings the data and modeling predictions into agreement.

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What about the flow reactor results?

- The picture is not clear at the moment as the gas dynamic effects seen behind a reflected shock wave are not present in the flow reactor studies.
- However, the high sensitivity of the near third explosion limit region to small perturbations in concentration and temperature may be responsible for the variability observed in the ignition results.
- Other mechanisms such as wall catalysis, boundary layer effects etc., may be important and remain a topic of future work.

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Conclusions

- These studies revealed that the autoignition process for syngas is intrinsically variable in terms of the observed ignition delay time for operating conditions at which these studies were conducted.
- The source of this unexpected variability is not yet clearly understood, but does present a major uncertainty with respect to the use of syngas under lean premixed conditions.

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Project Team Members

- Dr. Geraldine Mouis, Research Staff Member
- Ms. Michelle Christensen, Graduate Student
- Dr. Sibtosh Pal, Senior Research Staff Member

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Acknowledgments

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F. L. Dryer, Princeton University;
E. L. Petersen, Texas A&M; T. A. Litzinger, Penn State

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Additional slide

Experimental Operating Conditions

Typical conditions for autoignition studies of syngas mixtures (H_2/CO_2)

phi	Mixed temp entrance of tube Beginning of run F	Mixed temp end of tube Beginning of run	Clamshells higher than flow temp	Mixed temp entrance of tube end run	Mixed temp end of tub end of run F	Fuel heated or hot	Injector inside clamshells	% H2 of fuel	Chamber pressure psia
1	780	835	yes	820	870	no	outside	75	135 to 145
0.6 or 0.5	840	960	yes	880	975	yes	outside	75 to 78	125 to 140
0.5	830	830	no	920	880	yes	Inside	75	125 to 135
0.5	820	820	no	900	870	no	Inside	75	230 to 250

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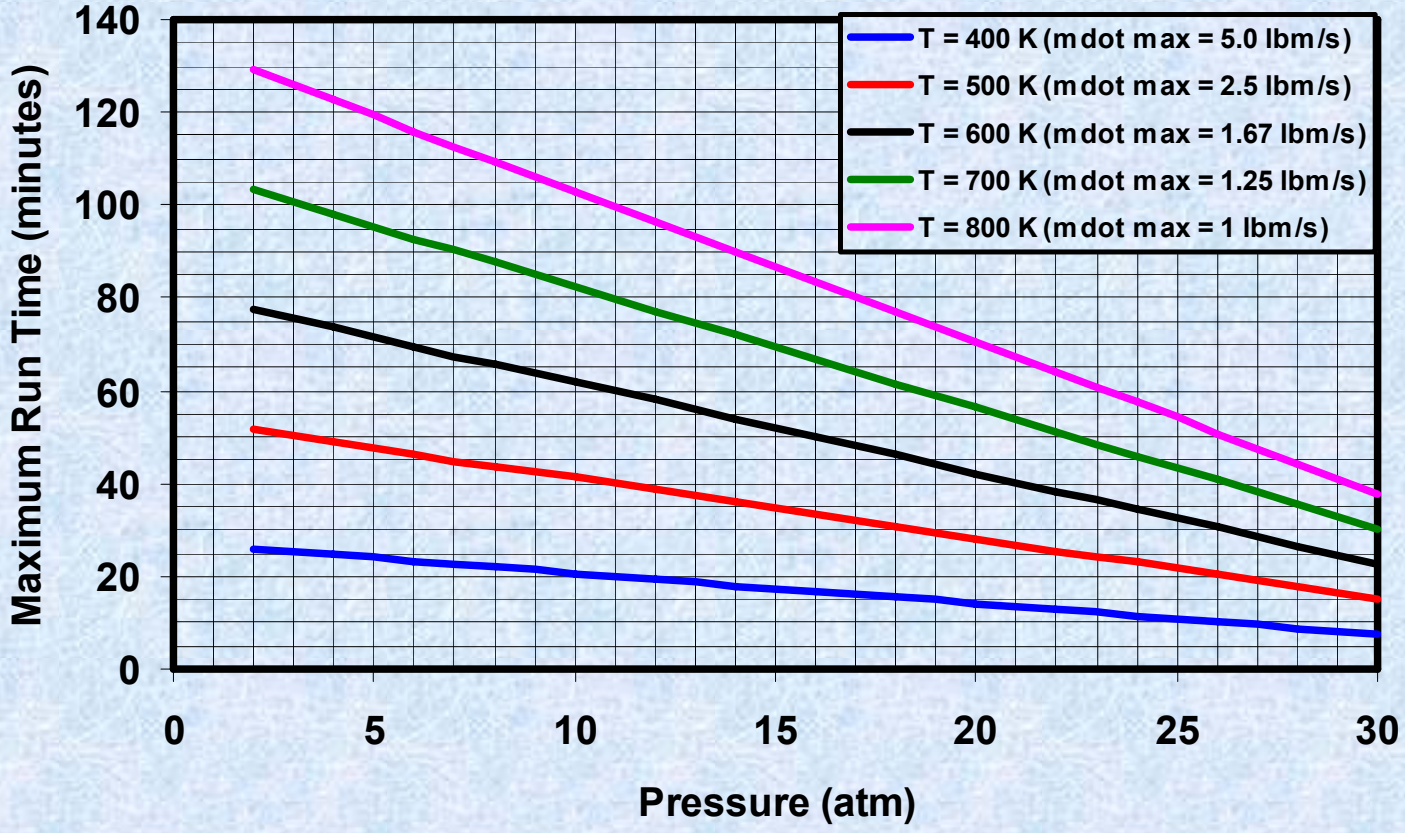
Questions?

Maximum Run Time vs. Pressure
(for 4.3 cm diameter tube)



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Thermocouple positions in inches

probe config2												
	T1	T2	T3	T4	T5	T6						
" from outlet Flange	96	84	72	60	48	36						
" from injection point	2.2	14.2	26.2	38.2	50.2	62.2						
" from 1st flange	0	12	24	36	48	60						
probe config1			T1	T2	T3	T4	T5	T6				
" from outlet Flange			72	60	48	36	24	12				
" from injection point			26.2	38.2	50.2	62.2	74.2	86.2				
" from 1st flange			24	36	48	60	72	84				
Inner wall	T2	T3	T4	T5	T6	T7	T8	T9	T10	T11	T12	T13
" from outlet Flange	94.225	77.875	61.525	58.225	37.525	34.225	29.875	25.525	22.25	17.875	14.625	12.25
" from injection point	3.975	20.325	36.675	39.975	60.675	63.975	68.325	72.675	75.95	80.325	83.575	85.95
" from 1st flange	1.775	18.125	34.475	37.775	58.475	61.775	66.125	70.475	73.75	78.125	81.375	83.75
Spacing between inner wall thermpcouples												
		T2-T3	T3-T4	T4-T5	T5-T6	T6-T7	T7-T8	T8-T9	T9-T10	T10-T11	T11-T12	T12-T13
		16.35	16.35	3.3	20.7	3.3	4.35	4.35	3.275	4.375	3.25	2.375
Outer wall	T1	T2	T3	T4	T5	T6						
" from outlet Flange	98	78	48	30	18	8						
" from injection point	0.2	20.2	50.2	68.2	80.2	90.2						
" from 1st flange	-2	18	48	66	78	88						

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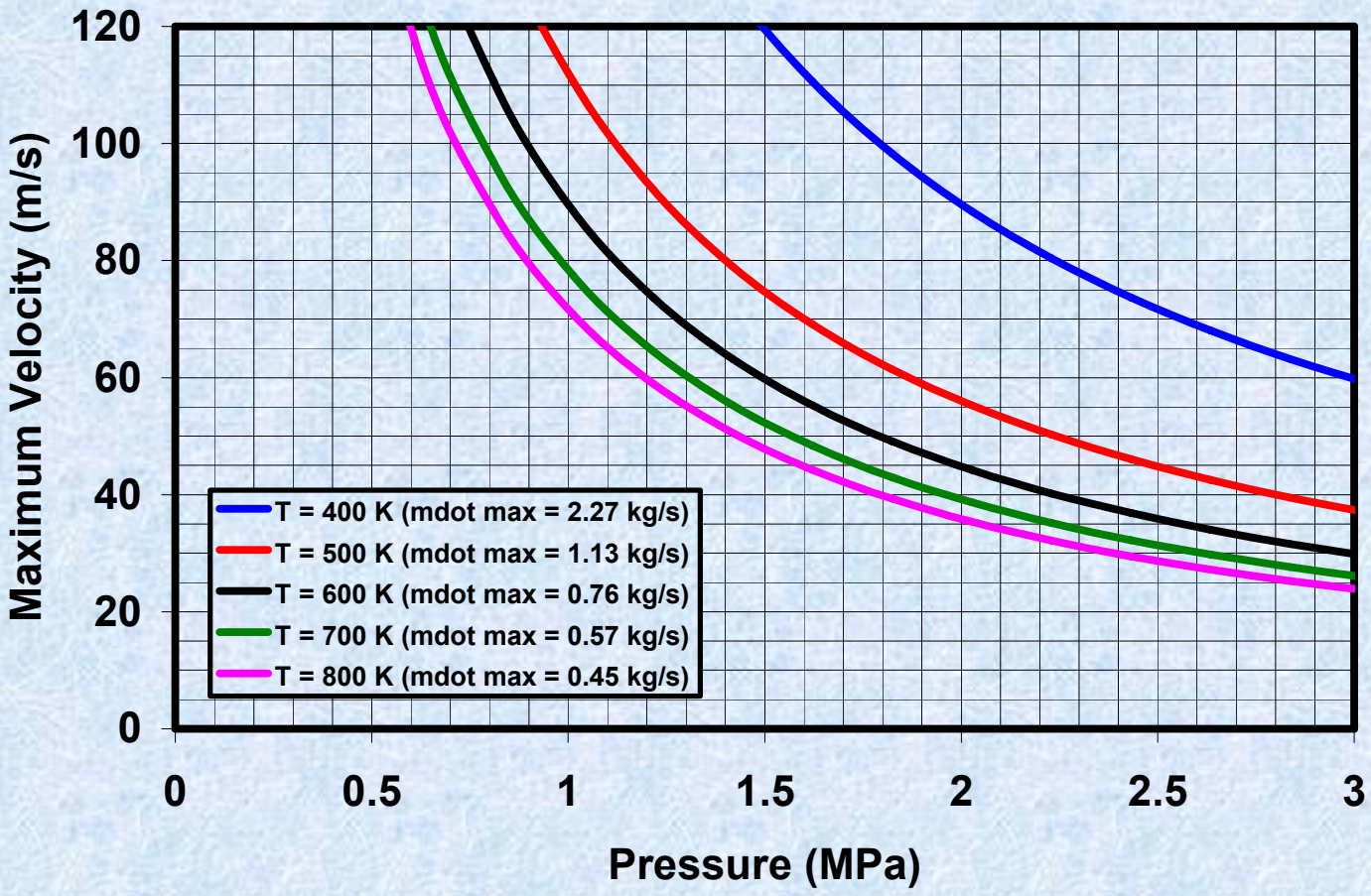
Maximum average air velocity in a 43-mm diameter flow reactor versus pressure. Note that with addition of fuel, the average velocities will be somewhat greater.



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