Ignition, turbulent flame speeds, and emissions from high hydrogen blended fuels

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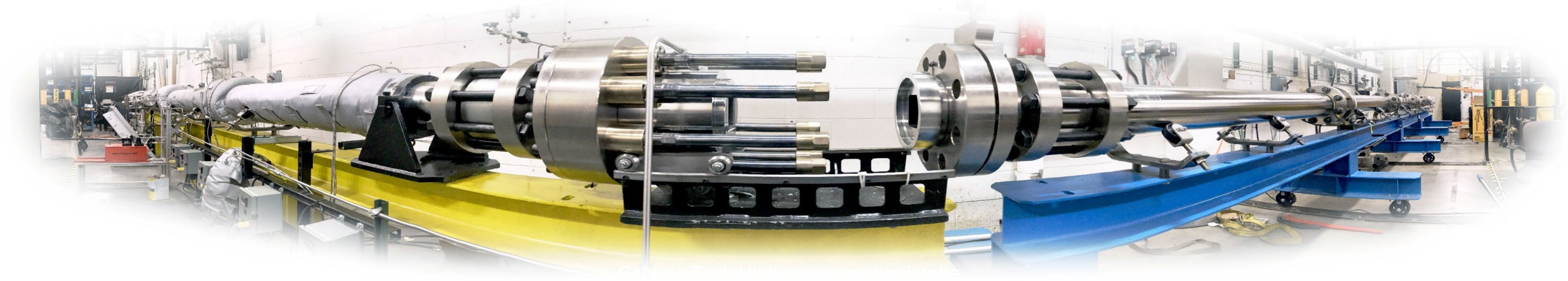
UTSR Workshop

Background and Motivation

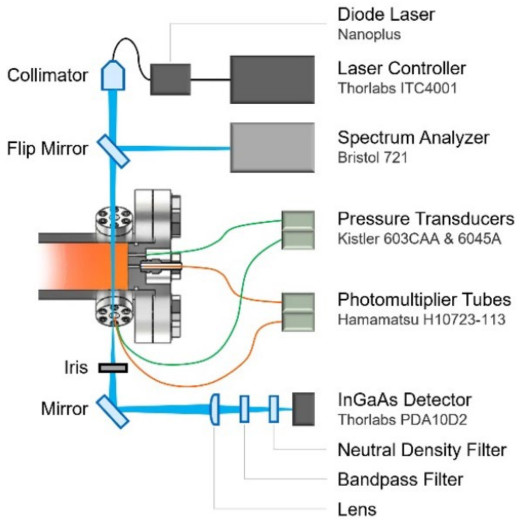
- Improve understanding of fundamental phenomena of hydrogen containing fuels for gas turbines.
- Pure hydrogen (H_2), carbon free hydrogen carrying fuels (such as ammonia, NH_3), mixtures of them and with natural gas
- Lots of data on autoignition delays and flame speeds exist, what is new?
  - Inconsistent trends on experimental data
  - Not much data at practical conditions (e.g., most data are in highly diluted environments)
  - Performance of existing kinetic models diverges significantly

Task 2: Investigation of Autoignition of Ammonia/Hydrogen

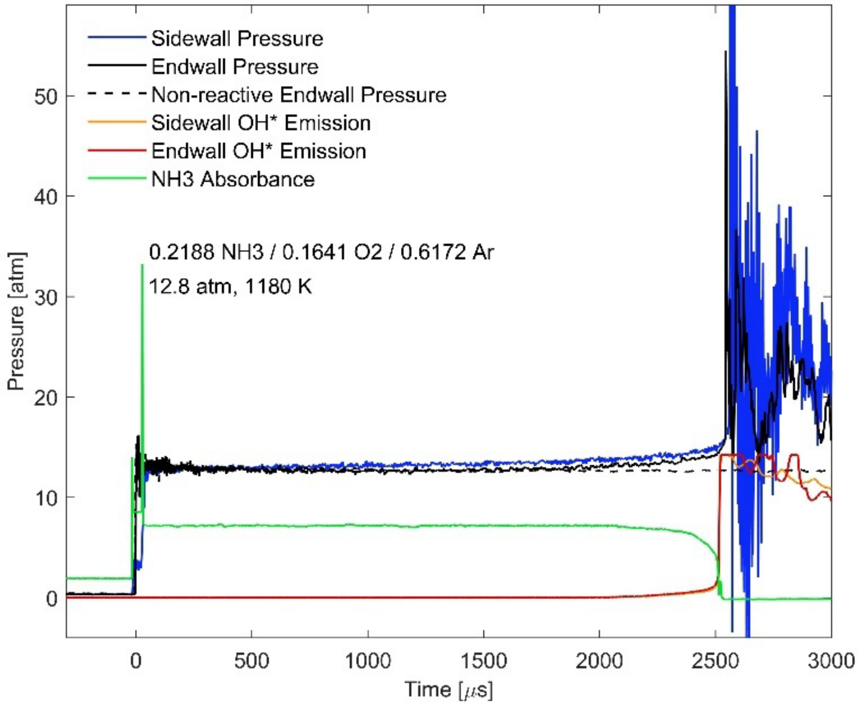


- Existing data are mostly in highly diluted environments
- Fuels: pure NH_3 and NH_3/H_2mixture
- Temperature range: 1100 K to 2200 K
- Equivalence ratio: 0.5, 1 and 2
- Pressure: ~10-20 atm
- Facility: high pressure shock tube

Schematic of experimental setup at the measurement section

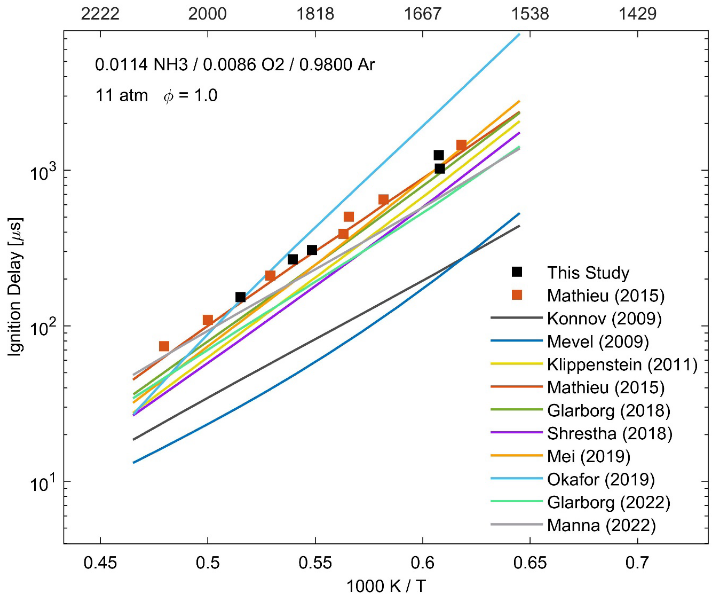


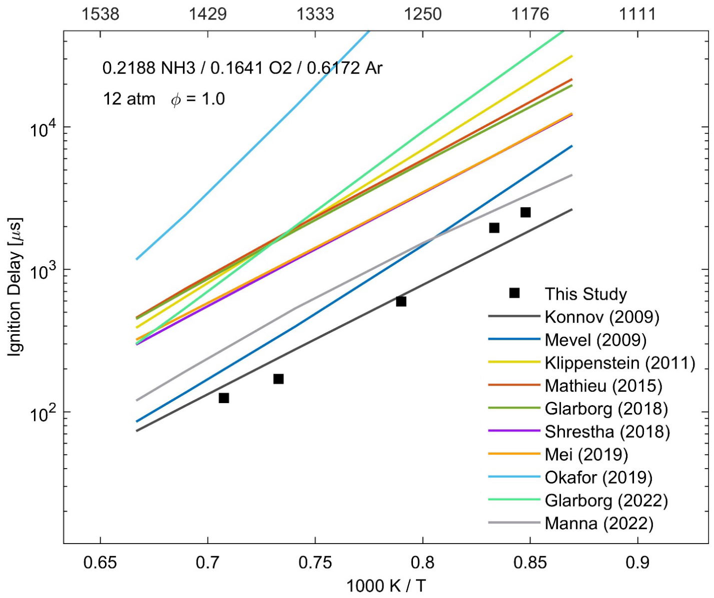
stoichiometric $NH_3/O_2/Ar$ mixture with 22% fuel at 12.8 atm and 1180 K.

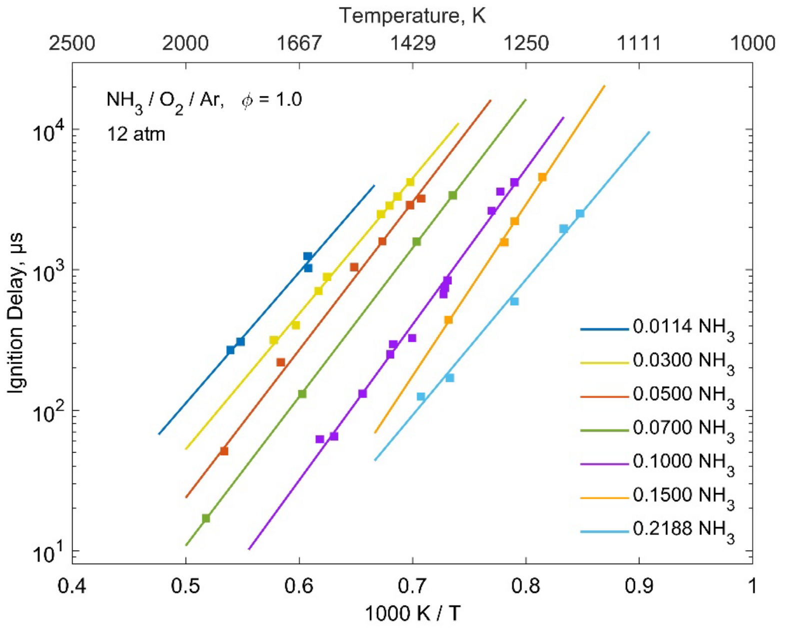


IDTs of NH_3

- There exists fuel concentration effect
- No model can reproduce experiments well at all conditions



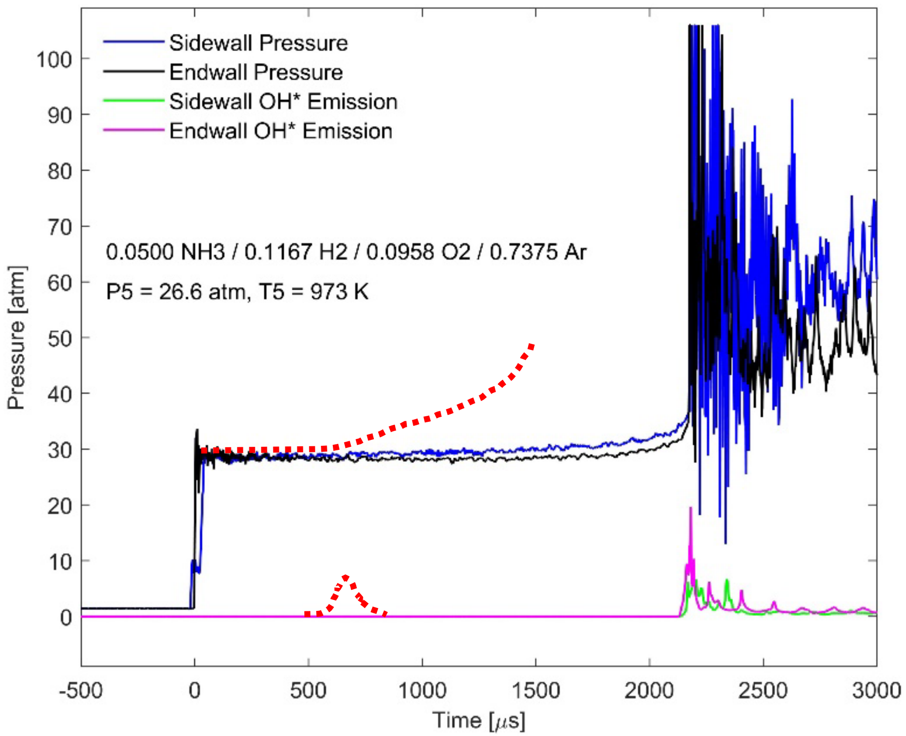


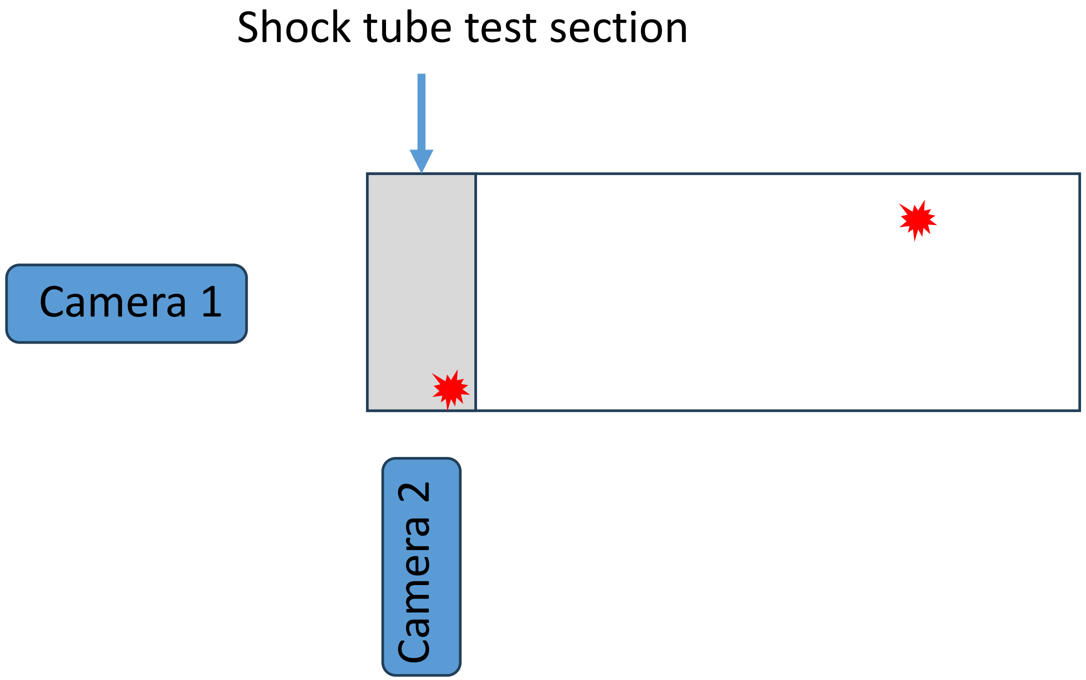


O. Mathieu, E.L. Petersen, *Combust. Flame* 162 (2015) 554-570.
R. Mevel, S. Javoy, F. Lafosse, N. Chaumeix, G. Dupre, C.E. Paillard, *Proc. Combust. Inst.* 32 (2009) 359-366.
A.A. Konnov, J. De Ruyck, *Combust. Sci. Technol.* 168 (2001) 1-46.

IDTs of NH_3/H_2

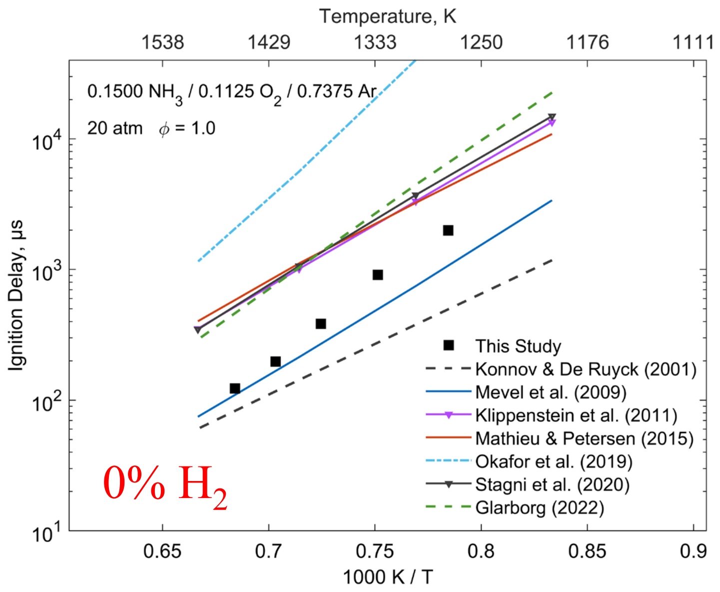
- NH_3/H_2 mixture to improve flame stabilization
- Rich NH_3 flame produce very significant amount of H_2
- Carefully selected experimental conditions
  - Ovoid premature ignition events for H_2

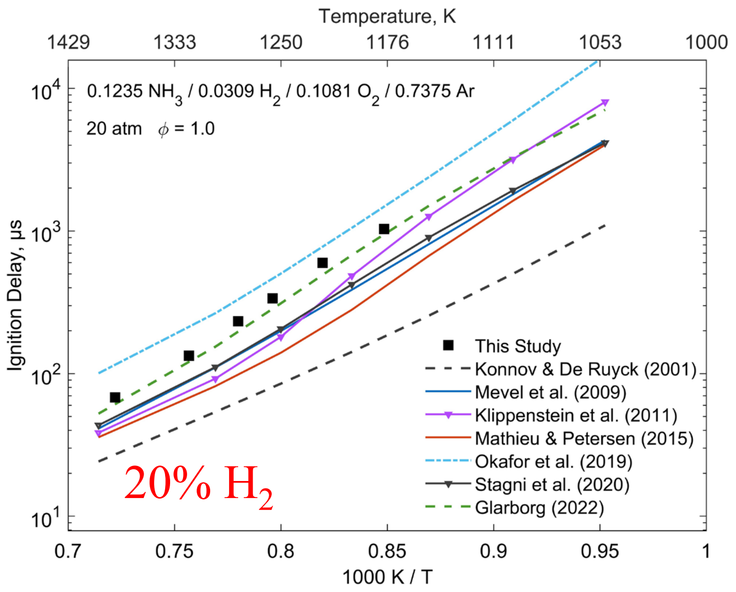


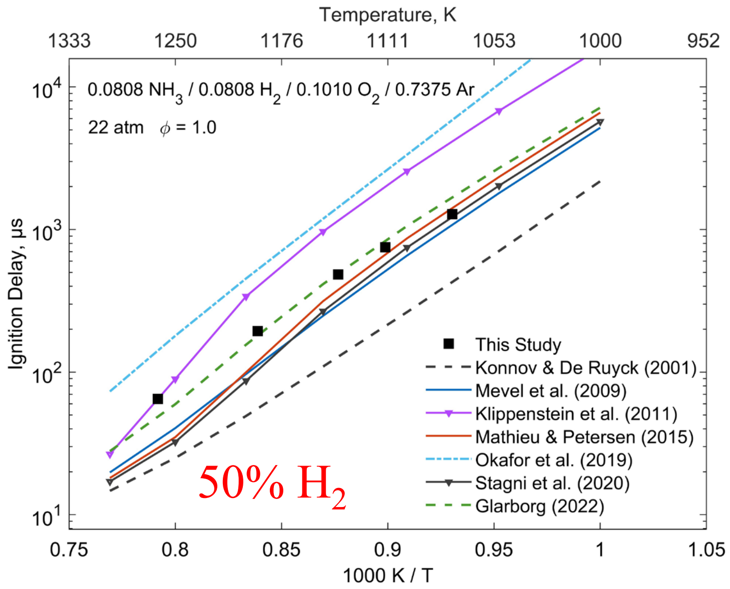


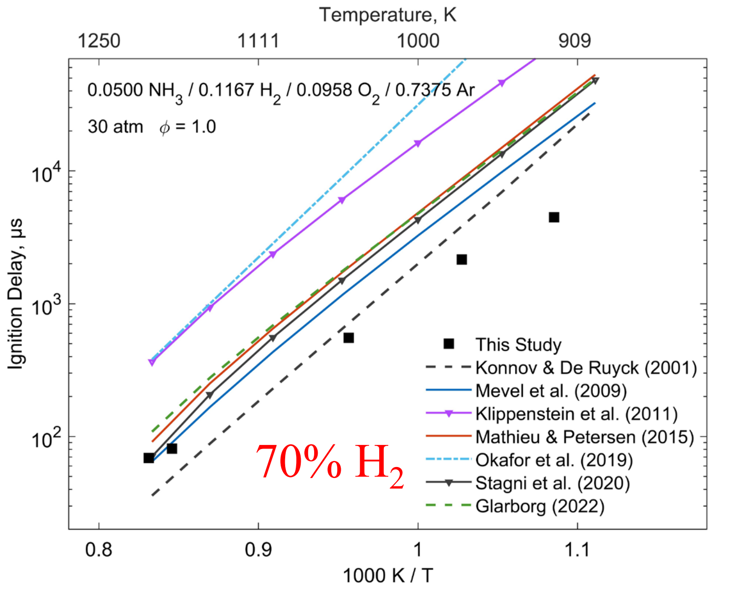
IDTs of NH_3/H_2

- Results & observations
- Good agreement with Glarborg (2022) at 20% and 50% hydrogen in fuel
- Can't fine one model fits all





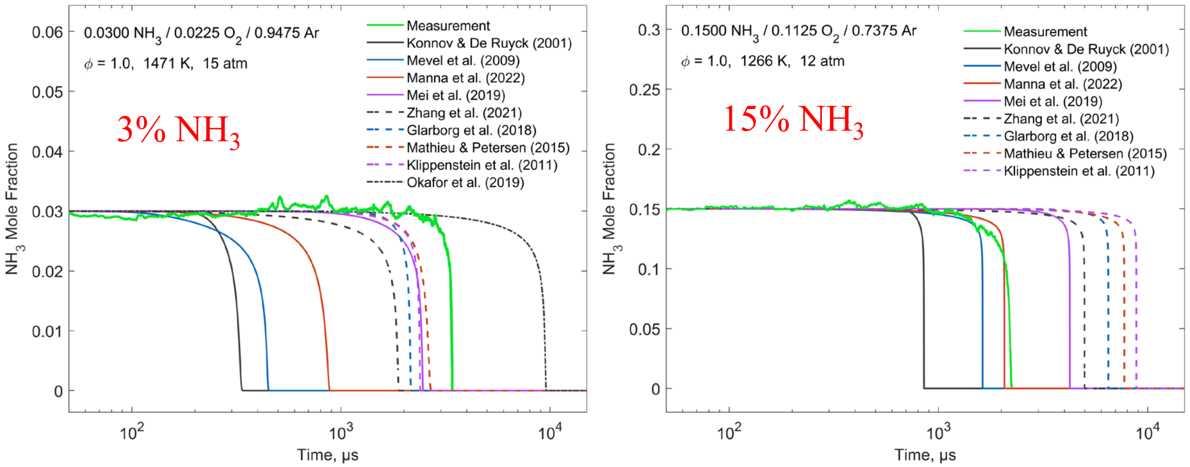




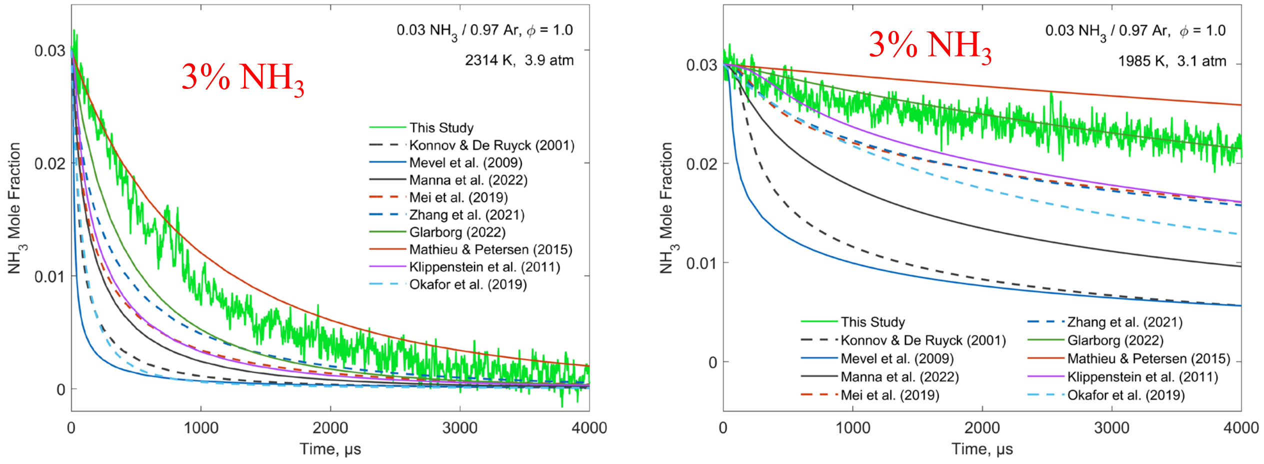
NH_3 Sensor & Speciation

- NH_3 absorption feature consisting of three closely spaced R-branch transitions in the ν_2+ν_3 combination band near 2.2 μm
  - adequate line strengths, relatively weak temperature dependence, and good spectral isolation from other possible interfering species commonly found at high-temperature combustion conditions, such as H_2O and CO.
- Thoroughly characterized (manuscript under review)
  - Collisional broadening coefficients dependence on pressure & temperature

oxidation

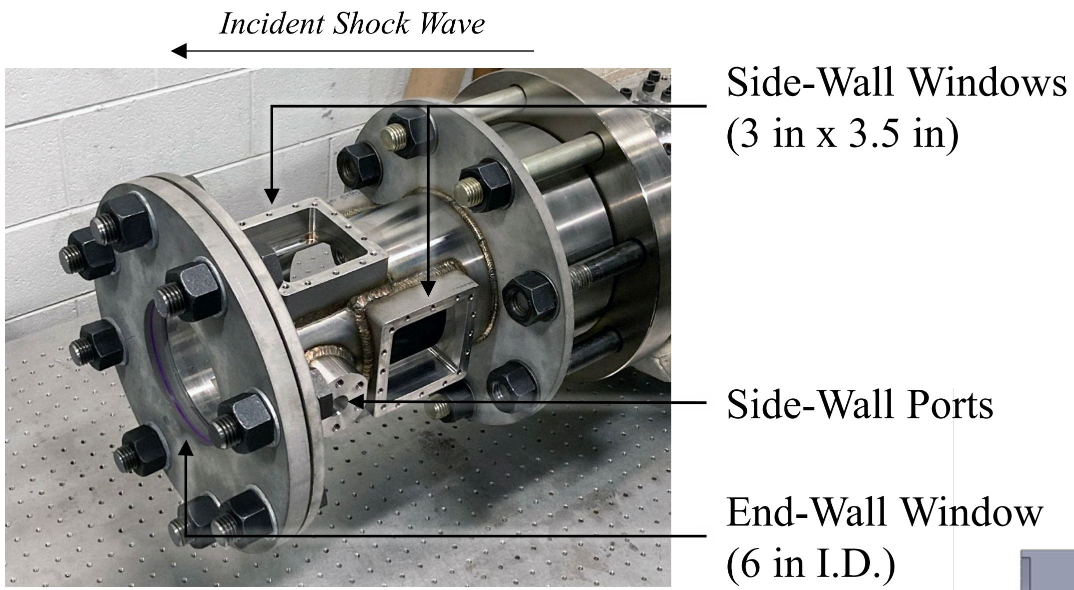


pyrolysis

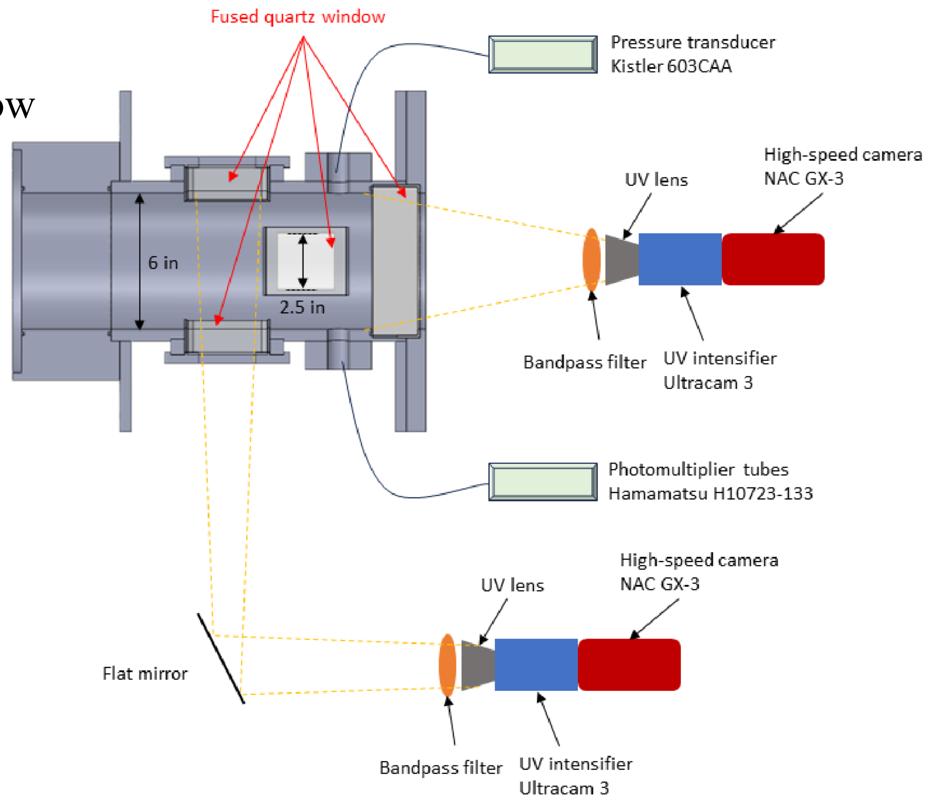


2D Imaging of Shock Tube

End View



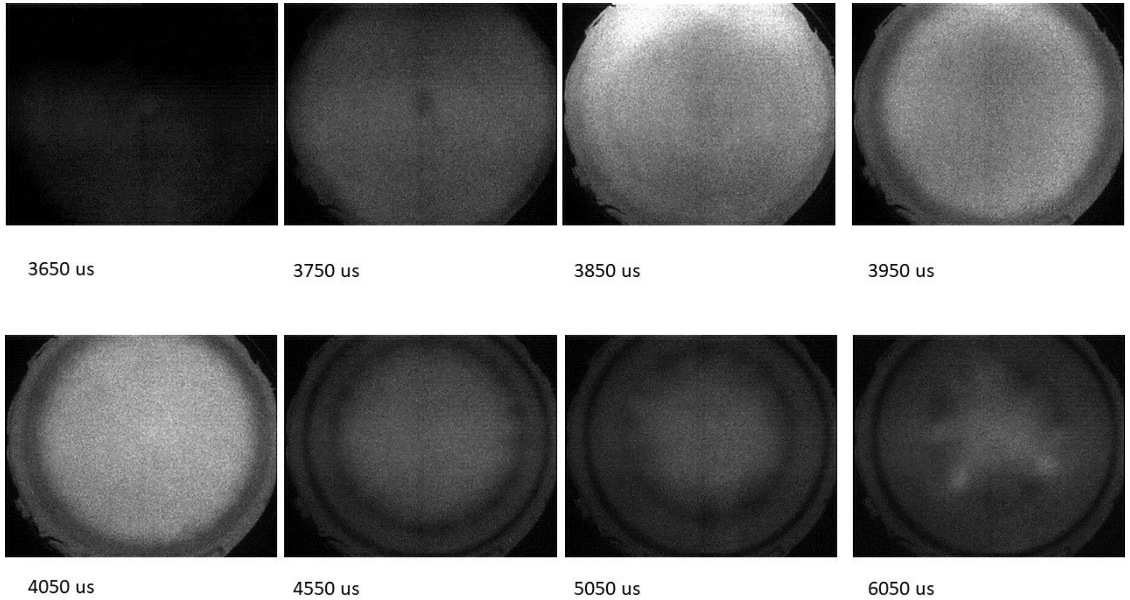
Isometric View



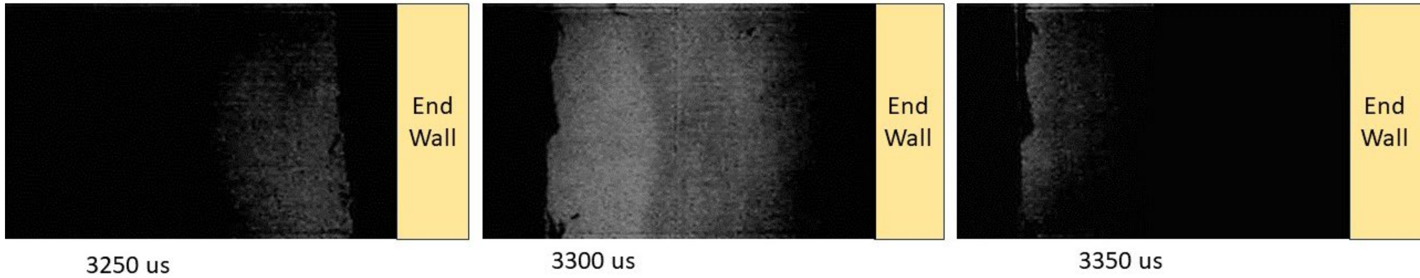
- 6-in-diameter optical access from end-wall and effective 3-in-by-7-in from side-wall
- 2D optical access allows examination of ignition uniformity and flame speed measurements

Preliminary Results

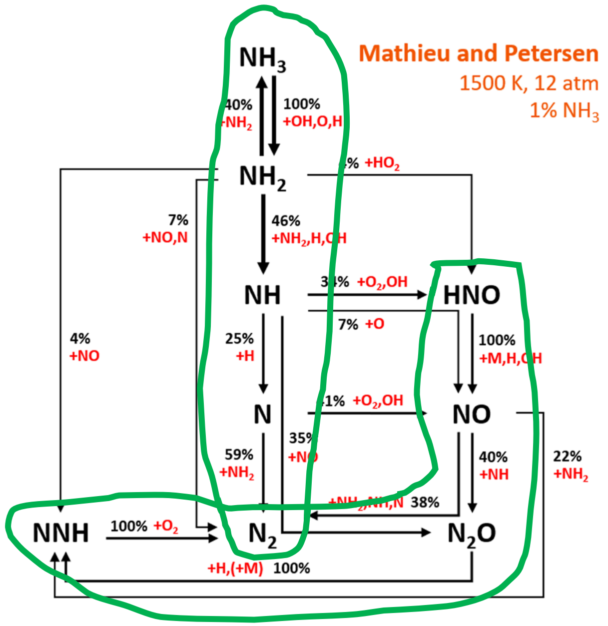
Highs-speed images for hydrogen mixture from end-wall
P=5.8 atm, T=1044 K
Measured 808 *μ* *vs* Computation 877 *μ*

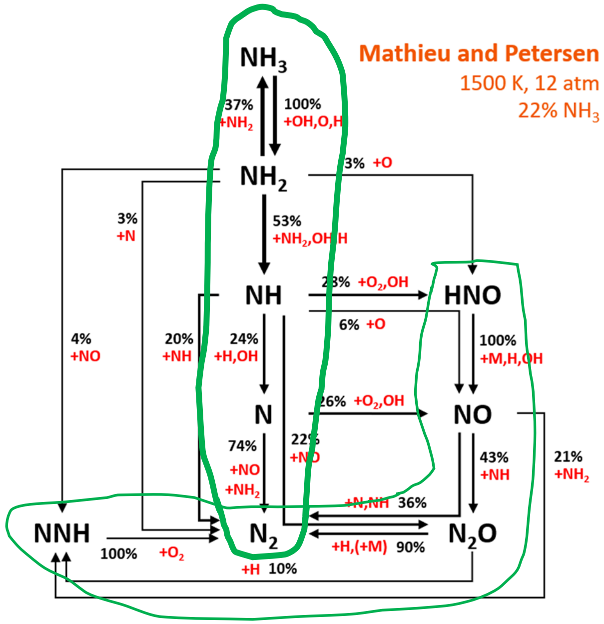


Highs-speed images for hydrogen mixture from sidewall
P=6.2 atm, T=1087 K
Measured 250/200 *μ* (P&OH) *vs* Computation 340/280 *μ*
(FFCM/NUIGMech 1.1)

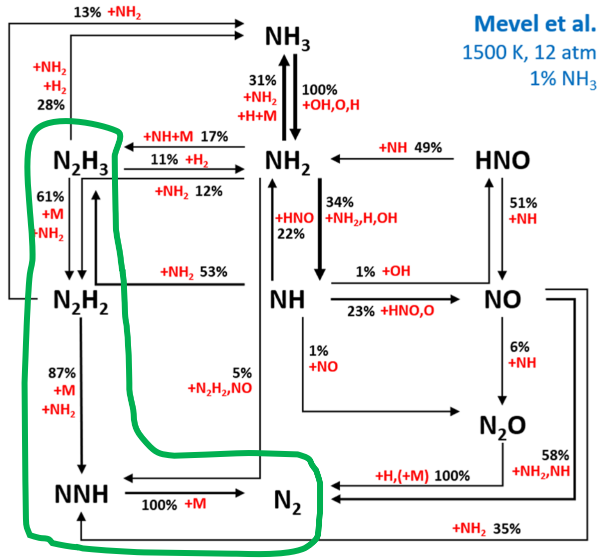


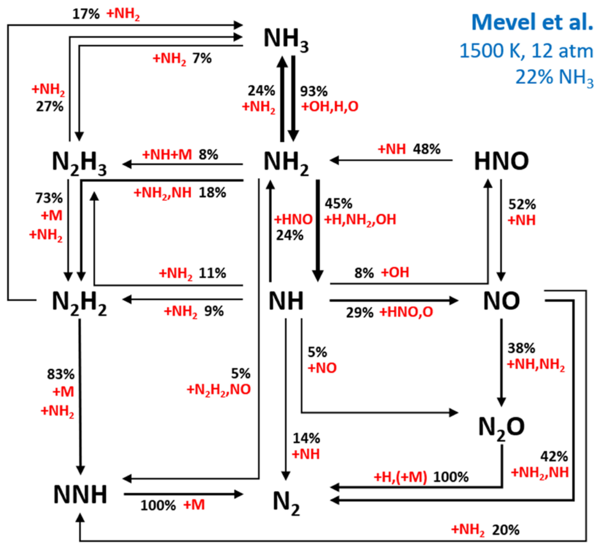
Mechanism Optimization : Reaction Pathway Analysis





- Low fuel
  - NH_2-NH-N-N_2
  - HNO-NO-N_2O-NNH-N_2
- High fuel
  - HNO-NO-N_2O-NNH-N_2 less important





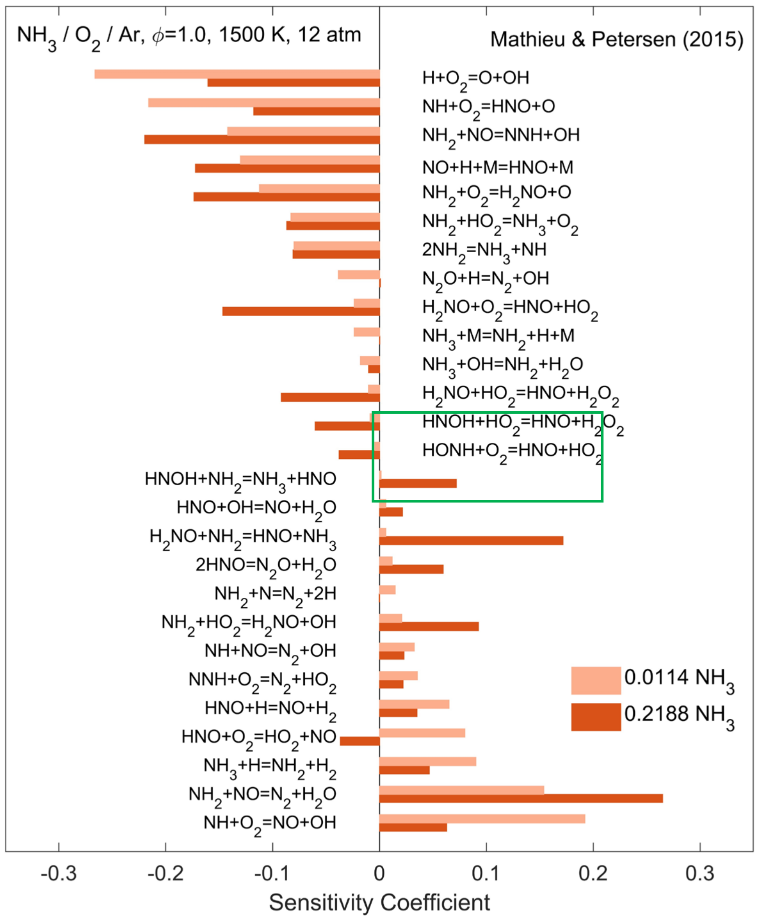
- Additional path through N_2H_3-N_2H_2-NNH-N_2

Mechanism Optimization : Reaction Pathway Analysis

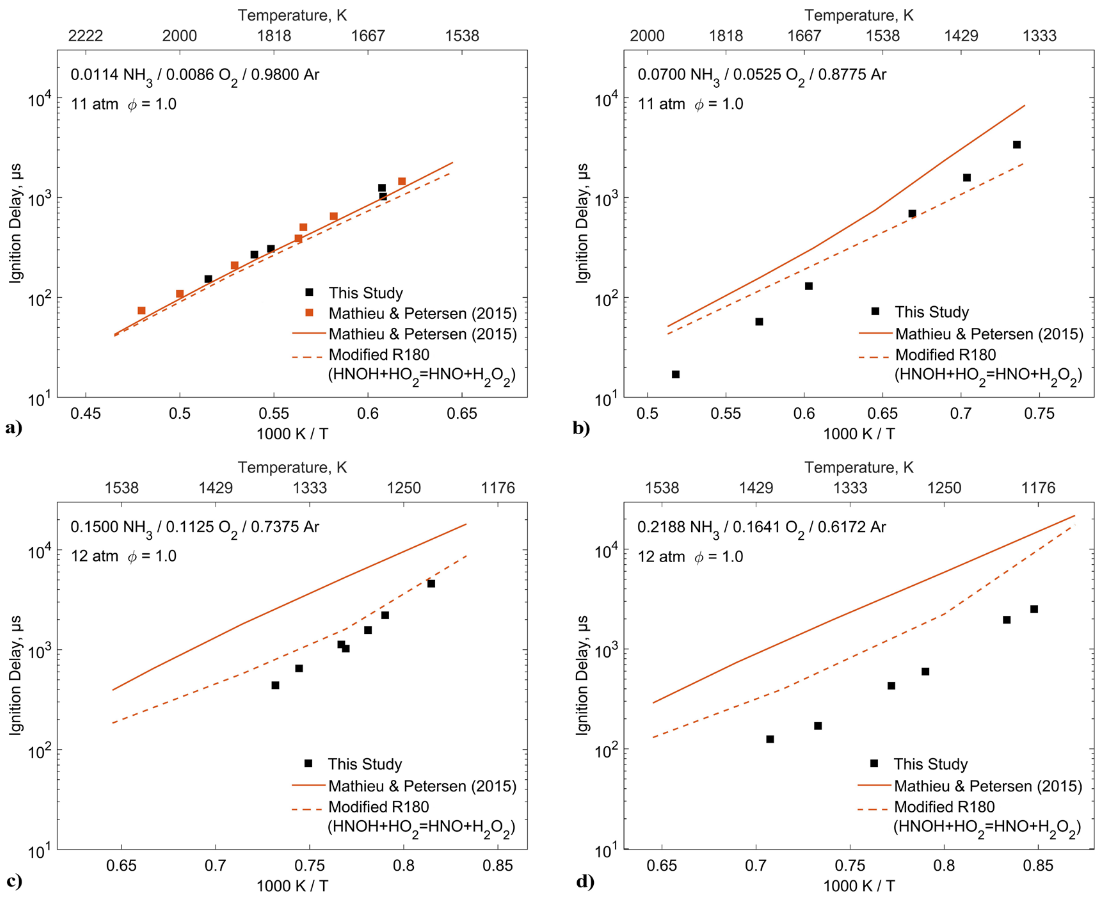
	Mathieu model	Mevel model
Promote ignition at high fuel	$NH_2 + NO \rightarrow NNH + OH$	$NH_2 + O_2 \rightarrow HNO + OH$ N_2H_3 and N_2H_2 decomposition
Promote ignition at low fuel	$NH + O_2 \rightarrow HNO + O$ $NH_2 + NO \rightarrow NNH + OH$	$NH_3 + NH_2 \rightarrow N_2H_3 + H_2$ N_2H_3 and N_2H_2 decomposition
Inhibit ignition at high fuel	$H_2NO + NH_2 \rightarrow HNO + NH_3$ $NH_2 + NO \rightarrow N_2 + H_2O$ $NH_2 + O_2 \rightarrow NO + OH$	$2NH_2 \rightarrow NH_3 + NH$ $NH_3 + H \rightarrow NH_2 + H_2$
Inhibit ignition at low fuel	$NH_2 + NO \rightarrow N_2 + H_2O$ $NH + O_2 \rightarrow NO + OH$	$NH_3 + H \rightarrow NH_2 + H_2$ $NH_2 + H \rightarrow NH + H_2$ N_2H_3 and N_2H_2 quench NH_2

Mechanism Optimization

- Important reactions vary among models
- Argument on the existence of N_2H_X
- Sensitivity analysis & reaction pathway analysis



Stoichiometric NH_3 mixtures with a) 1% NH_3, b) 7% NH_3, c) 15% NH_3, and d) 22% NH_3



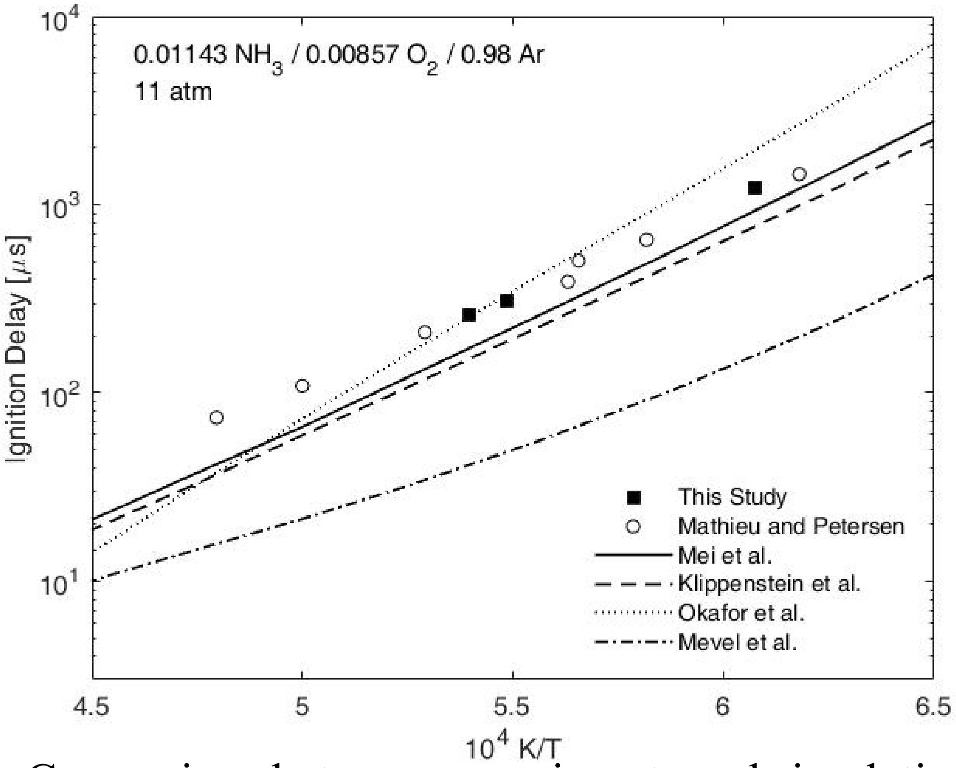
Conclusions from Ignition Study

- NH_3 IDTs have fuel concentration dependency; NH_3/H_2 mixture shows similar dependency on mixing ratio; no model can predict such dependencies well.
- NH_3 sensor was developed and characterized to probe pyrolysis and oxidation kinetics.
- Shock tube imaging capability was developed to examine ignition uniformity and flame speed measurement.
- Kinetic model optimization was explored.

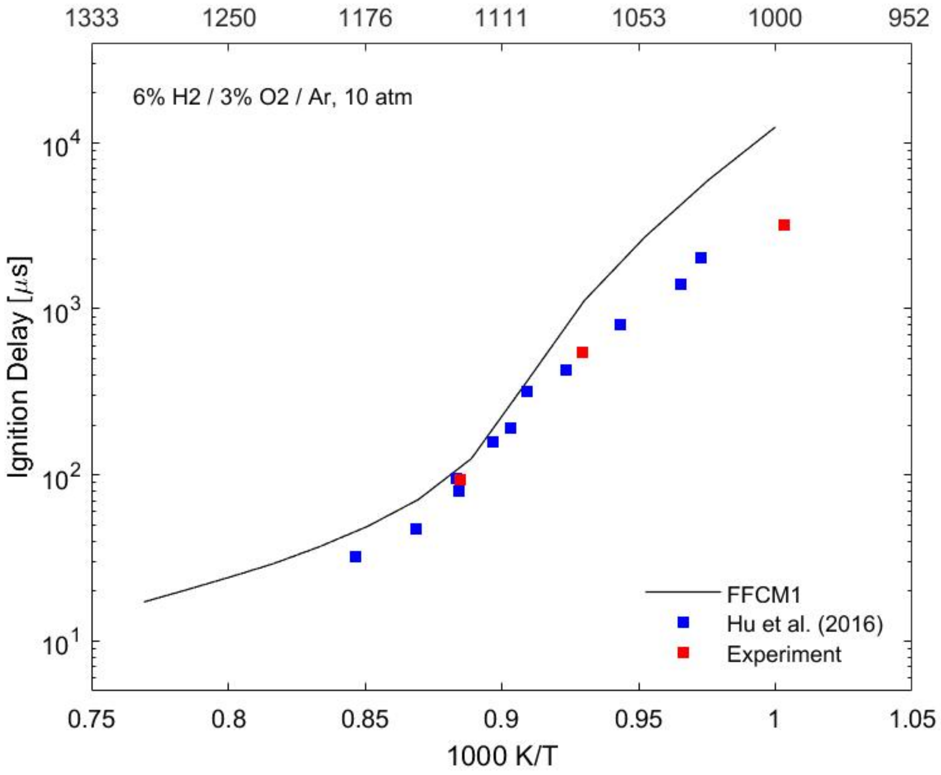
Thank you & Questions?

Benchmark of shock tube IDT measurement

- Repeat experiments reported in literature and compare with simulations



Comparison between experiments and simulation for IDTs of $NH_3/O_2/Ar$ mixture at 11 atm

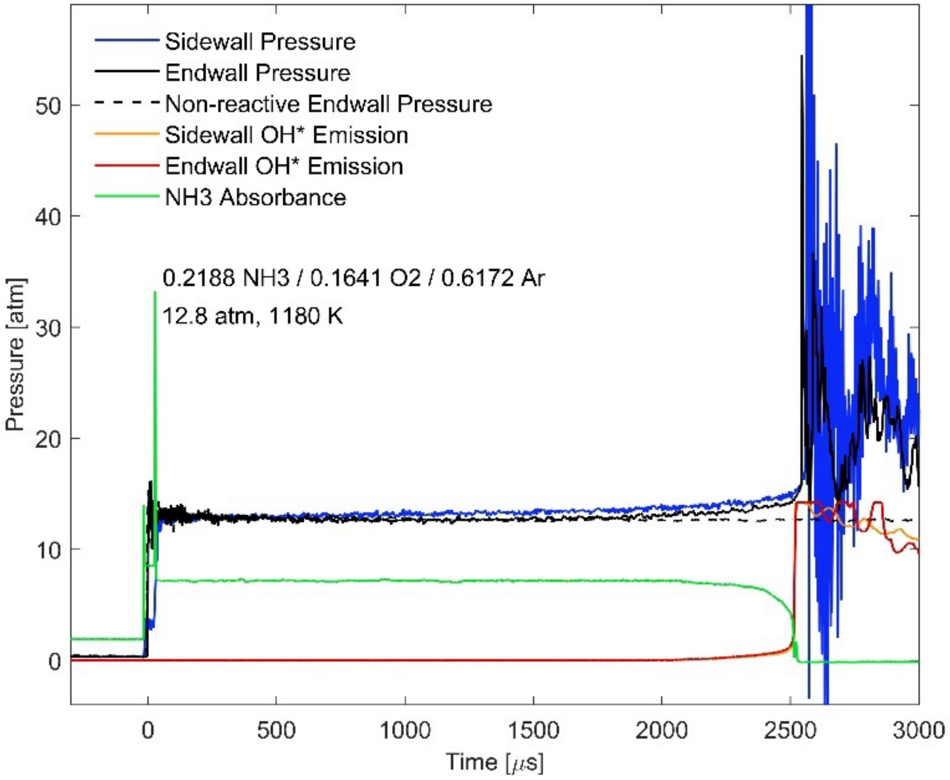


Comparison between experiments and simulation for IDTs of $H_2/O_2/Ar$ mixture at 10 atm

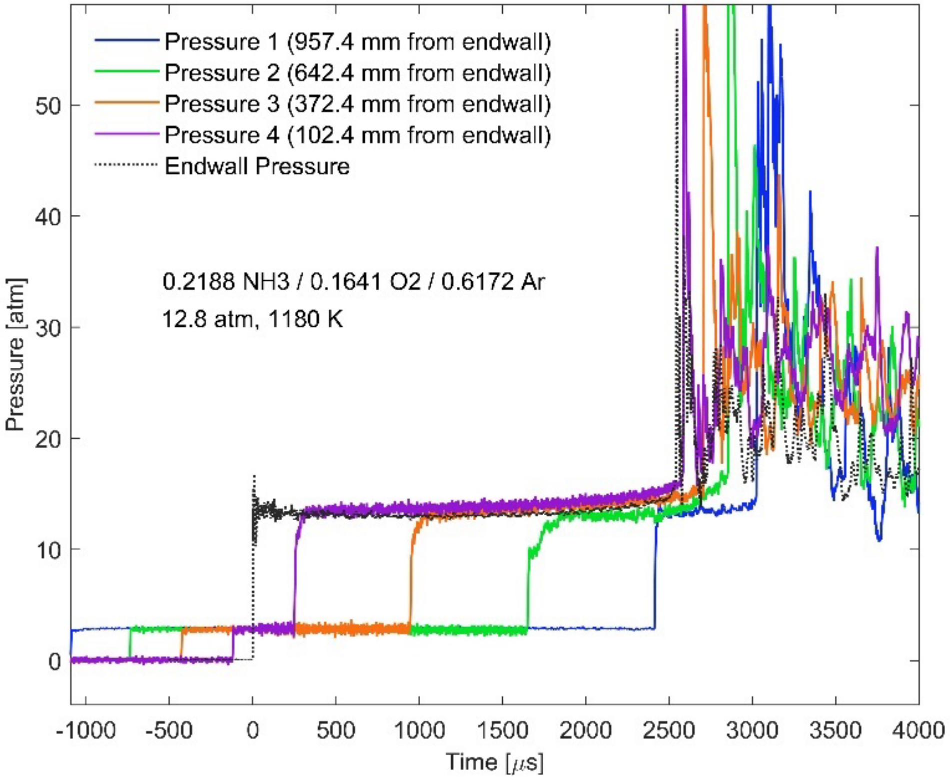
O. Mathieu and E. L. Petersen, *Combust. Flame*, vol. 162, no. 3, pp. 554–570, 2015
Hu, E., Pan, L., Gao, Z., Lu, X., Meng, X., & Huang, Z. (2016). *International Journal of Hydrogen Energy*, *41*(30), 13261-13280

Pressure Traces during IDT Measurement

- Clean Pressure traces, no sign of inhomogeneous ignitions



Signals at the measurement section from a typical experiment in this study, for a stoichiometric $NH_3/O_2/Ar$ mixture with 22% fuel concentration at 12.8 atm and 1180 K. OH* emission and NH_3 absorbance signals are of arbitrary units.



Pressure signals near the measurement section from a typical experiment in this study, for a stoichiometric $NH_3/O_2/Ar$ mixture with 22% fuel concentration at 12.8 atm and 1180 K