SAND2022-12002C

Characterization of Post-Detonation Fireballs at 1 MHz via LAS Measurements of Temperature, Pressure, CO and CO_2

Christopher S. Goldenstein, Charles Schwartz, Garrett C. Mathews, and Many Collaborators

School of Mechanical Engineering, Purdue University, West Lafayette, IN 47907

IEEE RAPID 2022

September 13, 2022

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia Light Speed Grand Challenge

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
Grand Challenges

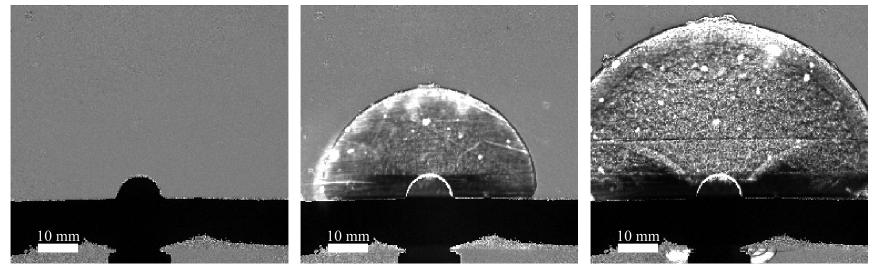
Three-year R&D effort
(October 2021-September 2023)
Engaging more than 30 Sandia staff, eleven faculty, and fourteen students

UNIVERSITY of FLORIDA

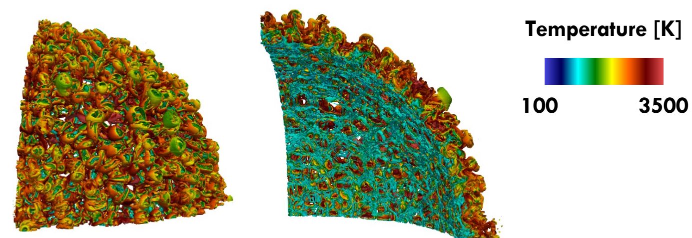
ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

PURDUE UNIVERSITY

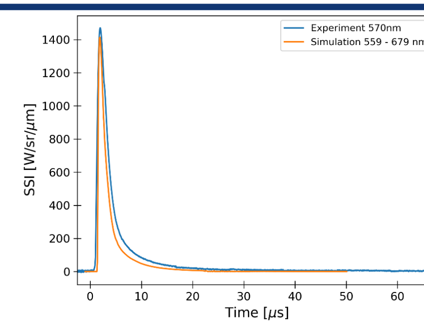
Advanced Experimental Diagnostics



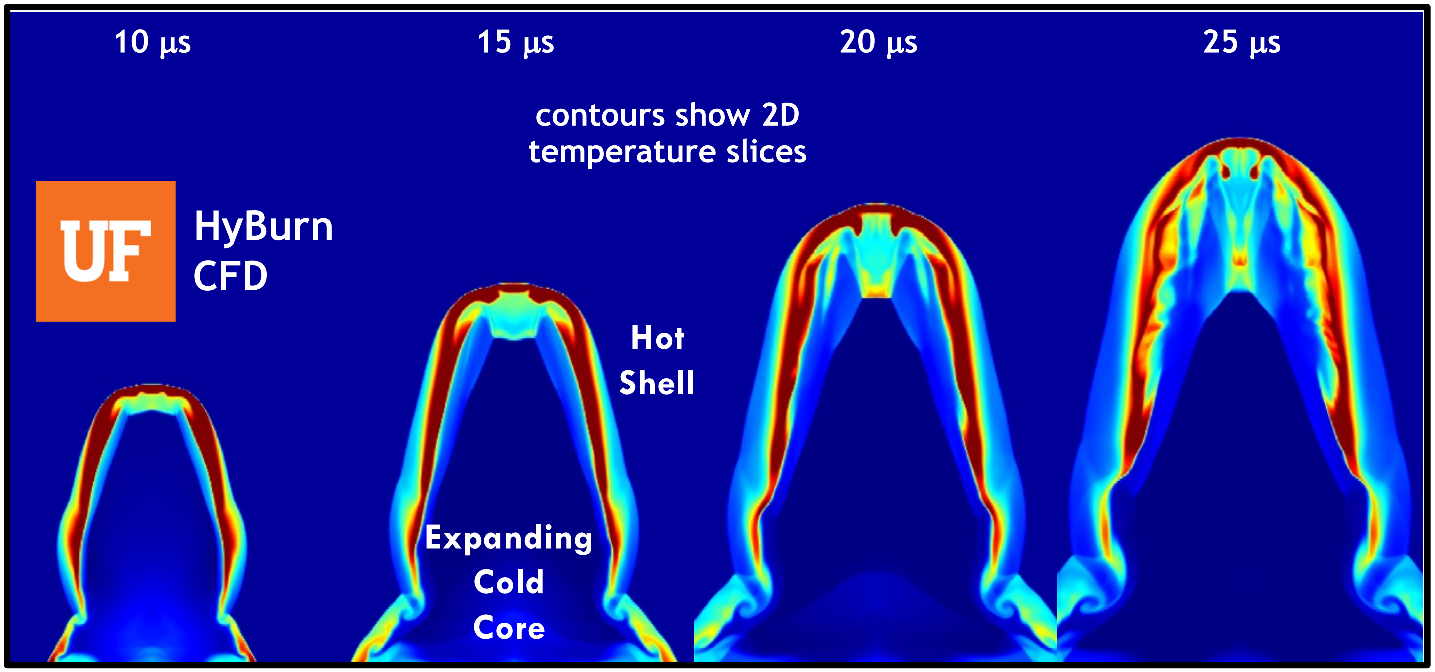
High-Fidelity Simulation



Optical Emission Predictions



Anatomy of a Post-Detonation Fireball



- Emission from hot particles and gaseous species originates from hot shell
- *But, cold core of expanded detonation products plays an important role*

Sandia Light Speed Grand Challenge

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
Grand Challenges

Our Goals

- Acquire ***T***, ***P***, **CO**, **CO_2** and H_2O measurements in post-det fireballs ***at ~ MHz*** rates to evaluate fireball+radiation model accuracy

Challenges

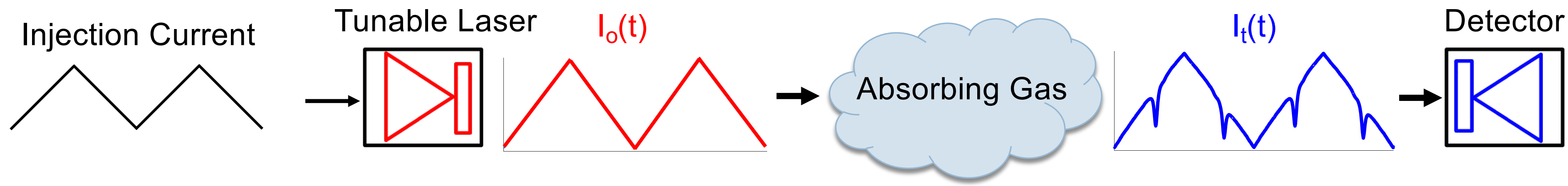
- Transmission losses
- Optical emission
- Small-scale fireballs
- Need ~μs resolution
- Line-of-sight nonuniformities

Solutions

- Optical engineering
- Spectral and spatial filtering
- Mid-infrared absorption
- DFB QCLs *with deep tuning* + wavelength selection
- *Wavelength selection + utilization of synthetic measurements from CFD results*

PURDUE ENGINEERING

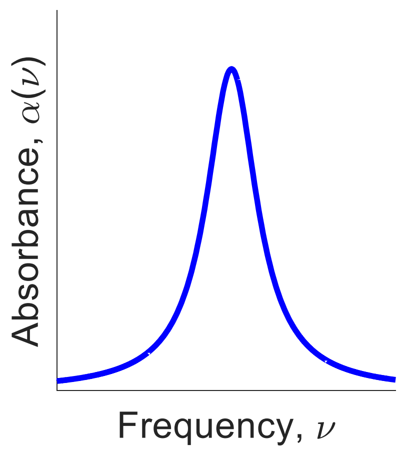
LAS Sensor Design: Diagnostic Technique



Spectral Absorbance: α(ν)

$$\alpha(\nu) = -\ln(I_t/I_0)$$

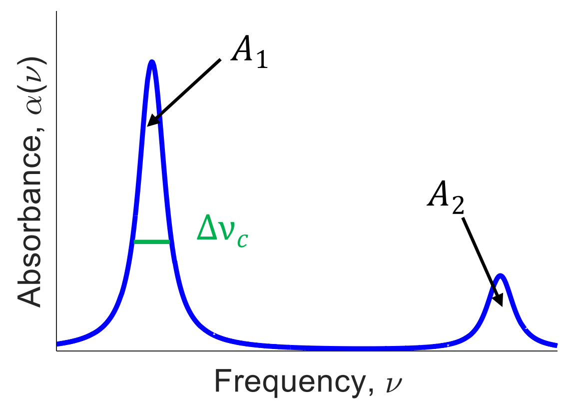
$$\alpha(\nu) = S(T)\phi_i(\nu)PX_iL$$



Measuring Gas Properties

Integrated Area: $A = S(T)PX_iL$

Lineshape: $\phi(\nu) = f(\Delta\nu_c, \Delta\nu_d, \nu)$



Collisional Width:

$$\Delta\nu_c = P\sum_A 2\gamma_{A-B}X_A$$ Pressure

↑ Broadening coefficient

$$\frac{A_2}{A_1} = \frac{S_2(T)}{S_1(T)} = f(T)$$ Temperature →

$$\frac{A_1}{S_1(T)PL} = X_i$$ Mole Fraction (PX_i, X_iL)

LAS Sensor Design: Wavelength Selection

Need mid-IR wavelengths

- Strong absorption needed for small scales and concentrations

Need high-E” transitions

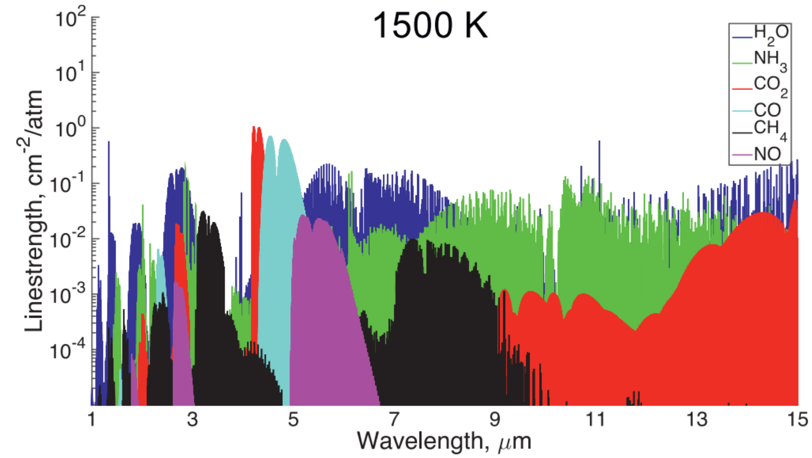
- Minimizes absorption in cold core & BL
  →eases interpretation of path-integrated absorption

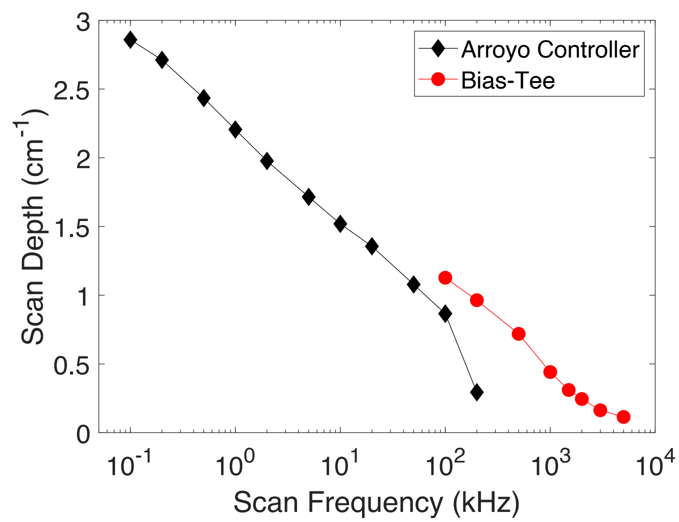
Need large ΔE” transitions

- Large temperature sensitivity

Need closely spaced transitions for near-MHz measurements

- Tuning amplitude of DFB QCLs is small at high-f→



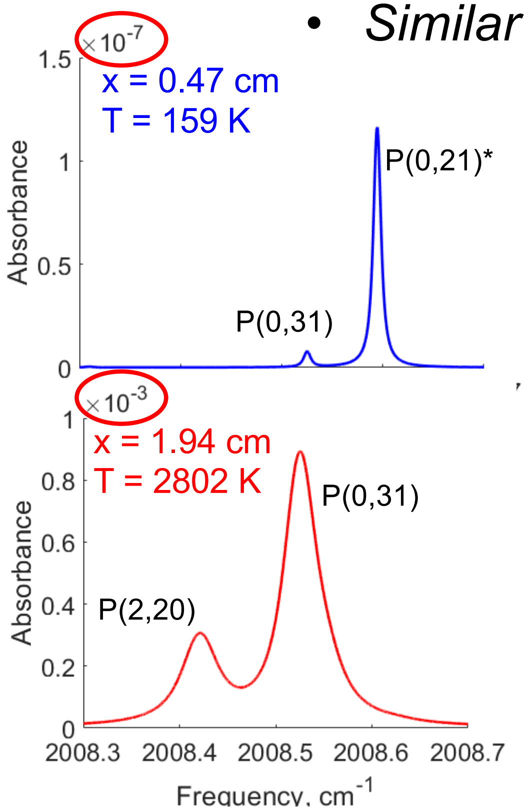


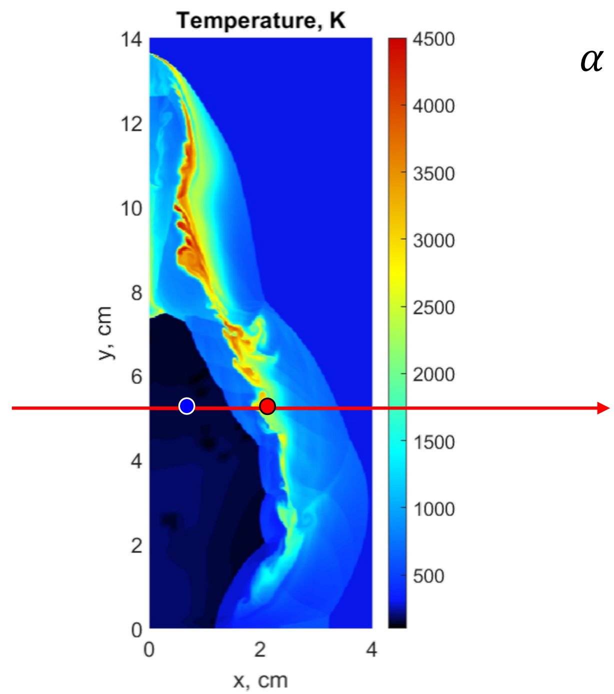
LAS Sensor Design: Wavelength Selection

QCL targets CO P(0,31) and P(2,20) transitions near 2008.5 cm^{-1} (~5 μm)

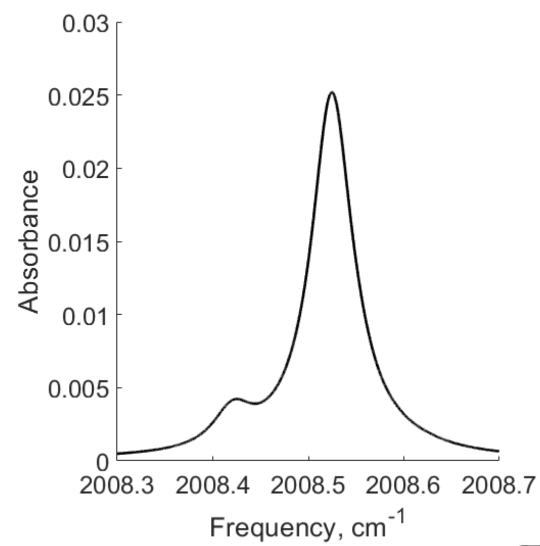
- E” ~1901 and 5052 cm^{-1}, ΔE”=3151 cm^{-1}
  - Measurements are deliberately biased to fireball’s hot outer shell!
    - *Similar approach for CO_2 diagnostic*

50,000 x Larger Signal!

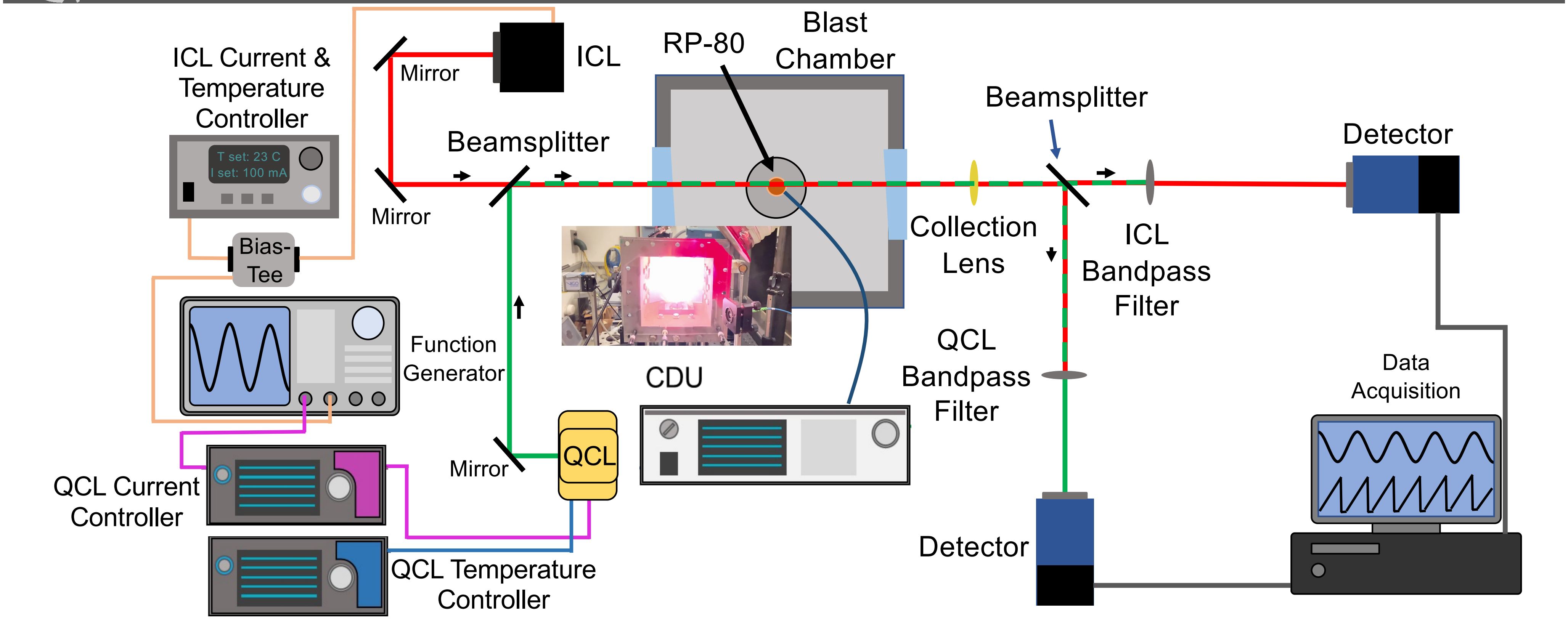




$$\alpha = \int_0^L S(T_i) P_{CO,i} \phi_i(\nu, \Delta\nu_c, \Delta\nu_d) dl$$



Experimental Setup for Simultaneous T, P, CO, CO_2

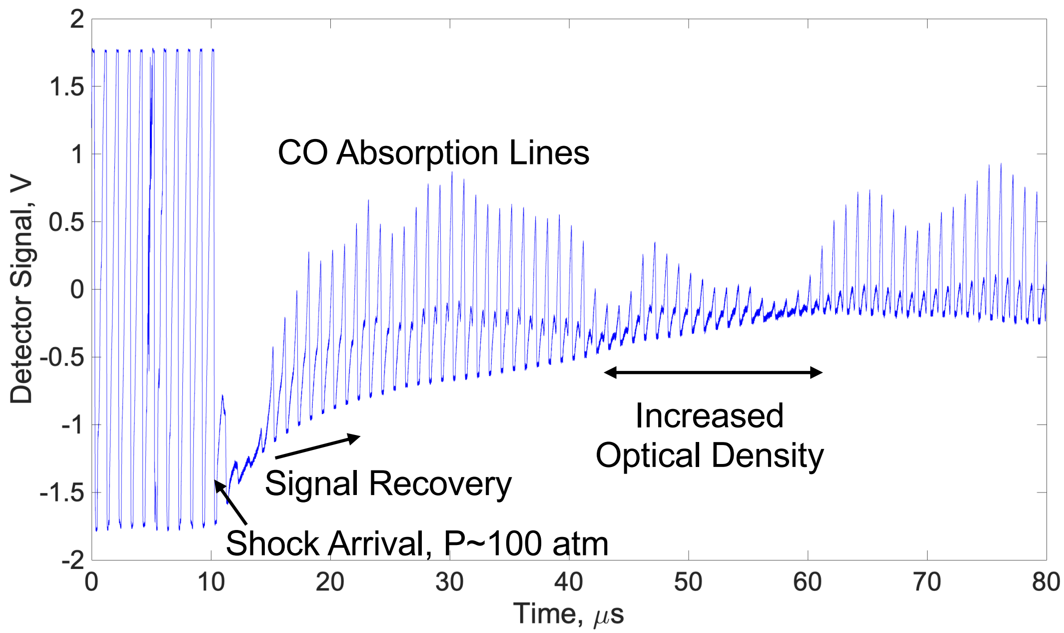


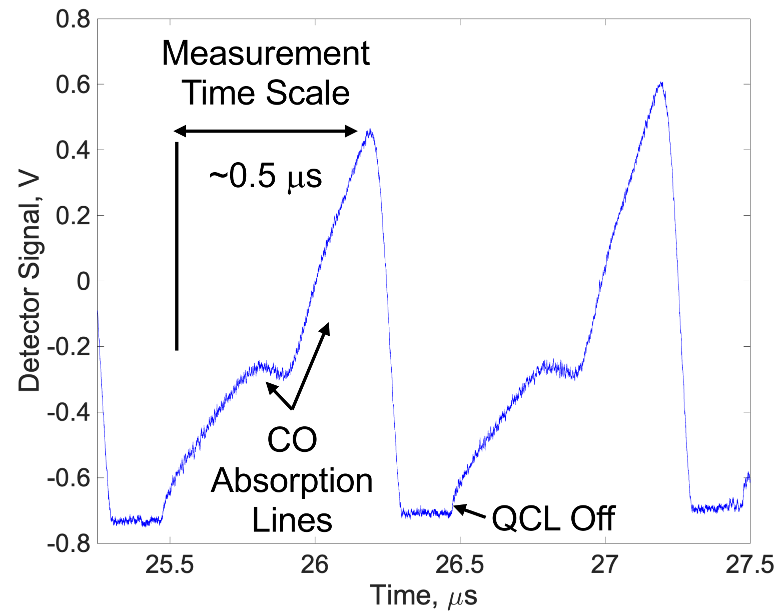
Key Details

- QCL scanned across CO transitions near 2008 cm^{-1} at 1 MHz
- ICL scanned across CO_2 transitions near 2384 cm^{-1} at 500 kHz

PURDUE ENGINEERING

Results: Raw Signal vs time





Key Takeaways

- Large optical losses, especially at shock arrival
- Each T, P, $P_{CO}L$ measurement acquired in ~0.5 µs
  - Beam steering and emission are "frozen" on measurement time scale

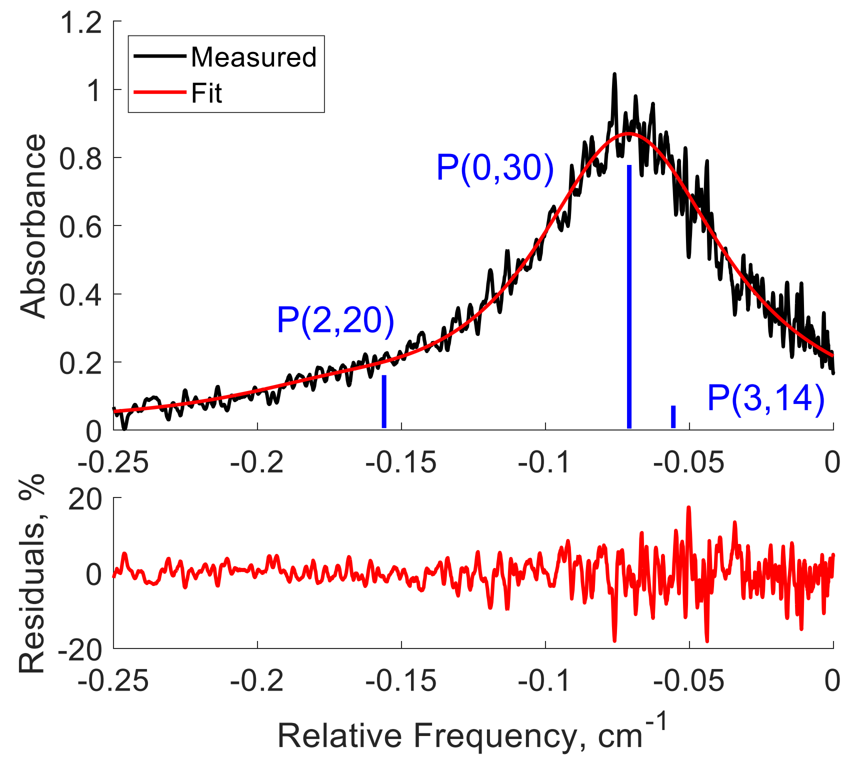
Results: Example Absorbance Spectrum

Key Takeaways

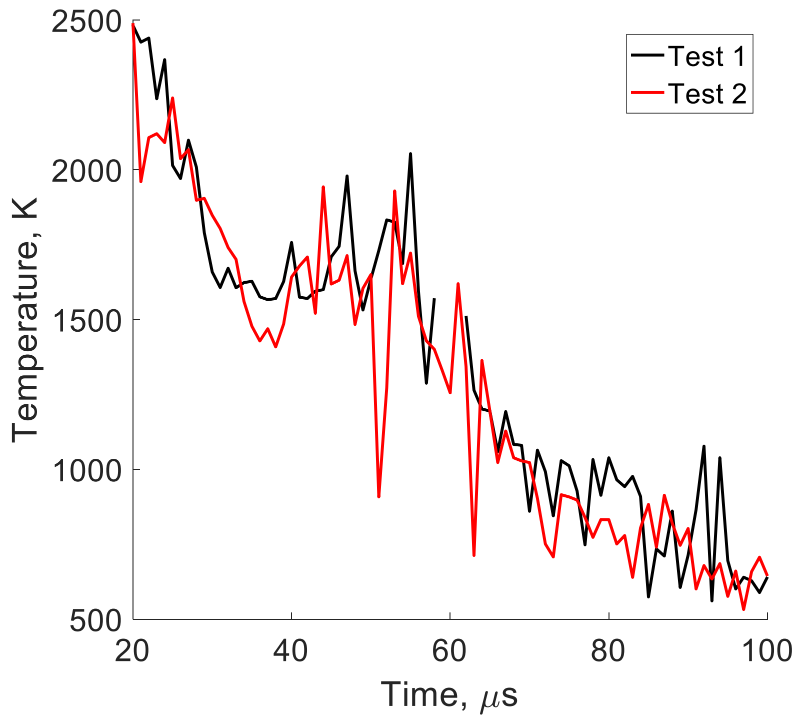
- Large absorbance
  - Relatively high-SNR (~100)
- Spectrum dominated by 2 lines
- Spectrum well modeled by uniform LOS absorption model using HITEMP2019
  - *Due to minimal abs. in cold core & BL via high-E" lines*
  - Single *T, P,* $P_{CO}L$ from each fit

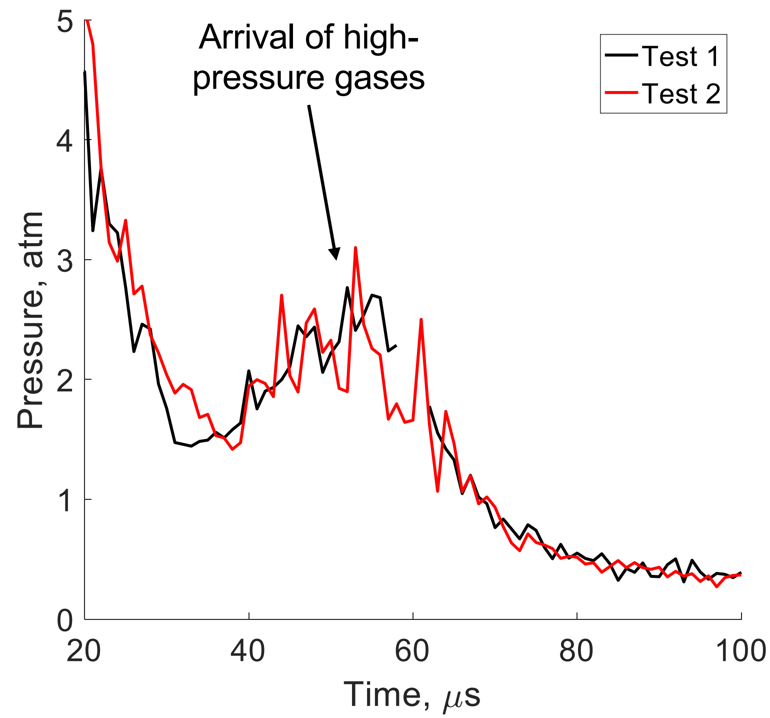
T = 1360 K,
P = 1.63 atm,
$P_{CO}L$ = 0.315 atm-cm

Example Single-Scan Measurement



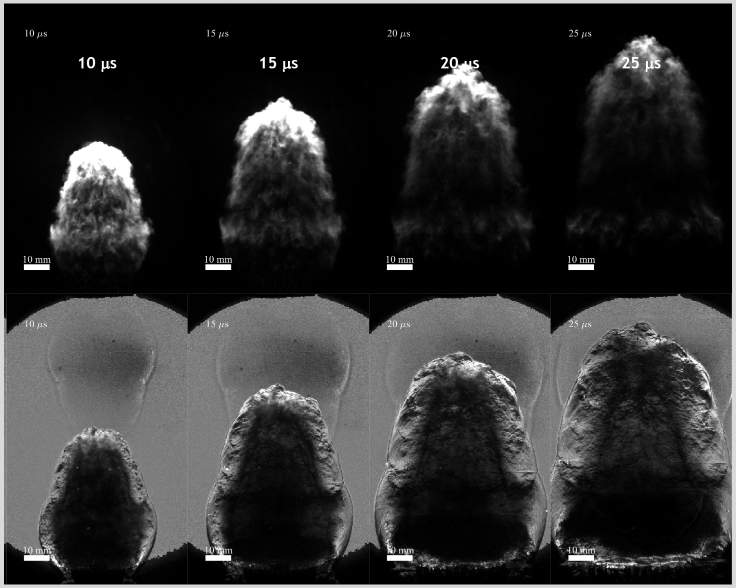
Results: Time Histories at *y* = 51 mm

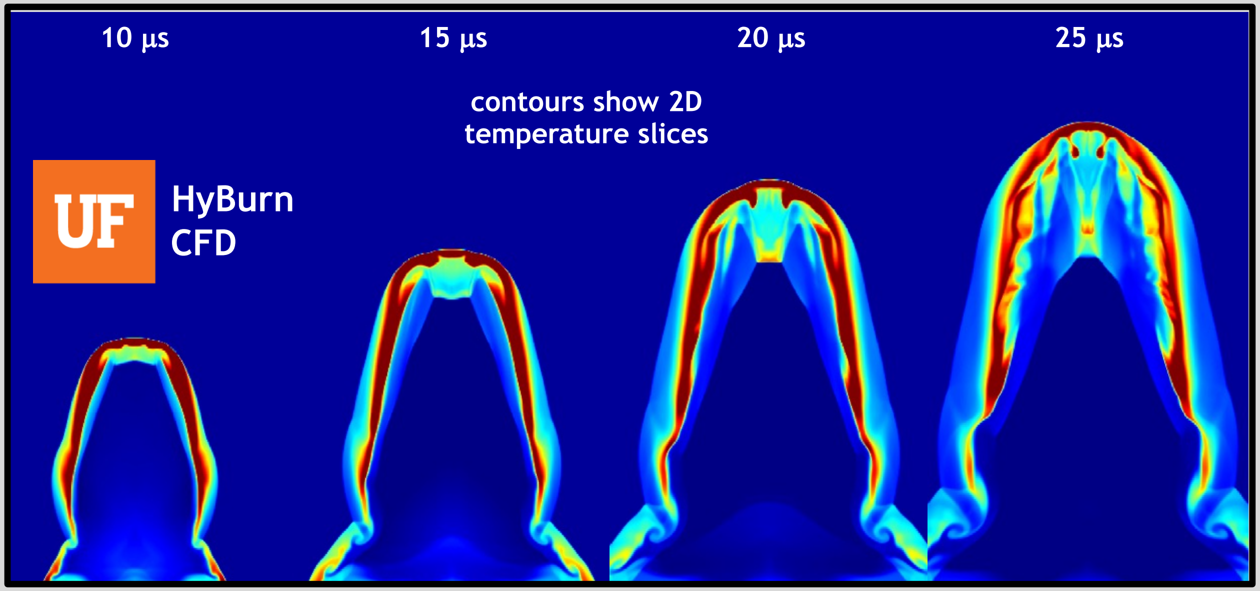




Key Takeaway

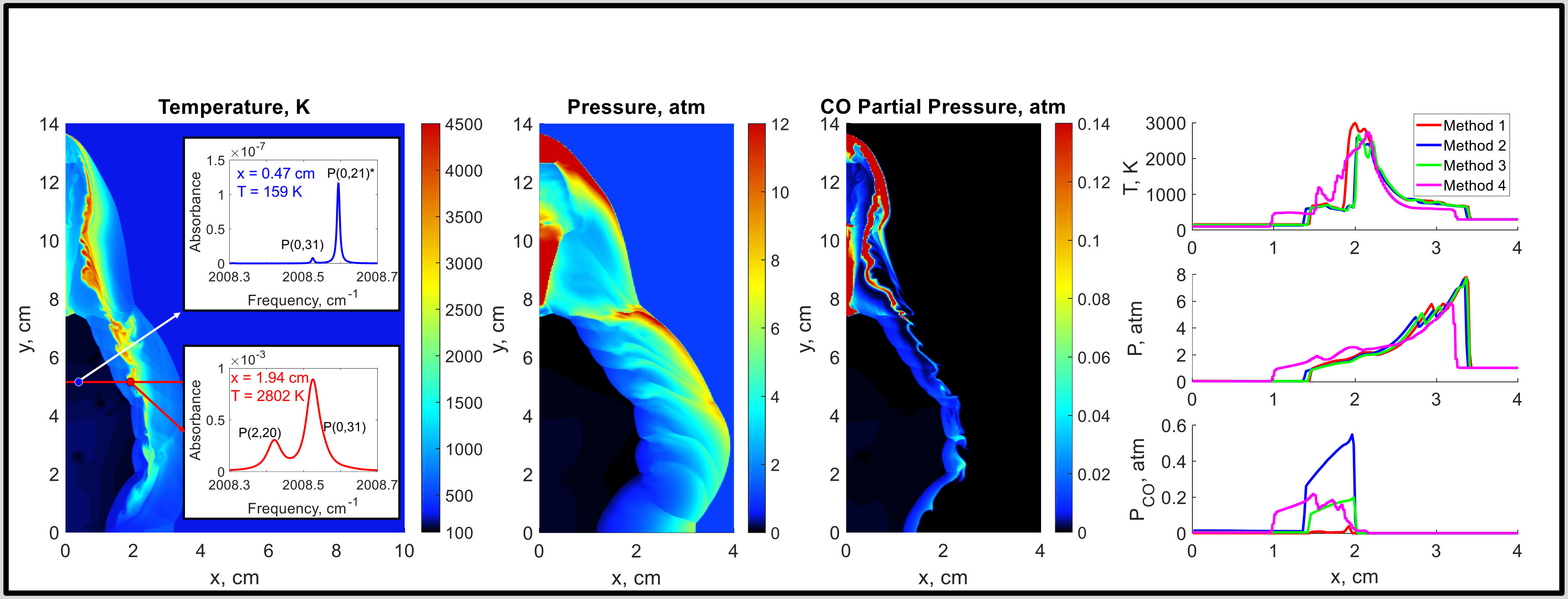
- Results are highly time resolved and repeatable





But how do you compare measurements to models recognizing they both have flaws?

Use CFD to simulate your spectroscopic measurements

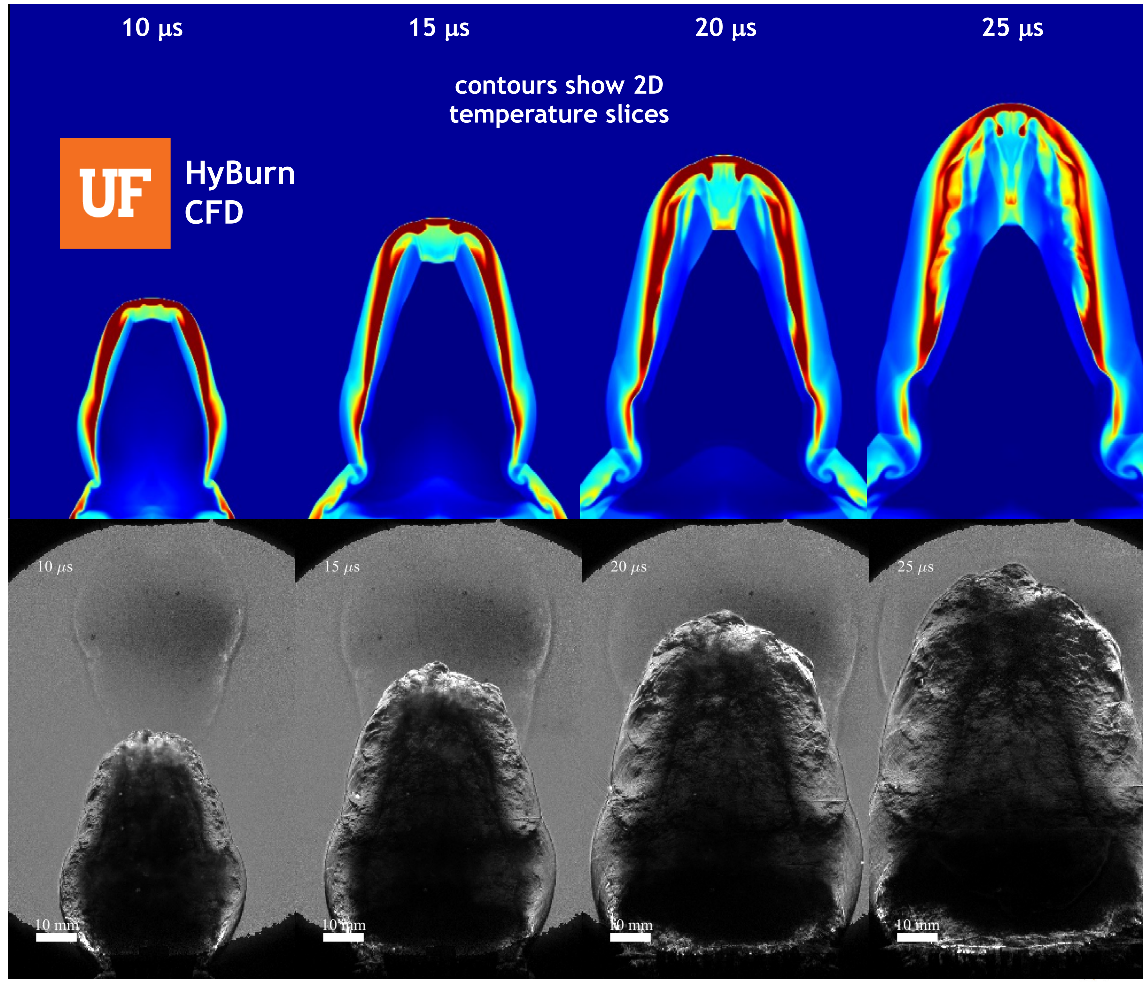


Compare experimental LAS measurements vs synthetic LAS measurements

Fireball Modeling

LABORATORY DIRECTED RESEARCH & DEVELOPMENT
Grand Challenges

Simulation Framework



Multi-physics requires several coupled computational tools

1. Hydrocode predicts explosive detonation and fragmentation

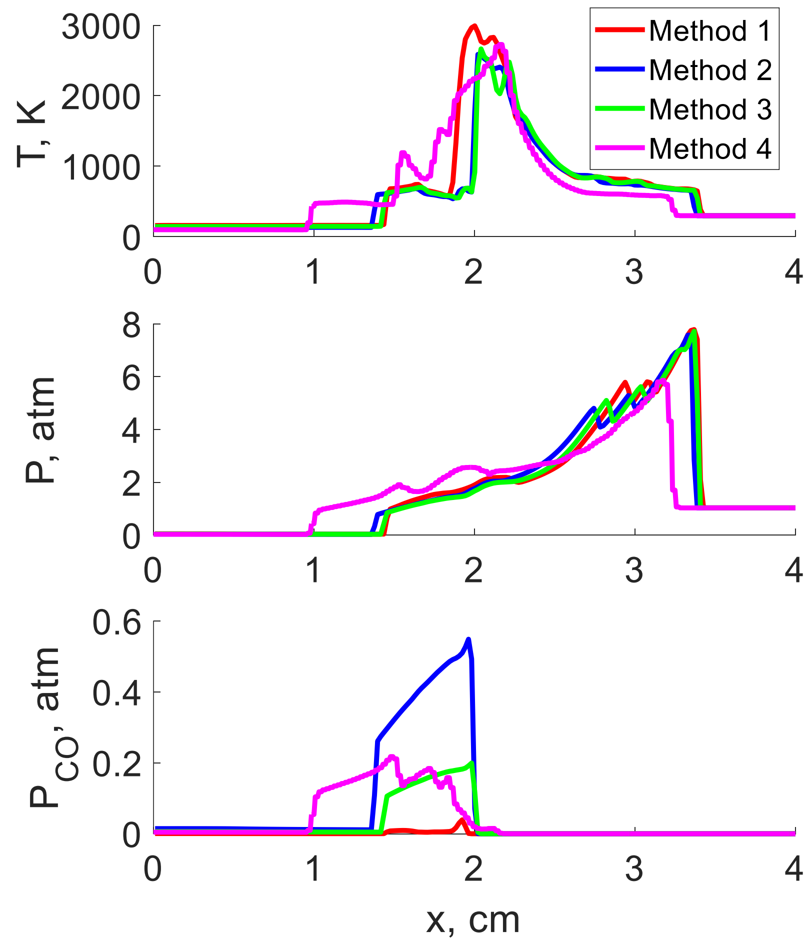
2. ***Fireball species initialized based on equilibrium and kinetics assumptions***

3. 3D reactive Large Eddy Simulation (LES) predicts fireball evolution

Fireball Modeling Assumptions

Evaluated 4 CFD Models

- **Method 1 (2D)**
  - Chemical equilibrium at 4 μs handoff to HyBurn
    →Very little CO
- **Method 2 (2D)**
  - K-W rules implemented at handoff time
    → Much more CO!
- **Method 3 (2D)**
  - Isentropic expansion from CJ state to 1500 K, afterwhich kinetics are frozen prior to handoff to HyBurn
- **Method 4 (3D)**
  - 3D version of Method 3



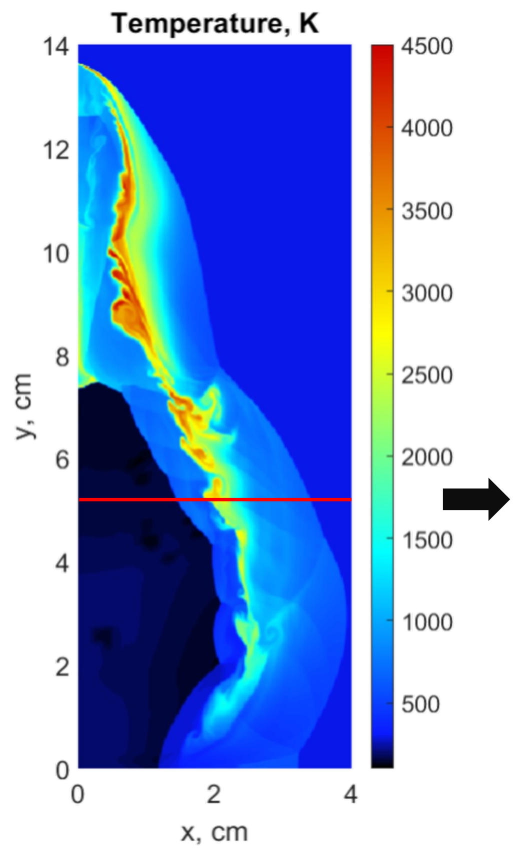
Results: Comparison with Synthetic LAS Measurements

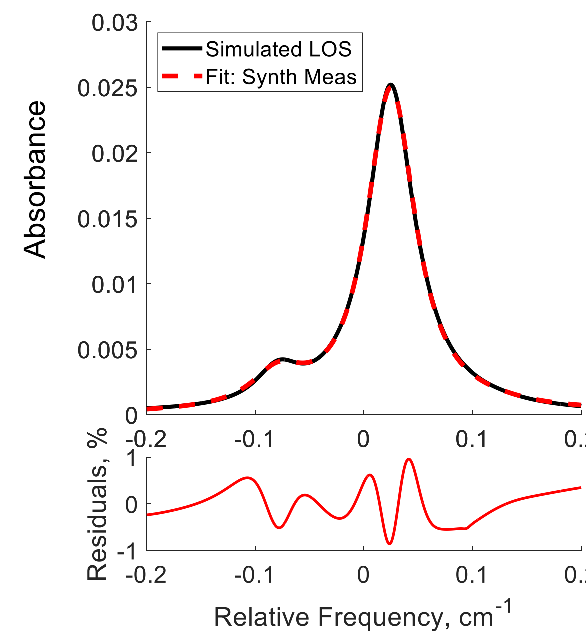
1. CFD provides
   - T, P, X_{CO}, X_{CO2}, X_{H2O}, X_{OH}, X_{NO} as f(x)
2. Used spectroscopic model to calculate path-integrated absorbance spectrum:

$$\alpha = \int_0^L S(T_i)P_{CO,i}\,\phi_i(\nu,\Delta\nu_c,\Delta\nu_d)dl$$

$$\alpha(\nu) = \sum_i S(T_i)P_{CO,i}\,\phi_i(\nu,\Delta\nu_c,\Delta\nu_d)dx$$

3. Fit a simulated spectrum *assuming uniform* LOS to synthetic measurement of $\alpha(\nu)$
   - ***Gives T, P, P_{CO}L to compare with measured values!***





Fitting results:
T = 1593.8 K
P = 1.14 atm
P_{CO} = 0.00044 atm

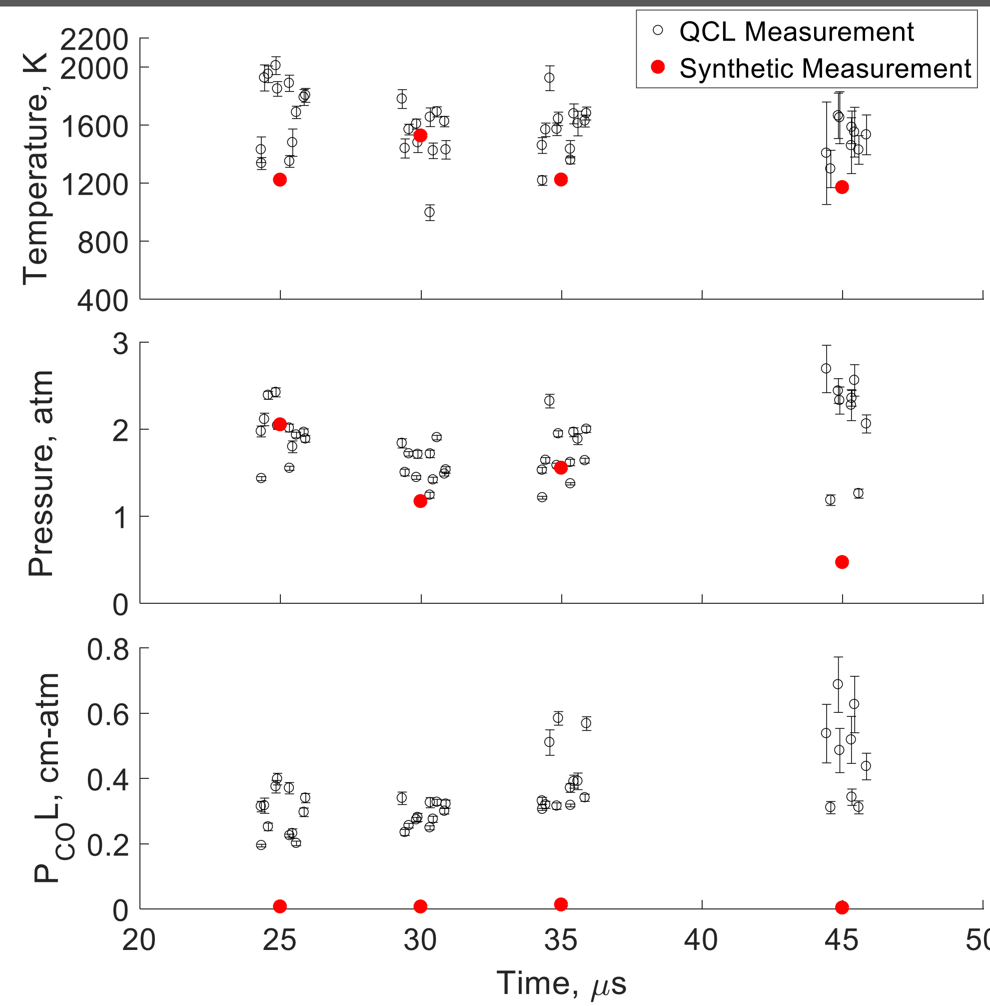
PURDUE ENGINEERING

Results: Comparison with Synthetic LAS Measurements

Key Takeaways for Method 1

- Measured T in general agreement with synthetic measurement
- Measured P in agreement between 25-35 μs
- *Measured $P_{CO}L$ is ~1 order of magnitude larger than synthetic measurement!*

Conclusion: Predicted X_{CO} in hot shell is wrong for Method 1



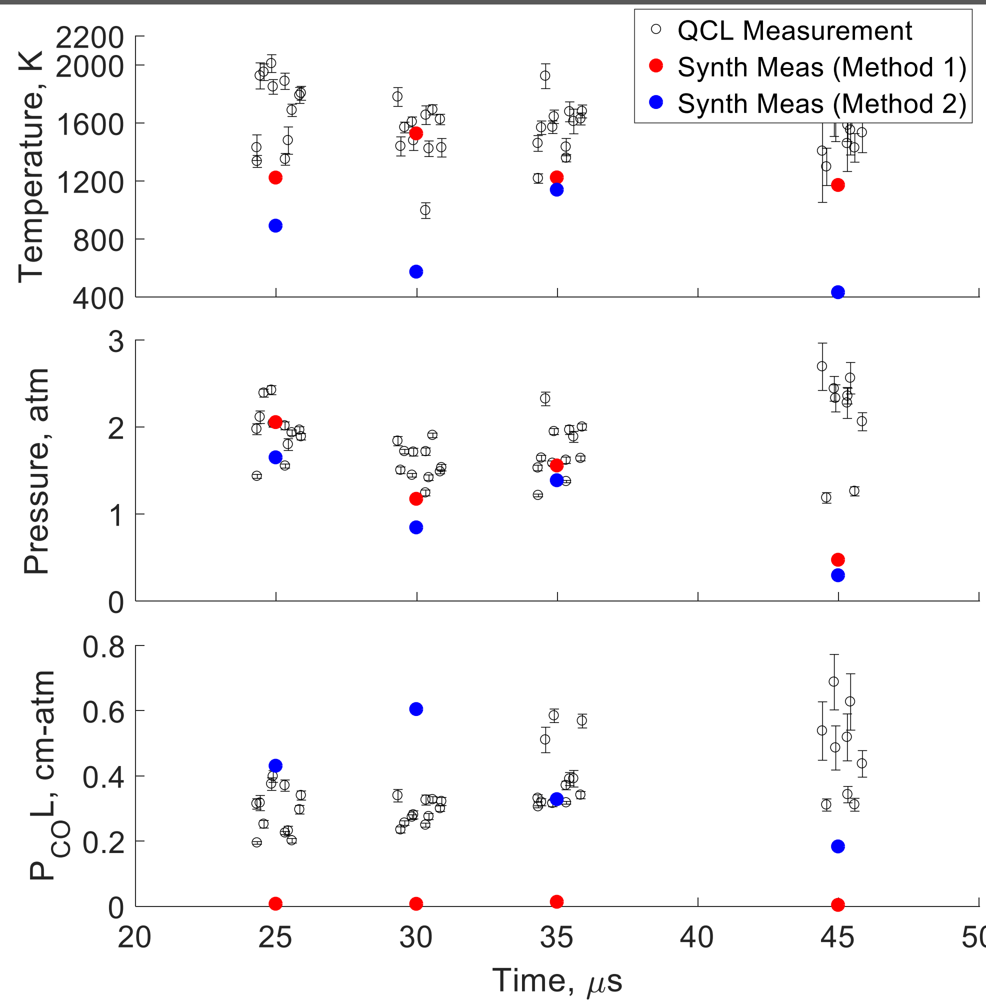
Results: Comparison with Synthetic LAS Measurements

Key Takeaways for Method 2

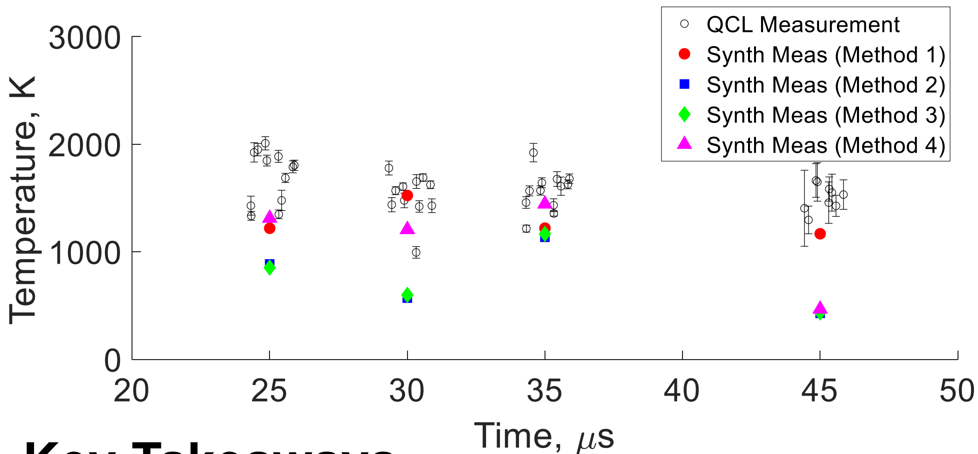
- Synthetic measurement of $P_{CO}L$ dramatically improved (correct order of magnitude)
  - Further suggests there is elevated CO in hot shell!
  - **But why?**
- Synthetic measurement of T and P exhibit significantly worse agreement

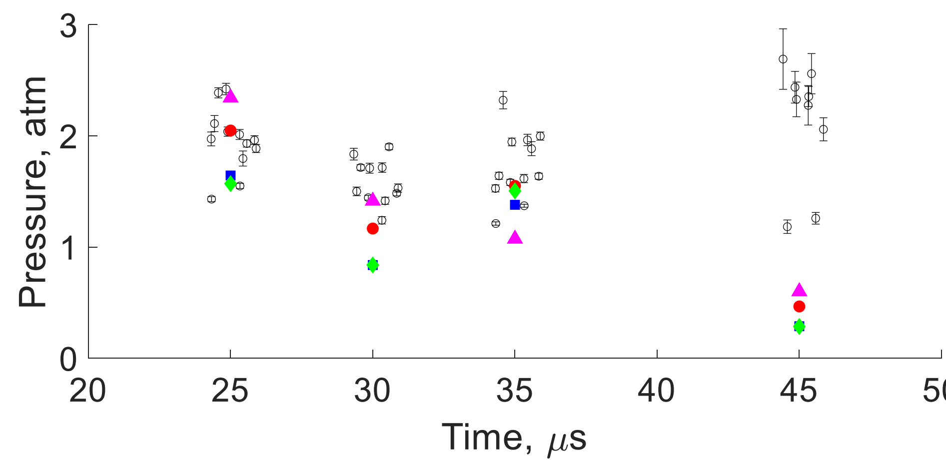
Need a more physical model which leads to more CO:

Methods 3 and 4→Freeze Out



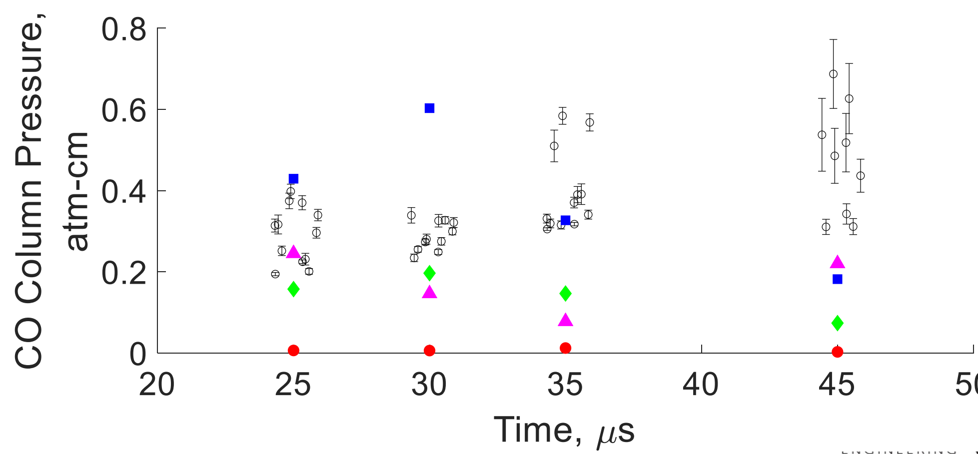
Results: Comparison with Synthetic LAS Measurements





Key Takeaways

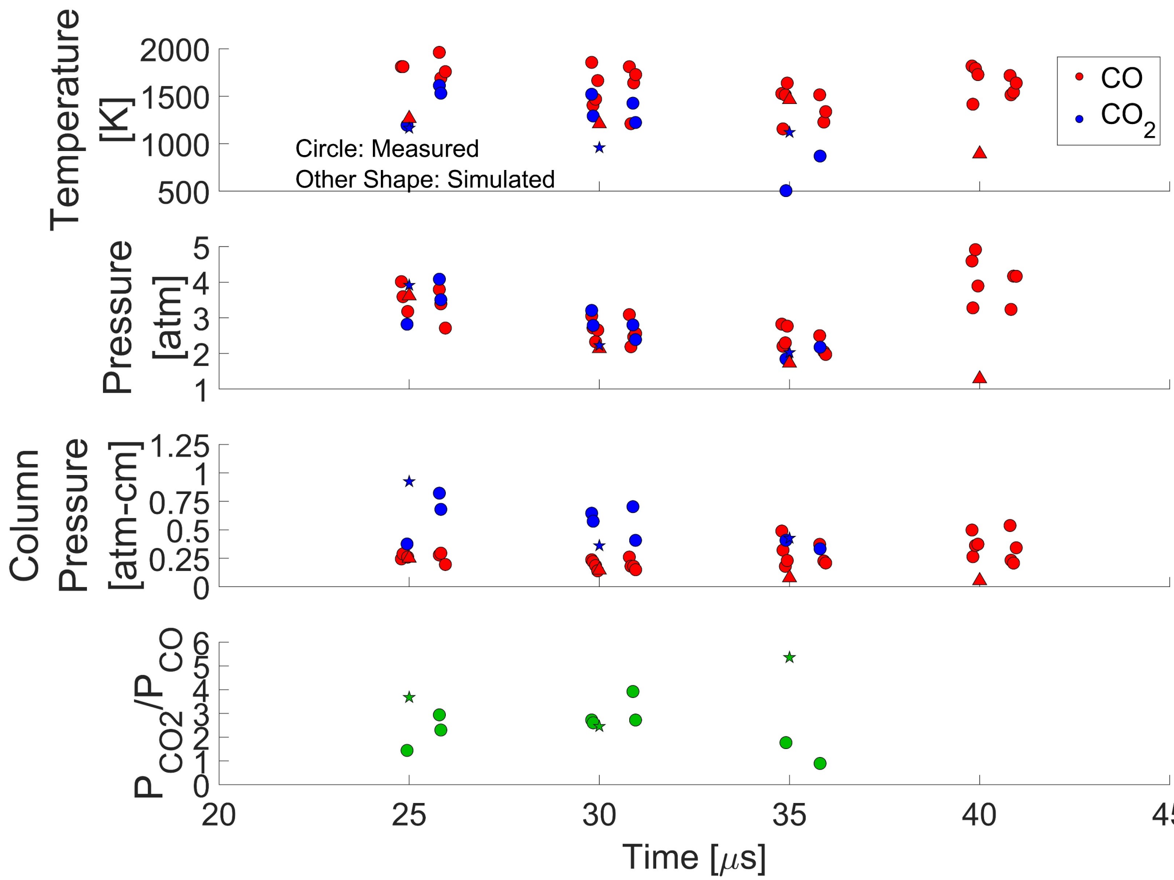
- **Method 3:** CO exhibits reasonable agreement, but *T* is consistently low
- **Method 4:** *T, P,* and CO exhibit good agreement with QCL measurements
  - ***Accounting for freeze out at 1500 K + 3D CFD is most accurate!***



Preliminary Results for CO_2

Key Takeaways

- **Method 4:** *T, P,* CO, and CO_2 exhibit good agreement with QCL and ICL measurements
  - ***CO_2/CO ratio* further suggests carbon freeze out is being handled appropriately**
  - ***Further improvements possible at longer times by accounting for soot oxidation in CFD???***



Conclusions

- QCLAS diagnostic applied to measure *T, P,* $P_{CO}L$ at 1 MHz in RP-80 fireballs
- ICLAS diagnostic applied to measure *T, P,* $P_{CO2}L$ at 500 kHz in RP-80 fireballs
- Measurements used to evaluate 4 CFD models
  - Illustrate importance of accounting for freeze out and 3D effects

Main Challenges Addressed:

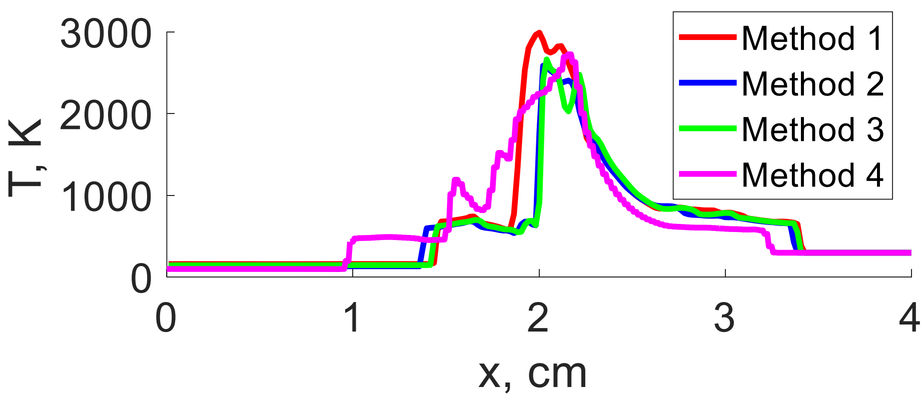
- Achieved MHz measurements in post-det fireballs
  →Wavelength selection + deep current modulation
- Overcame Extremely Nonuniform LOS
  →Wavelength selection + comparison with synthetic measurements
  →Dual-zone absorption model (see upcoming Proc. Comb. Inst. paper)

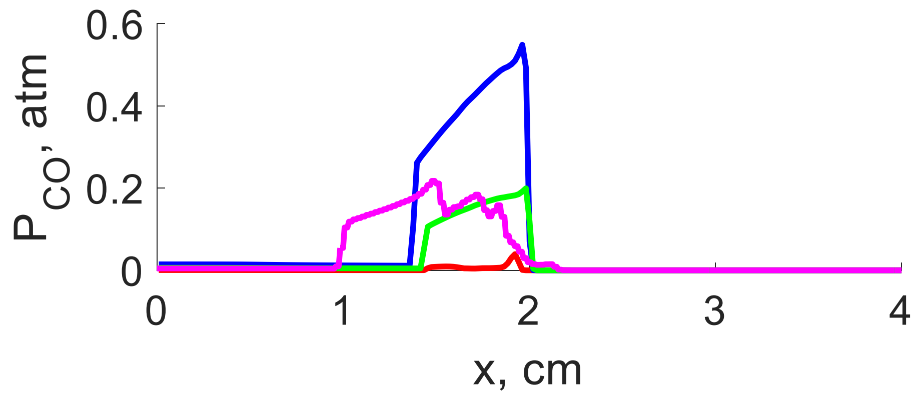
PURDUE ENGINEERING

Conclusions

Caveat: Accuracy of T, P, and CO ***profiles*** remains uncertain, BUT:

- Comparing experimental and synthetic LAS measurements *bounds the models*
- *This approach combined with reasonable, scientific arguments enables us to evaluate the accuracy of fireball models and model assumptions*





Acknowledgements

- **2016 DTRA YIP,** Dr. Allen Dalton and Dr. Jeff Davis
- **Sandia National Laboratories**

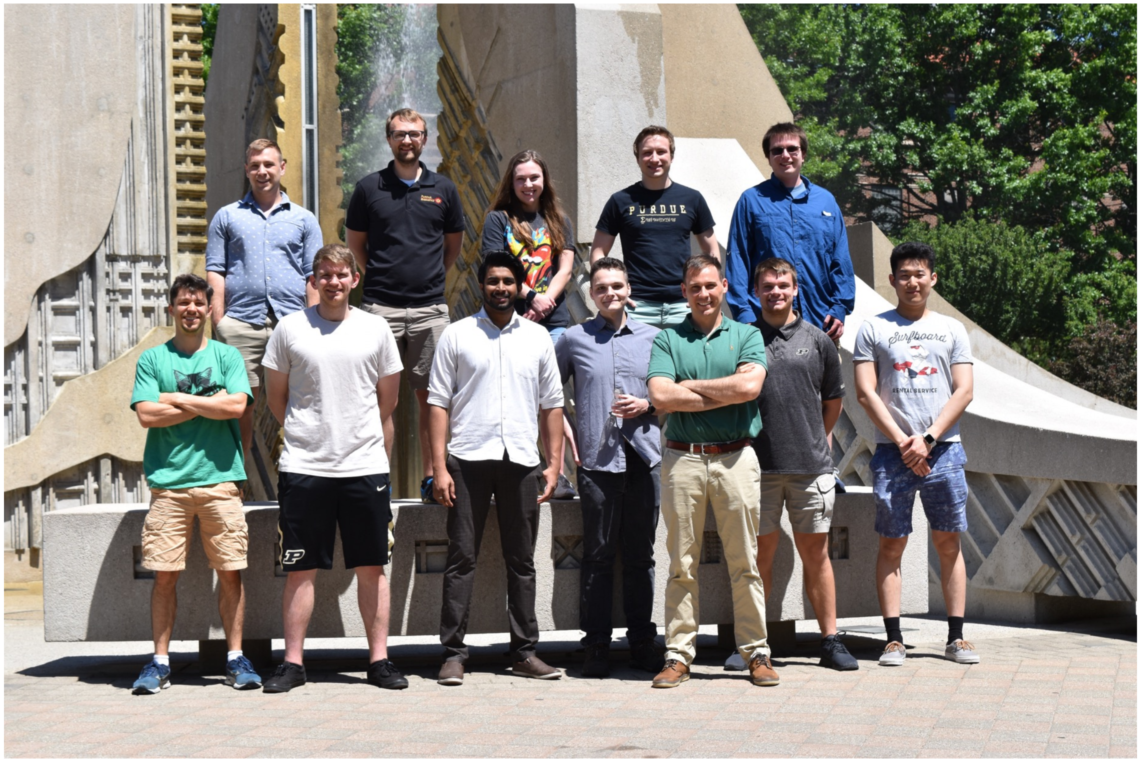
This work was supported by the Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories, which is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. This presentation describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

- **LAS Measurements:** Garrett Mathews, Charlie Schwartz (Purdue)
- **Detonator Testing:** Mateo Gomez, Prof. Steve Son (Purdue)

- **CFD**
  - Anthony Egeln Jr. and Prof. Ryan Houim (University of Florida)
  - Dr. Marco Arienti and Andrew Thompson (SNL)

- **Project Guidance and Leadership**
  - Dr. Dan Guildenbecher and Dr. Marc Welliver (SNL)

Acknowledgements



Learn more about us at: www.GoldensteinGroup.com

Key Papers

[1] G. C. Mathews and C.S. Goldenstein, Near-GHz scanned-wavelength-modulation spectroscopy for MHz thermometry and H_2O measurements in aluminized fireballs of energetic materials, *Applied Physics B* 126 (2020)

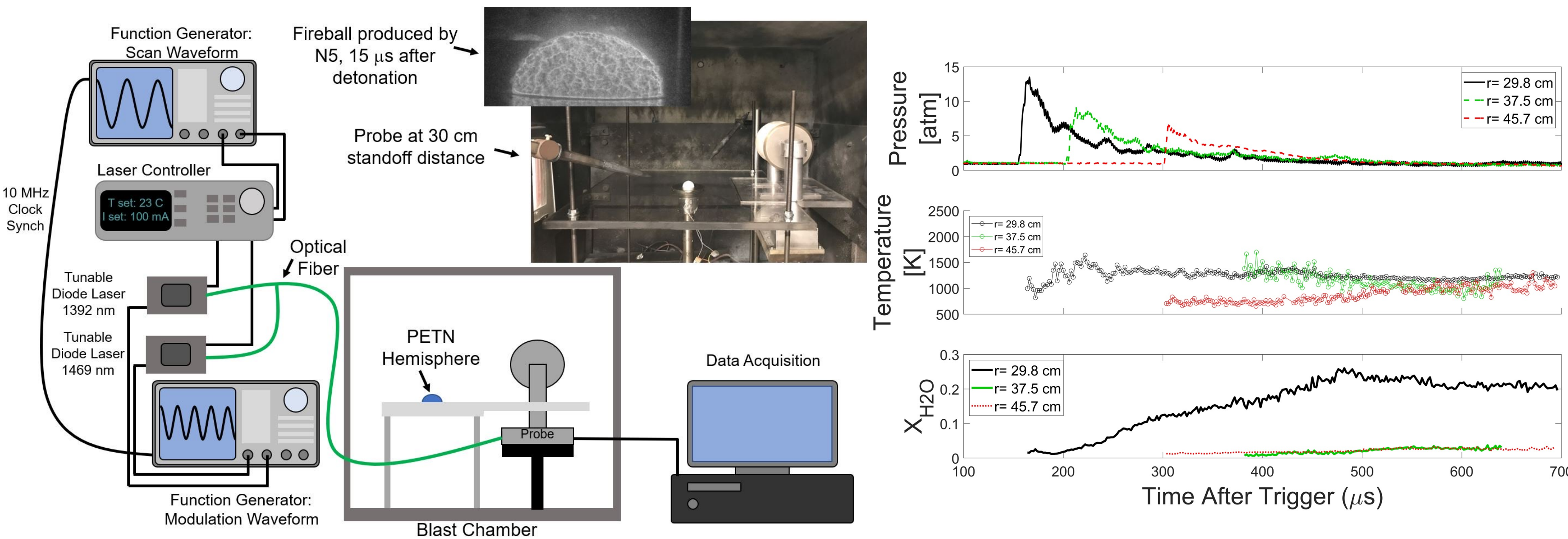
[2] G. C. Mathews et al., High-bandwidth absorption-spectroscopy measurements of temperature, pressure, CO, and H_2O in the annulus of a rotating detonation rocket engine, *Applied Physics B* 127 (2021)

[3] G. C. Mathews et al., Laser-Absorption-Spectroscopy Measurements of Temperature, Pressure, and CO at 1 MHz in Post-Detonation Fireballs, AIAA Scitech 2022 Forum, San Diego, CA, January 3-7, 2022

[4] G. C. Mathews et al., Experimental and Synthetic Laser-Absorption-Spectroscopy Measurements of Temperature, Pressure, and CO at 1 MHz for Evaluation of Post-Detonation Fireball Models, *Proceedings of the Combustion Institute, In Press (2023)*

PURDUE ENGINEERING

Aside: 500 kHz TDLAS at Larger Scale



- Measured T & H_2O at 500 kHz in fireballs of 25 g hemis at UIUC