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

PI: Wenting Sun

Co-PI: Tim Lieuwen, Vishal Acharya and Devesh Ranjan

School of Aerospace Engineering
Georgia Institute of Technology
Atlanta, GA 30332

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UTSR Project: DE-FE0032079   PM: Mark Freeman

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

Objectives

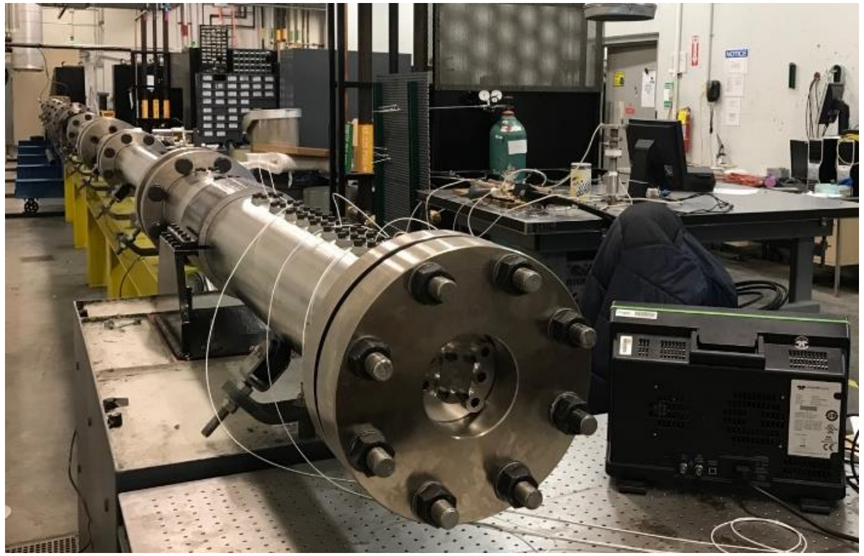
- Objective 1: Development of comprehensive database on autoignition delays for hydrogen containing fuels, including hydrogen/natural gas blends, pure hydrogen and ammonia, and ammonia/hydrogen blends at realistic gas turbine conditions (Task 2).
- Objective 2: Measurement of turbulent flame speeds and emissions of hydrogen containing fuels at different turbulence levels (Task 3).
- Objective 3: Measurement of laminar flame speeds of hydrogen containing fuels at high preheating conditions (Task 4).
- Objective 4: Validation and optimization of existing kinetic models using data obtained from experiments and development of reduced kinetic model specific for hydrogen containing fuels (Task 5).

Task 1: Project Management and Planning

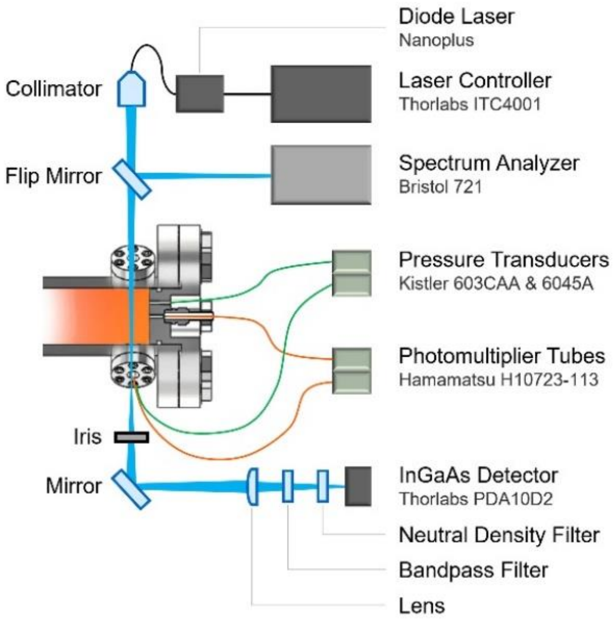
- We will manage and direct the project in accordance with a Project Management Plan to meet all technical, schedule and budget objectives and requirements.
- We will coordinate activities in order to effectively accomplish the work.
- We will update the Project Management Plan 30 days after award and as necessary throughout the project to accurately reflect the current status of the project.
- We will submit quarterly report, attend program review meetings, and arrange regular meetings with program manager.

Task 2: Investigation of Autoignition of Ammonia/Hydrogen

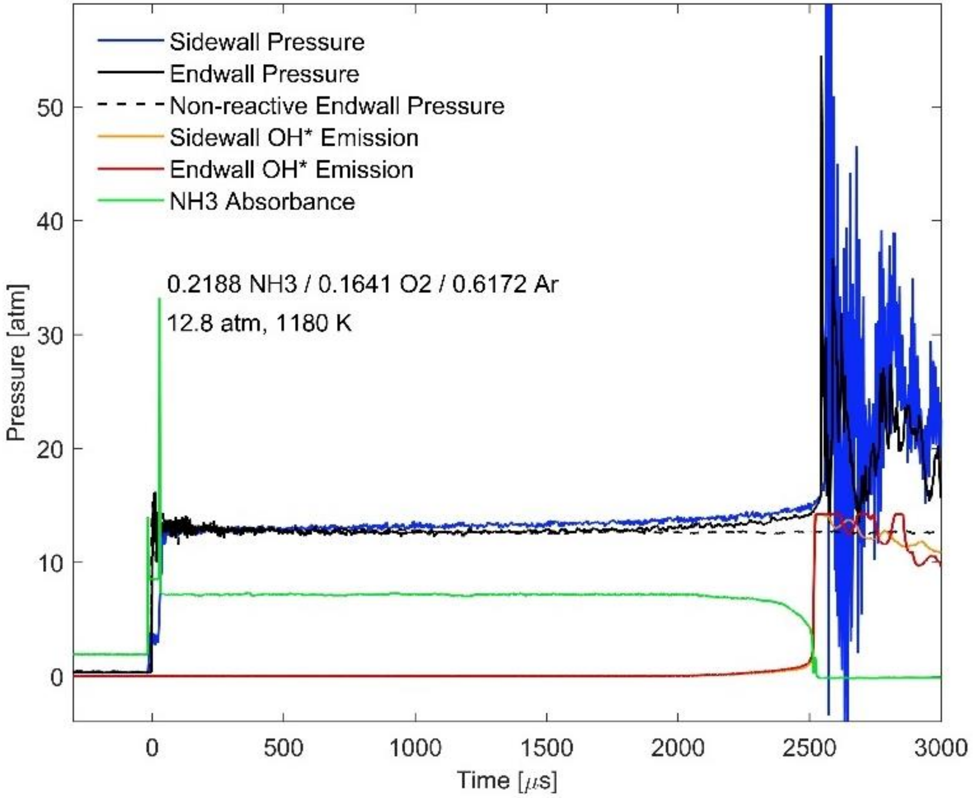
- Existing data are mostly in highly diluted environments
- Fuels: pure NH_3 and NH_3/H_2mixture
- Temperature range: 1100 K to 2200 K
- Equivalence ratio: 0.5, 1 and 2
- Pressure: ~10-20 atm
- Facility: high pressure shock tube



Schematic of experimental setup at the measurement section

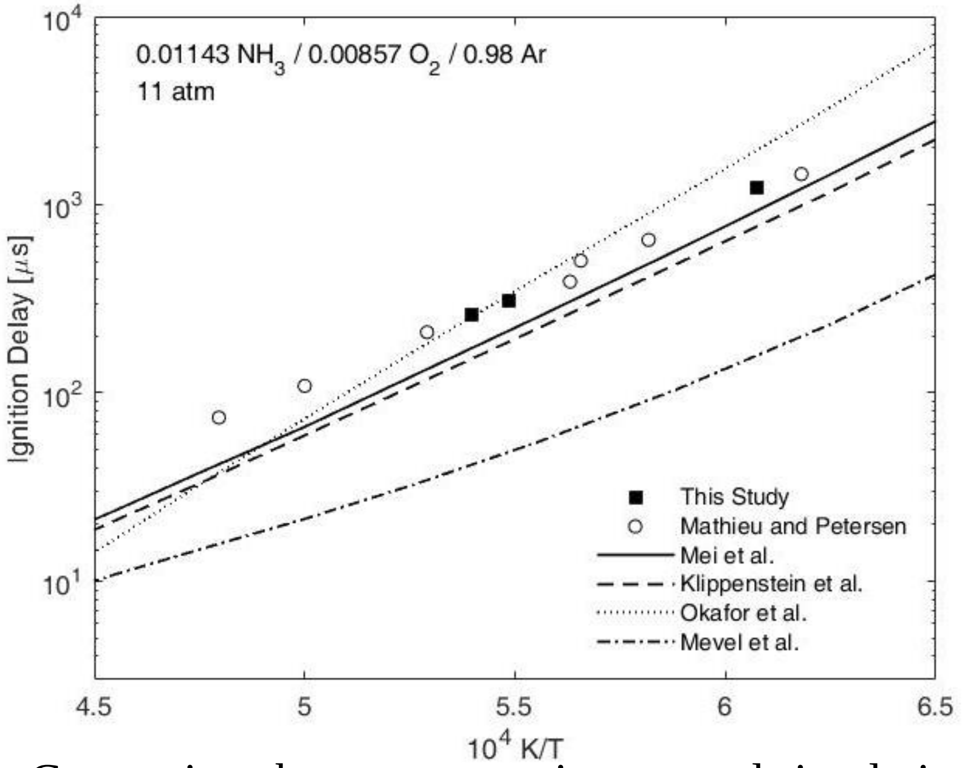


stoichiometric $NH_3/O_2/Ar$ mixture with 22% fuel at 12.8 atm and 1180 K.

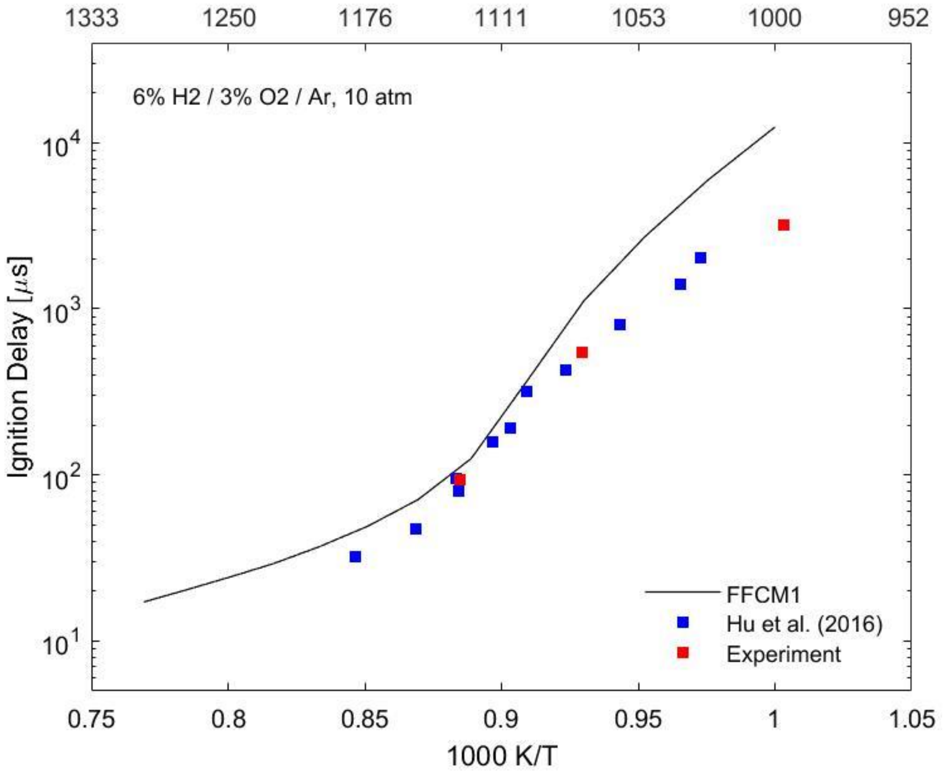


Benchmark of shock tube IDT measurement

- 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

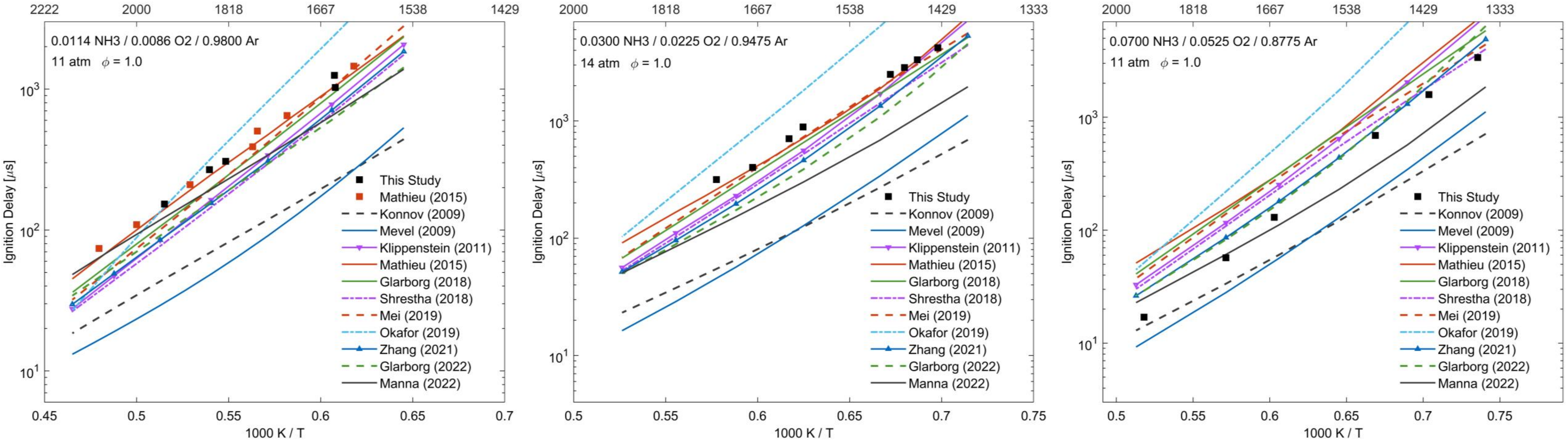


Comparison between experiments and simulation for IDTs of $H_2/O_2/Ar$ mixture at 10 atm

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

IDTs of NH_3

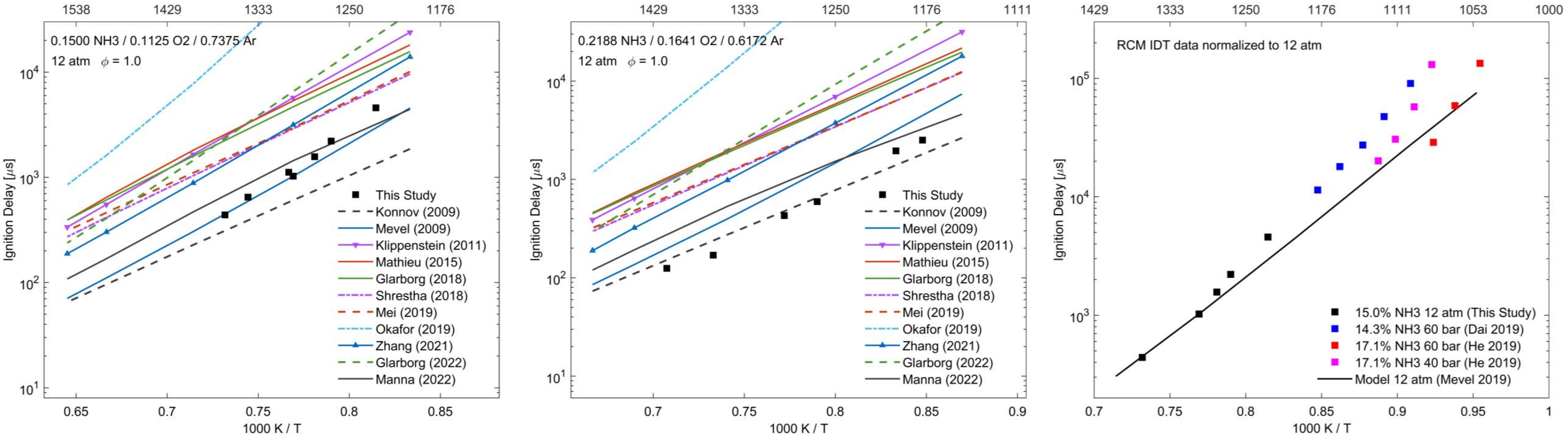
- Compared with different kinetic models
  - Good agreement with Mathieu & Petersen (2015) up to 3% ammonia
  - Deviation increases with the increase of fuel concentration
  - No model can reproduce experiments well at all conditions



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

- Agreement with Mevel et al. (2009) and Konnov & De Ruyck (2001) at 15-20% ammonia
- Validated with existing RCM (rapid-compression machine) data near 15% ammonia
- Clear trend observed. How to explain the fuel concentration dependence effect? (I don't know!!!)
- Publication: Peng, D. Ranjan, W. Sun, "A shock tube study of fuel concentration effect on high-pressure autoignition delay of ammonia" 2023 Applications in Energy and Combustion Science, 16, 100202



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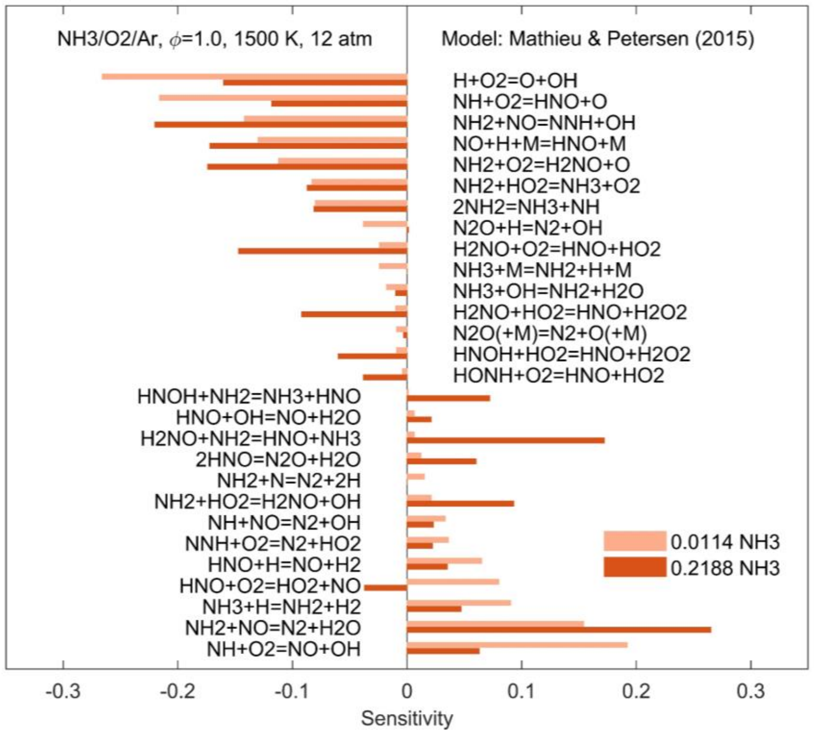
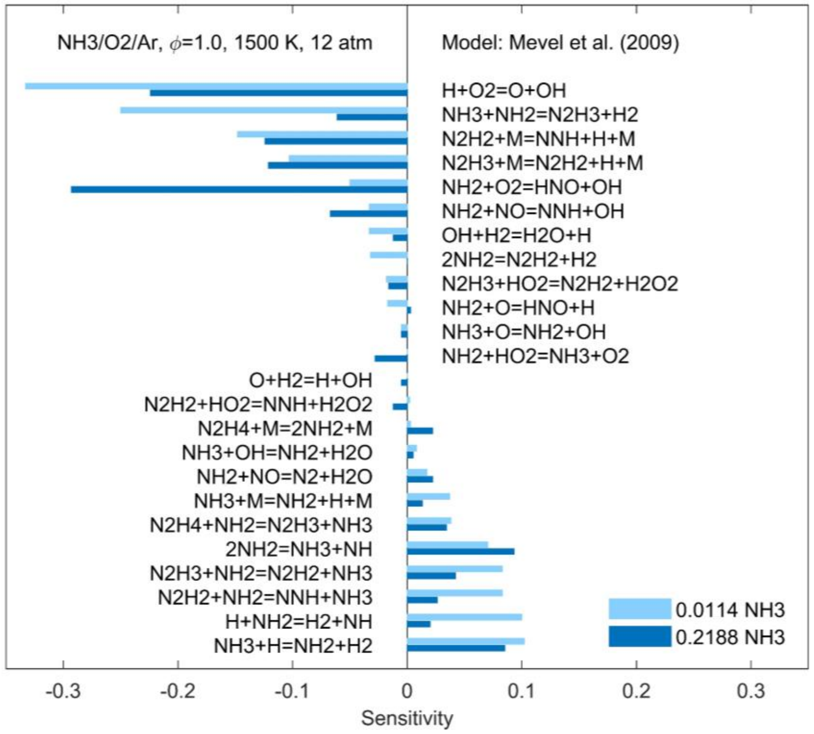
Sensitivity Analysis





- Compared with kinetic models by Mathieu & Petersen (2015) and by Mevel et al. (2009), each having good agreement with experiments at 1% and 22% ammonia, respectively

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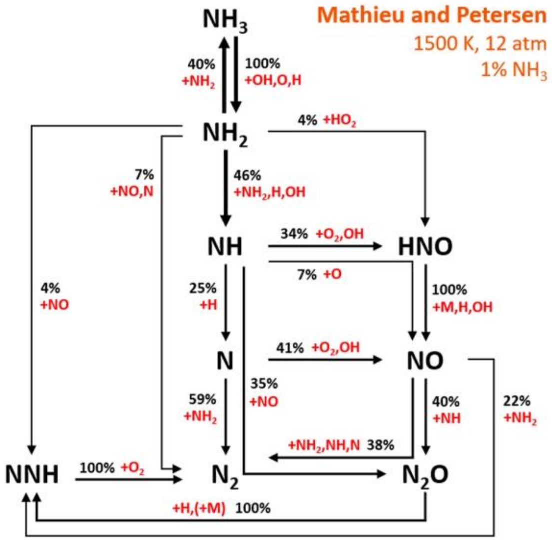
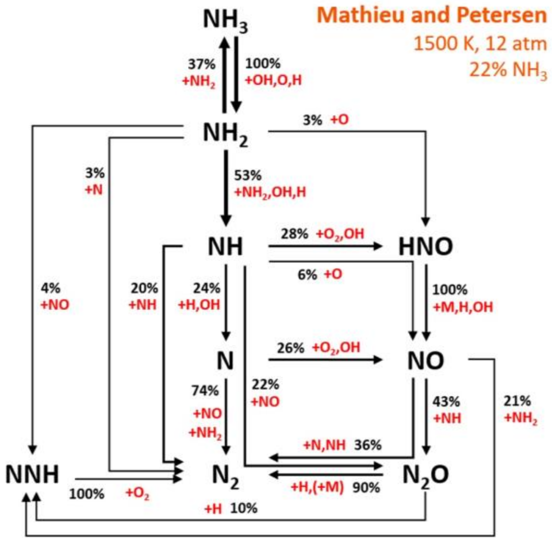
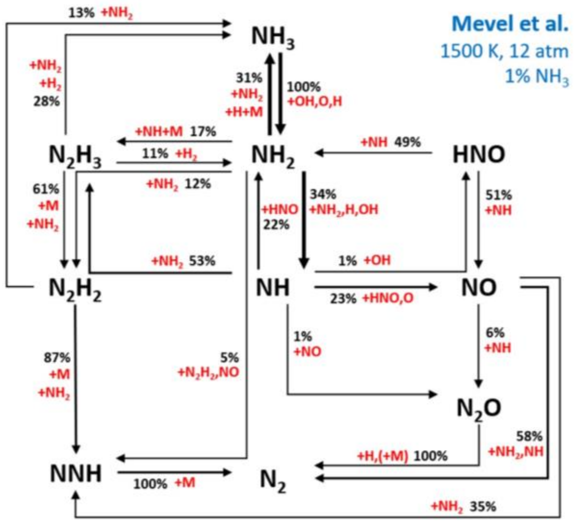
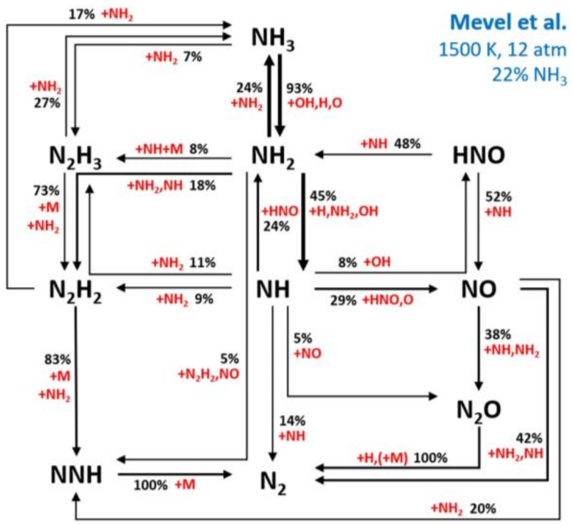
Reaction Pathways Analysis









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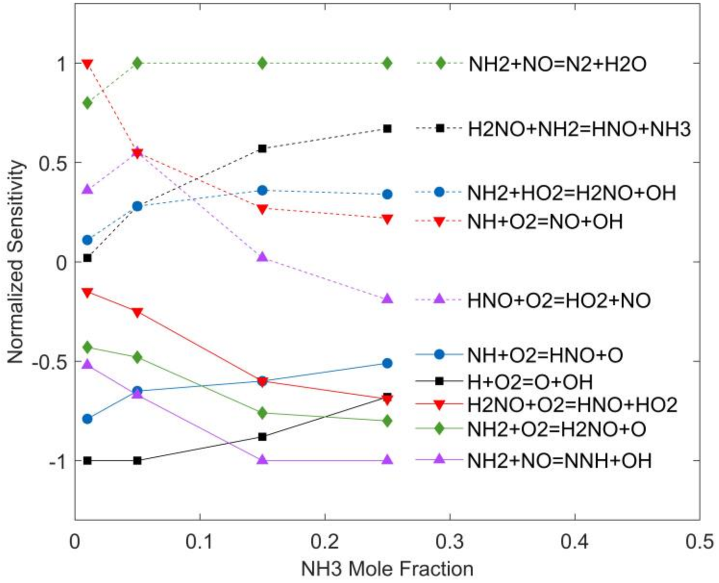
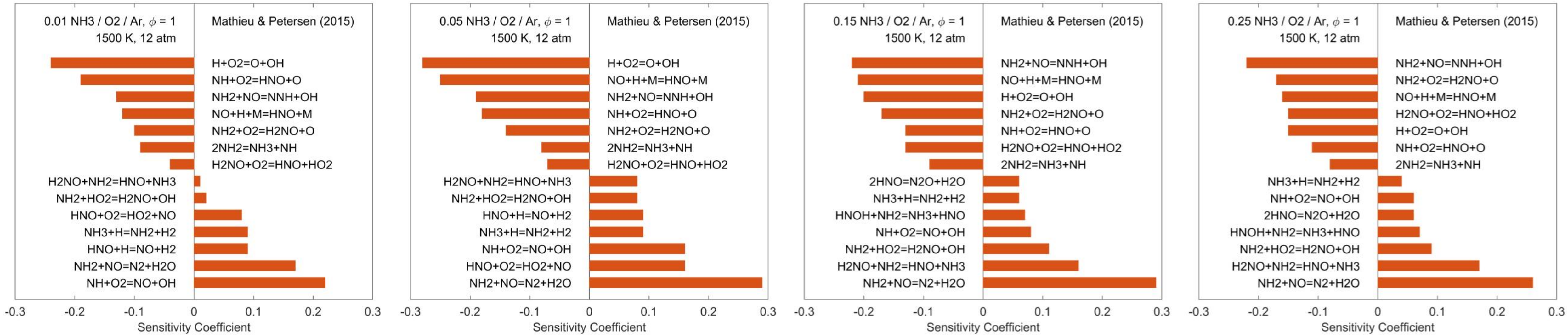
IDTs of NH_3 – Sensitivity on Fuel Concentration

- As fuel concentration increases from 1% to 25% (model by Mathieu and Petersen, 2015)
  - The strongest ignition promoter changes from $H+O_2=O+OH$ to $NH_2+NO=NNH+OH$
  - The strongest ignition inhibitor changes from $NH+O_2=NO+OH$ to $NH_2+NO=N_2+H_2O$
  - $H_2NO+O_2=HNO+HO_2$ vs. $H_2NO+NH_2=HNO+NH_3$ increasingly promote and inhibit ignition, respectively

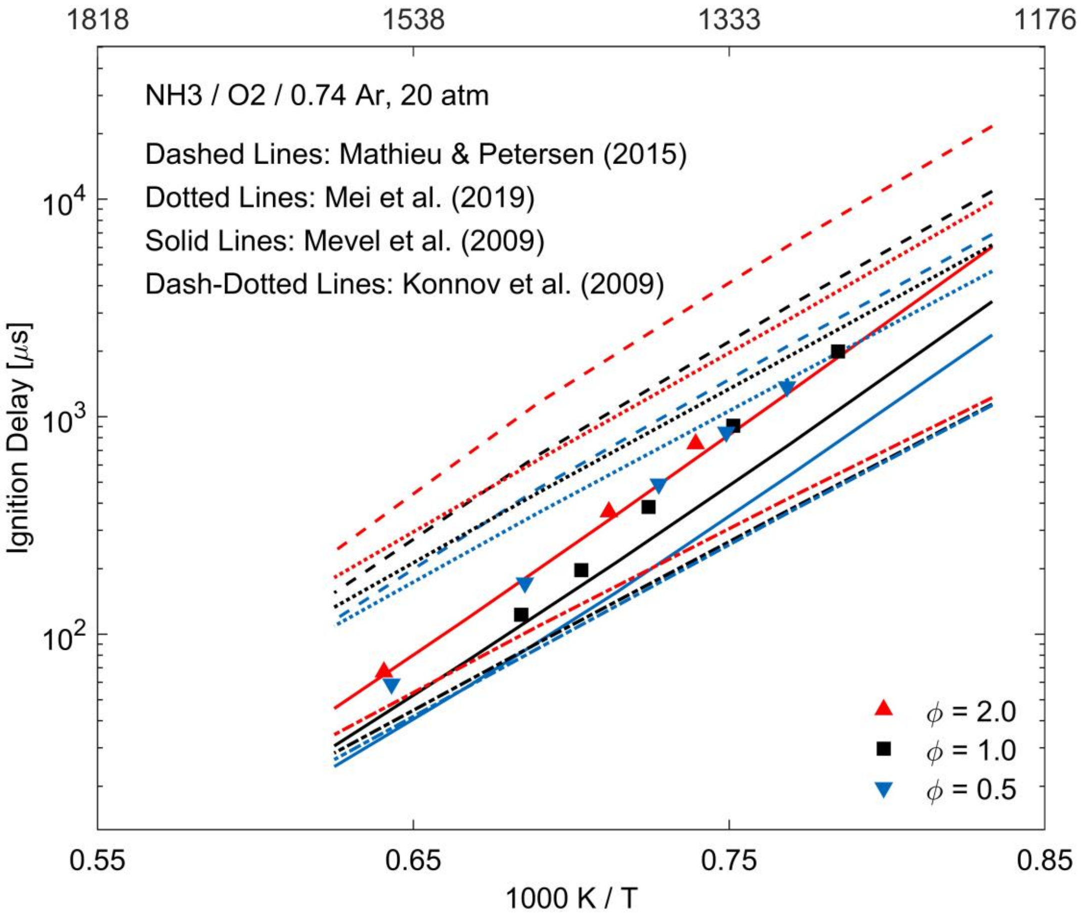




O. Mathieu, E.L. Petersen, *Combust. Flame* 162 (2015) 554-570.

IDTs of NH_3 – Equivalence Ratio Effect

- Compared with existing kinetic model at equivalence ratios of 0.5, 1.0, and 2.0
- IDTs not very sensitive to equivalence ratio
- Most models predict increased IDT with increased equivalence ratio
- Models by Mathieu and Petersen (2015) and Mevel et al. (2009) show the strongest dependence on equivalence ratio
- Model by Konnov et al. (2001) predicts the least significant equivalence ratio effect



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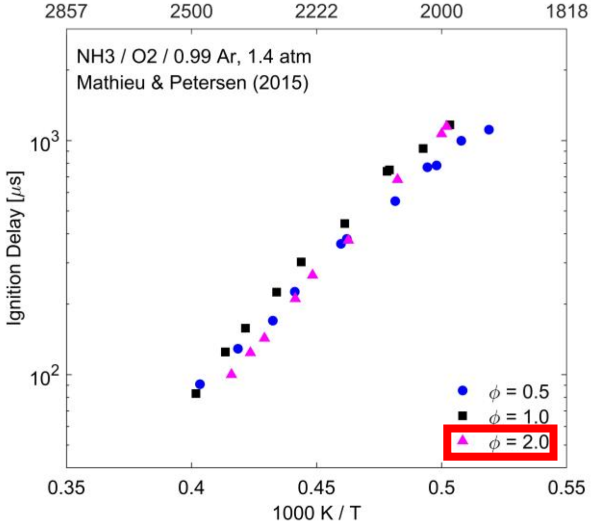
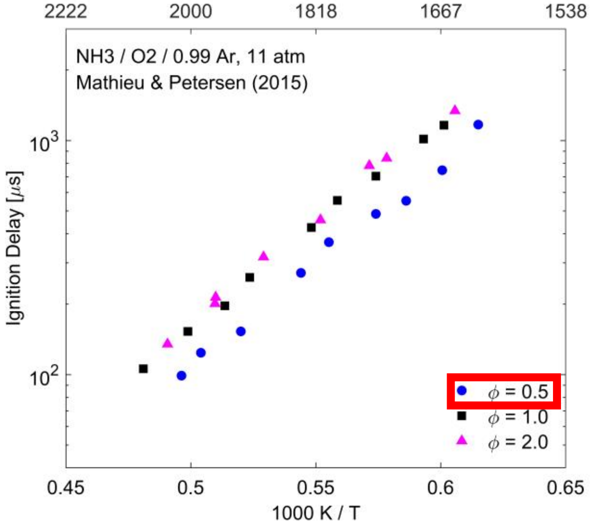
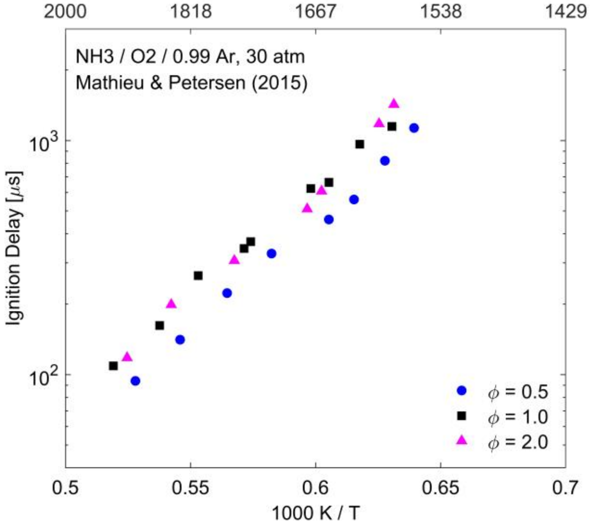
A.A. Konnov, J. De Ruyck, *Combust. Sci. Technol.* 168 (2001) 1-46.
B. Mei, X. Zhang, S. Ma, M. Cui, H. Guo, Z. Cao, Y. Li, *Combust. Flame* 210 (2019) 236-246.

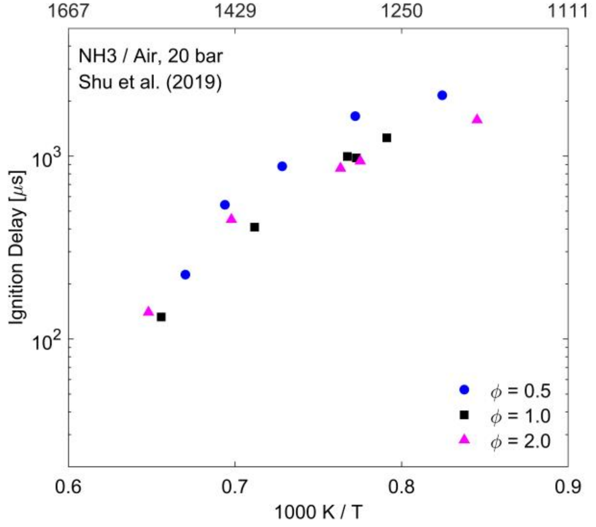
IDTs of NH_3 – Equivalence Ratio Effect from literature

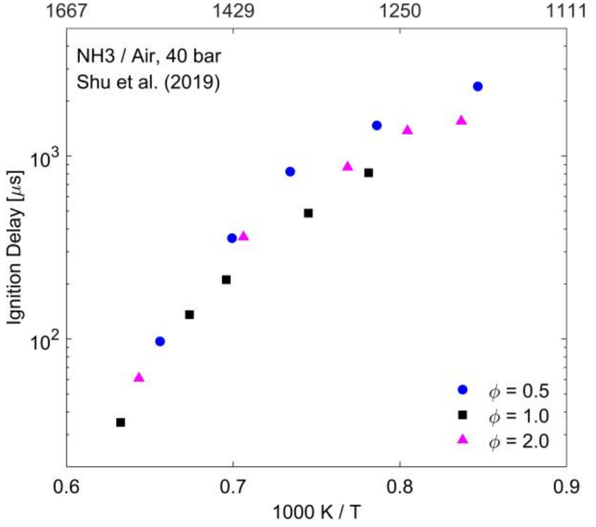
- IDTs in literature do not show consistent trend
- Effect of equivalence ratio appears to depend on mixture and conditions
- <u>No clear trend observed</u>

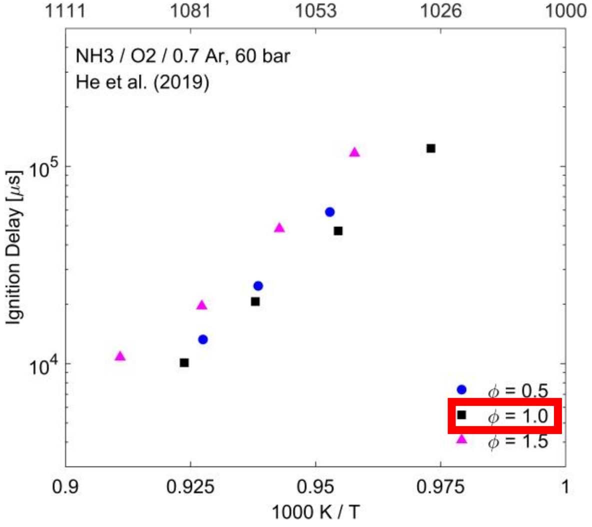


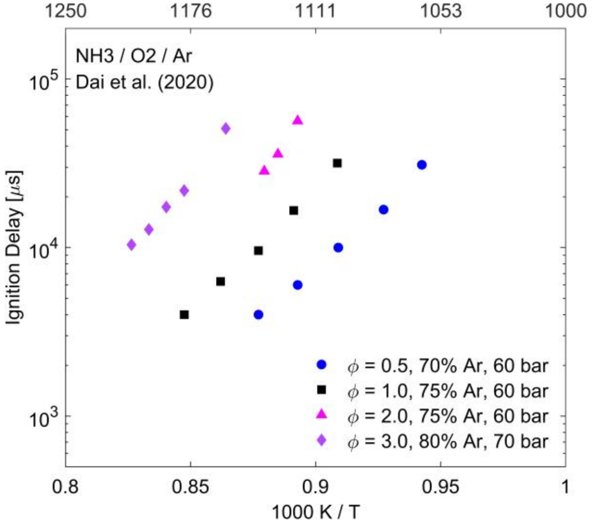








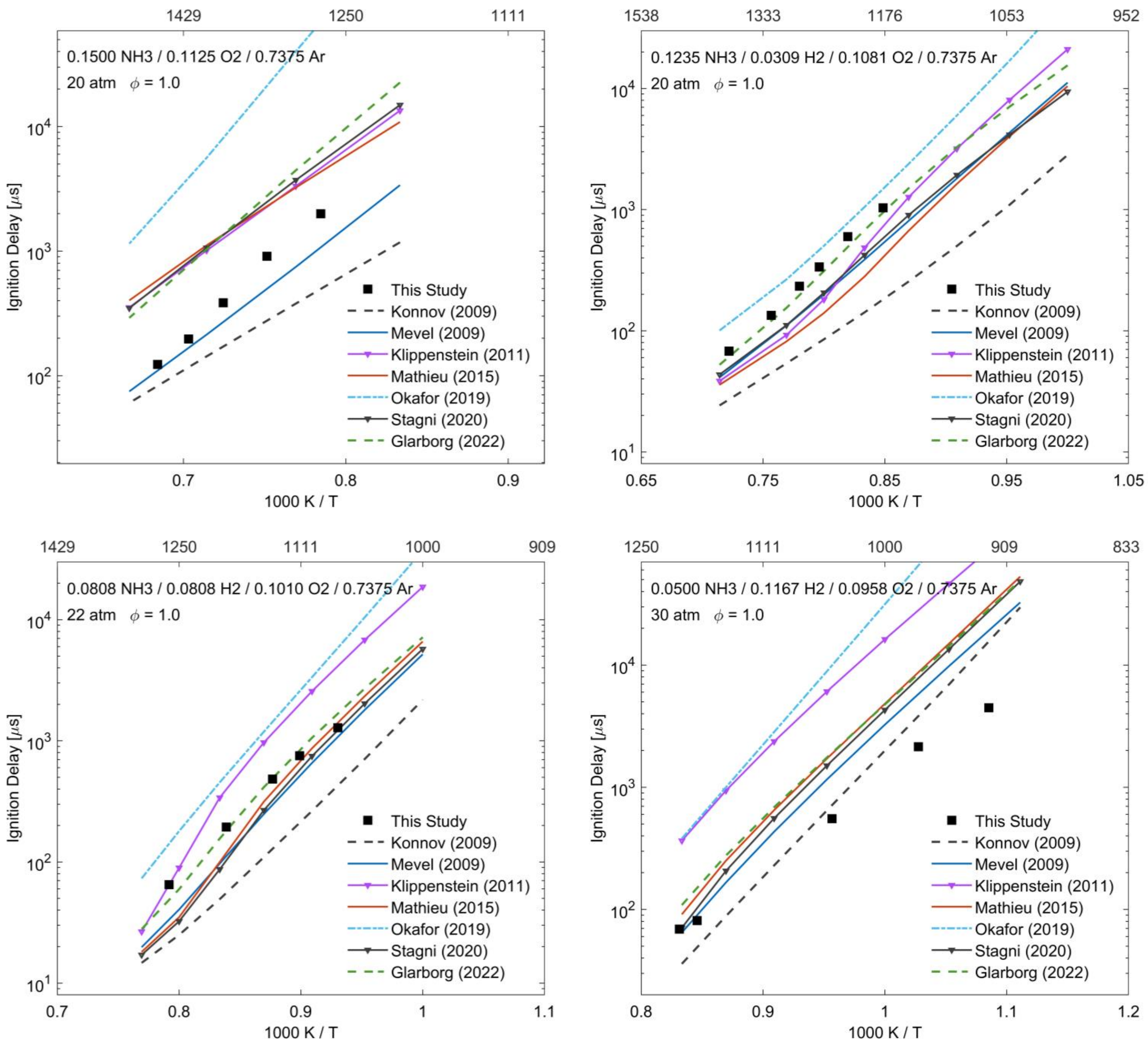




O. Mathieu, E.L. Petersen, *Combust. Flame* 162 (2015) 554-570.
B. Shu, S.K. Vallabhuni, X. He, G. Issayev, K. Moshammer, A. Farooq, R.X. Fernandes, *Proc. Combust. Inst.* 37 (2019) 205-211.
X. He, B. Shu, D. Nascimento, K. Moshammer, M. Costa, R.X. Fernandes, *Combust. Flame* 206 (2019) 189-200.
L. Dai, S. Gersen, P. Glarborg, H. Levinsky, A. Mokhov, *Combust. Flame* 215 (2020) 134-144.

IDTs of H_2/NH_3

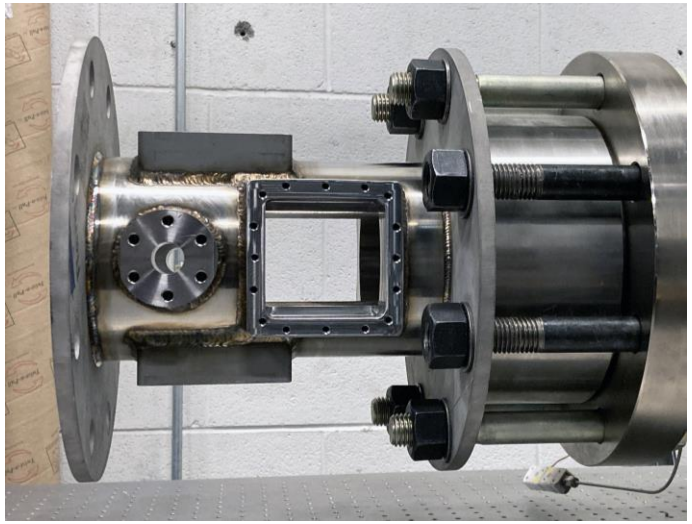
- IDTs with 0 to 70% hydrogen in fuel
- Compared with different kinetic models
  - Good agreement with Glarborg (2022) at 20% and 50% hydrogen in fuel
  - Most models over-predict IDT at 70% hydrogen in fuel; over-prediction increases towards lower temperatures (well-known H_2 IDT issue at low T)
- Need 2D optical access to examine ignition quality with H_2 addition



P. Glarborg, *Combust. Flame* 257 (2023) 112311.

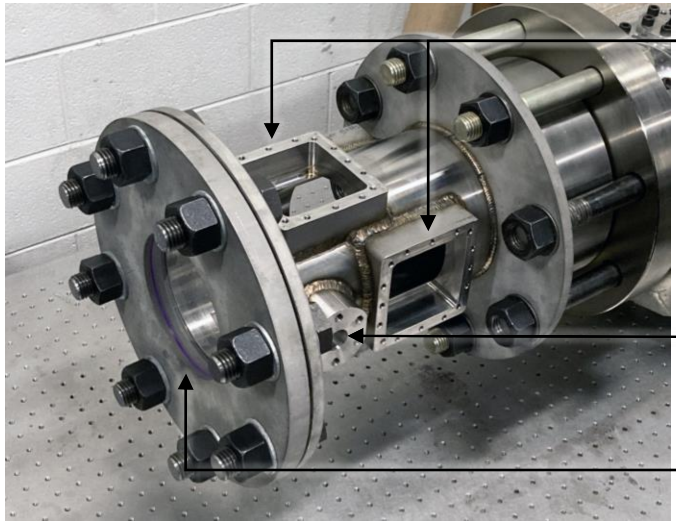
Task 4: Measurement of laminar flame speeds of hydrogen containing fuels at high preheating conditions

Incident Shock Wave ←



Side View

End View



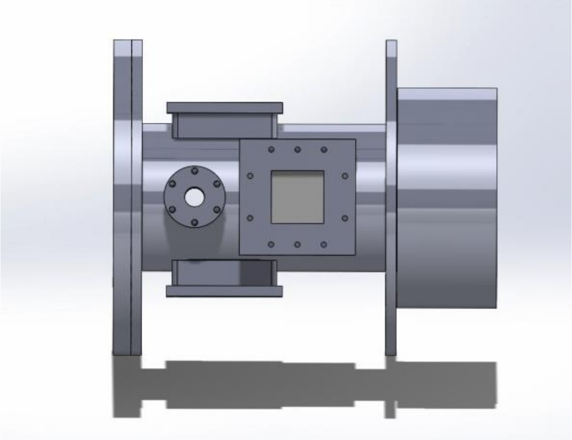
Isometric View

Side-Wall Windows
(3 in x 3.5 in)

Side-Wall Ports

End-Wall Window
(6 in I.D.)

- 6-in-diameter optical access from end-wall and effective 3-in-by-7-in from side-wall
- 2D optical access allows flame speed measurements and examination of ignition uniformity for H_2
- Currently validating performance with IDT experiments and setting up instrumentation for optical measurements



Complete Side View

Conclusions from Ignition Study

- NH_3 IDTs obtained at different fuel concentrations. No kinetic model can predict the IDTs at all conditions.

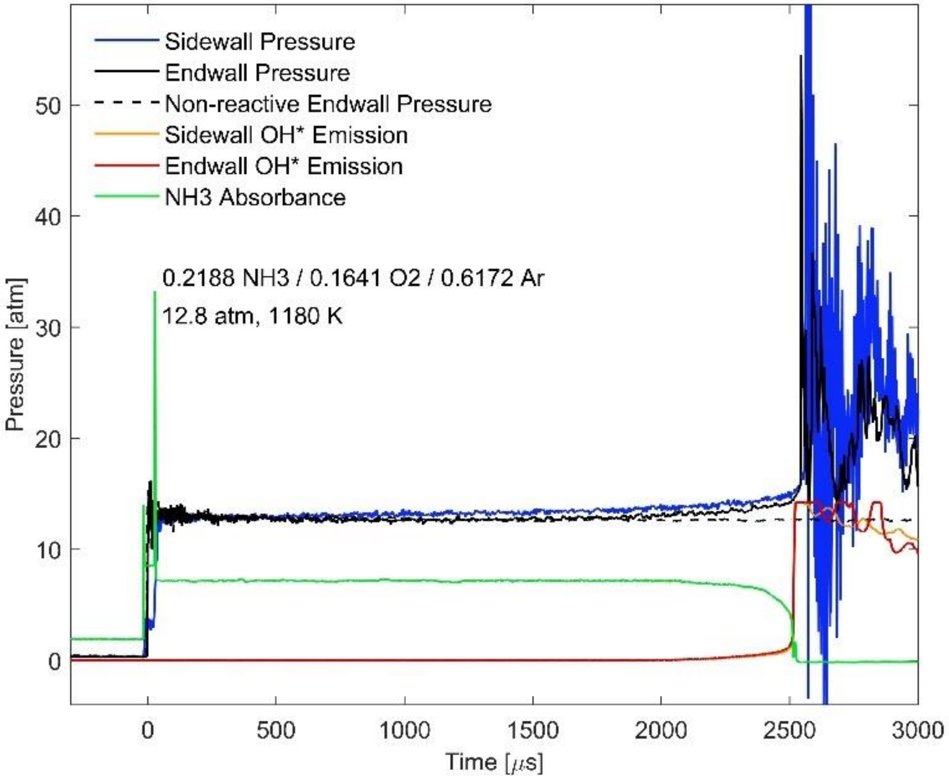
- NH_3 IDTs show no clear trend on equivalence ratio dependence

- Discrepancy on NH_3/H_2 IDTs is observed and being investigated

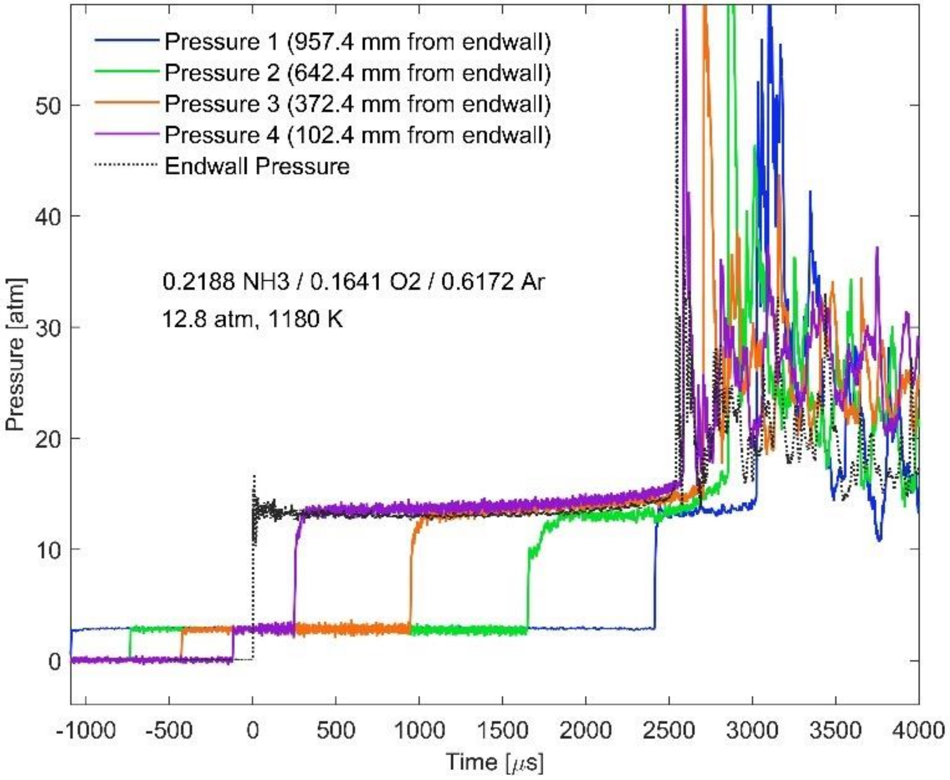
Thank you & Questions?

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