SAND2022-8049C

MHz LAS Diagnostics for *T*, *P*, and *X* Measurements in Post-Detonation Fireballs of Energetic Materials

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Gordon Research Conference
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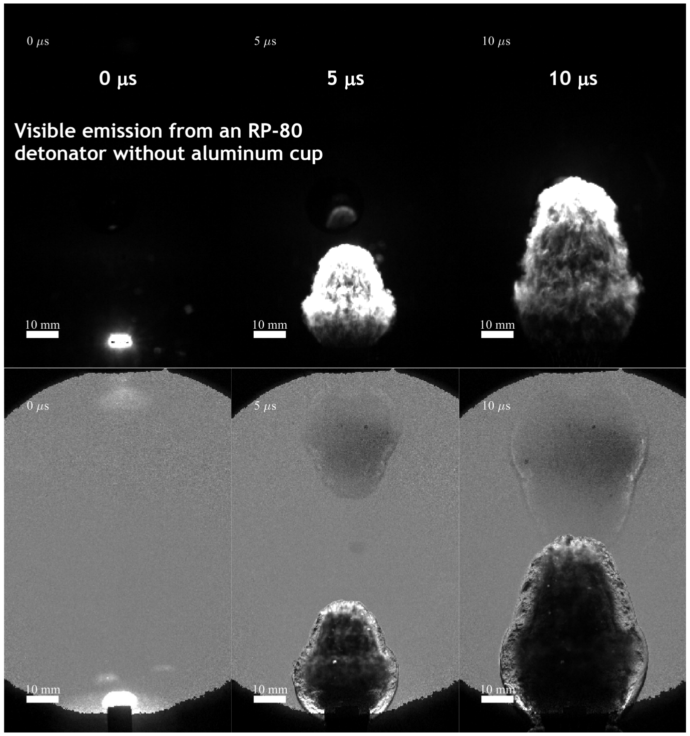
Outline

- Introduction to Sandia *Light Speed Grand Challenge Project*
- Laser Absorption Spectroscopy Sensor Design
    - Addressing Nonuniform Line-of-Sight
- Experimental Setup
- Results
- Evaluation of CFD Models
- Conclusions, Future Work, Acknowledgements



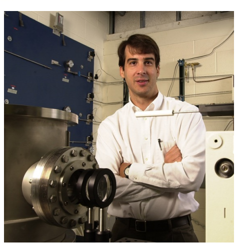
Sandia Light Speed Grand Challenge

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

UF UNIVERSITY of FLORIDA

ILLINOIS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN



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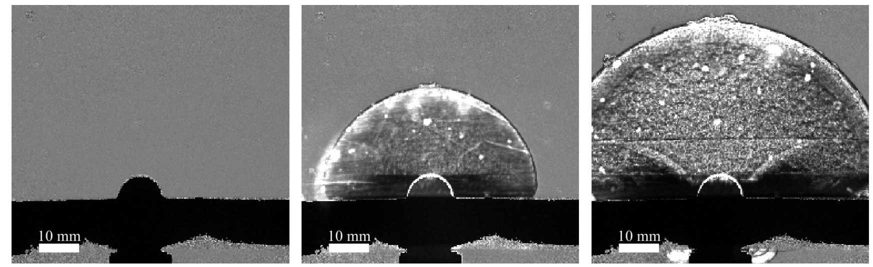
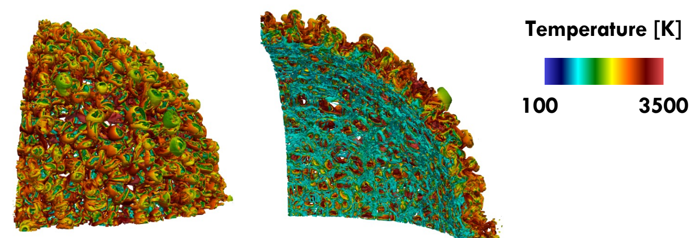
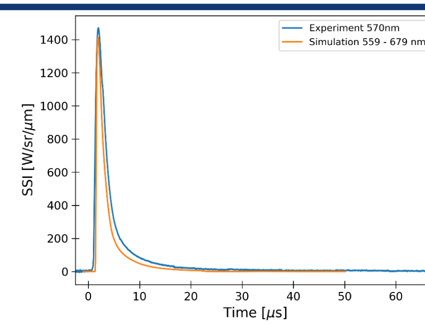
Advanced Experimental Diagnostics



High-Fidelity Simulation



Optical Emission Predictions



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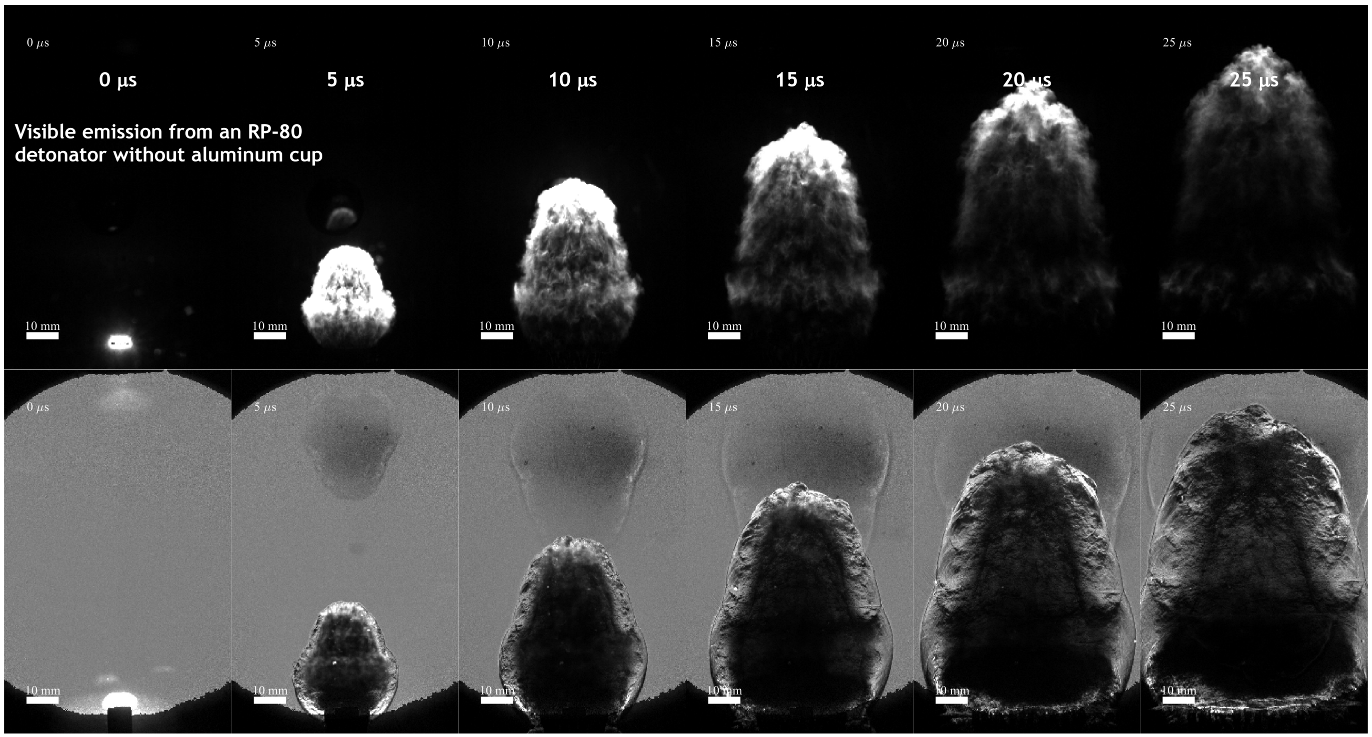
The Beginning

- Characterization of RP-80 fireballs using emission and schlieren imaging



- Results illustrate structure of fireball and regions of peak luminosity

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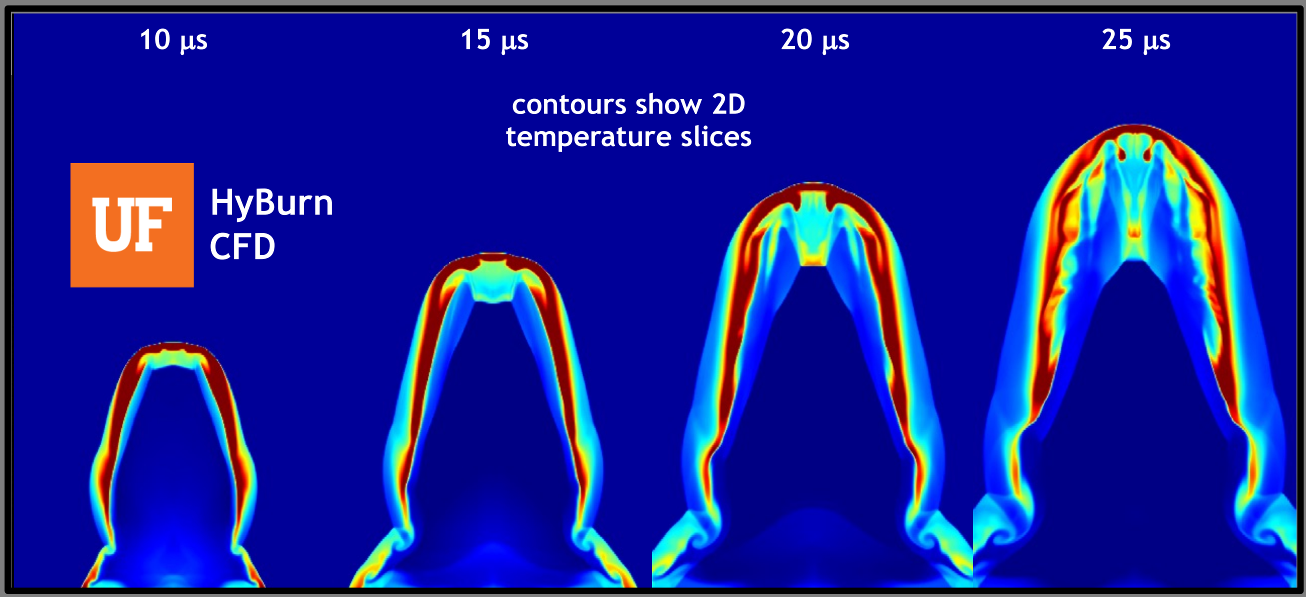
But when measured and modeled emission don't agree, how do you know what is responsible?!?

Emission = f(T, P, X)



Need laser diagnostics to characterize T, P, and species in hot outer shell!

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Grand Challenges

Our Goals

- Acquire temperature, H_2O, CO measurements in post-det fireballs at ~ MHz rates to evaluate fireball model accuracy

Challenges

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

Solutions

- Optical engineering
- Spectral and spatial filtering
- DFB QCLs *with bias-tee* + wavelength selection
- Wavelength selection *+ utilization of synthetic measurements from CFD results*

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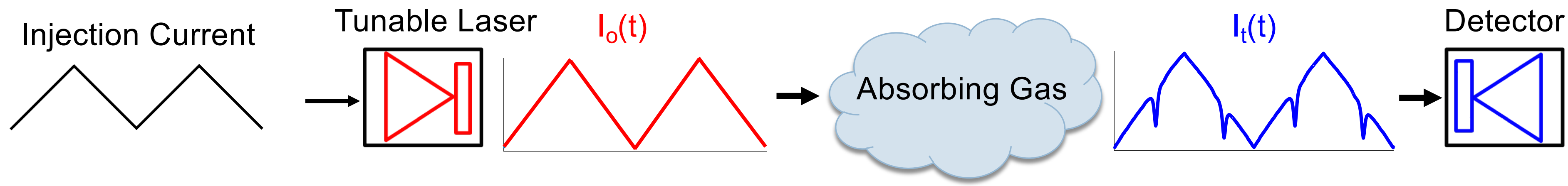
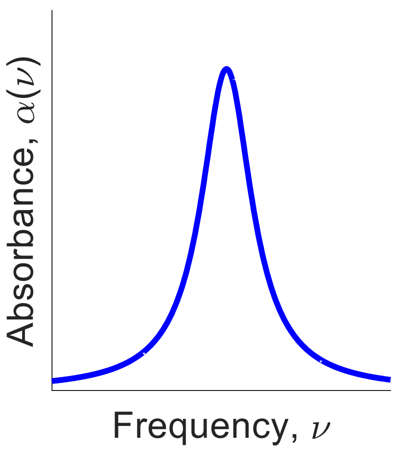
LAS Sensor Design: Diagnostic Technique



Spectral Absorbance: α(ν)

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

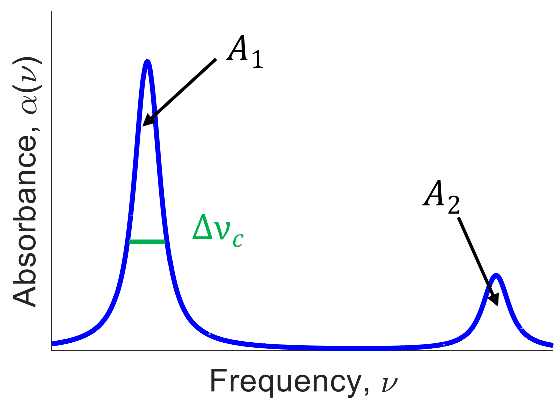
$$\alpha(\nu) = S(T)\phi_i(\nu)PX_iL$$



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)

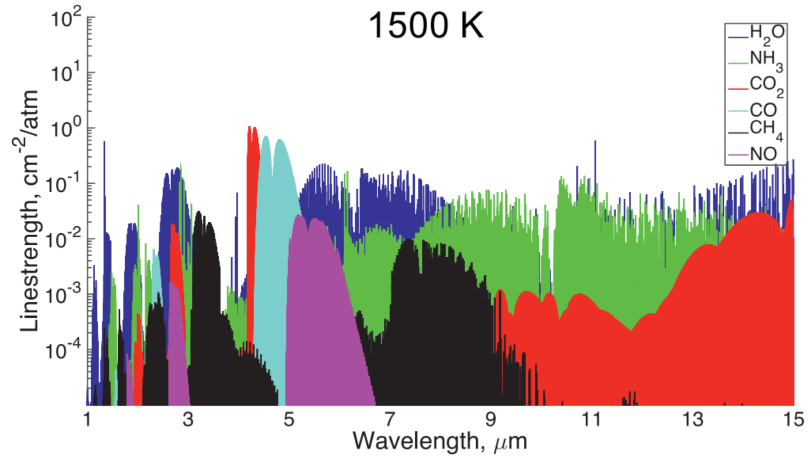
LAS Sensor Design: Wavelength Selection

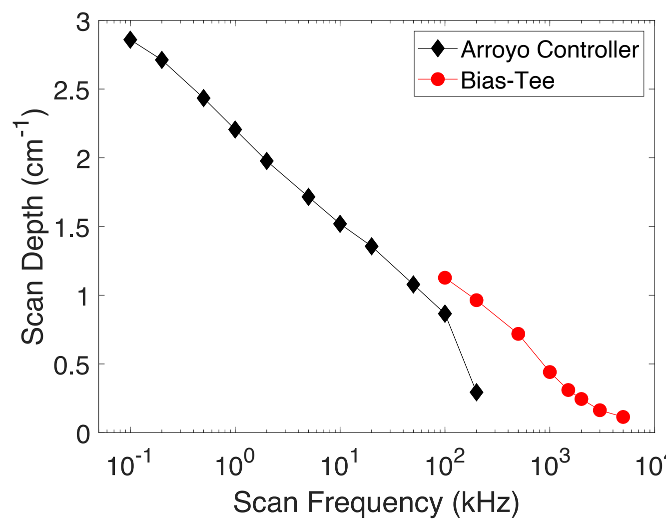
Need mid-IR wavelengths
- Strong absorption needed for small scale and concentrations→

Need high-E” transitions
- Minimizes absorption in cold core→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→



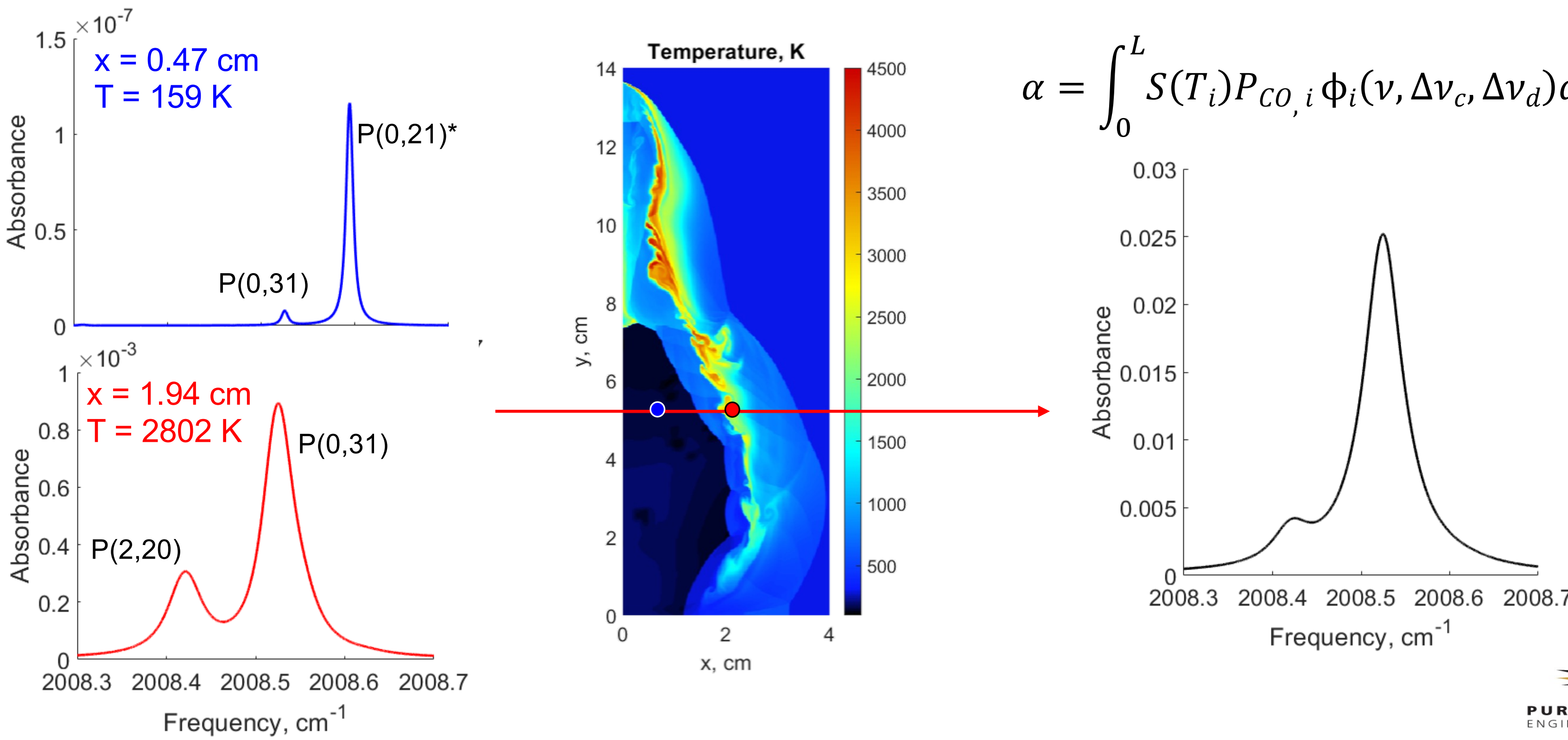


LAS Sensor Design: Wavelength Selection

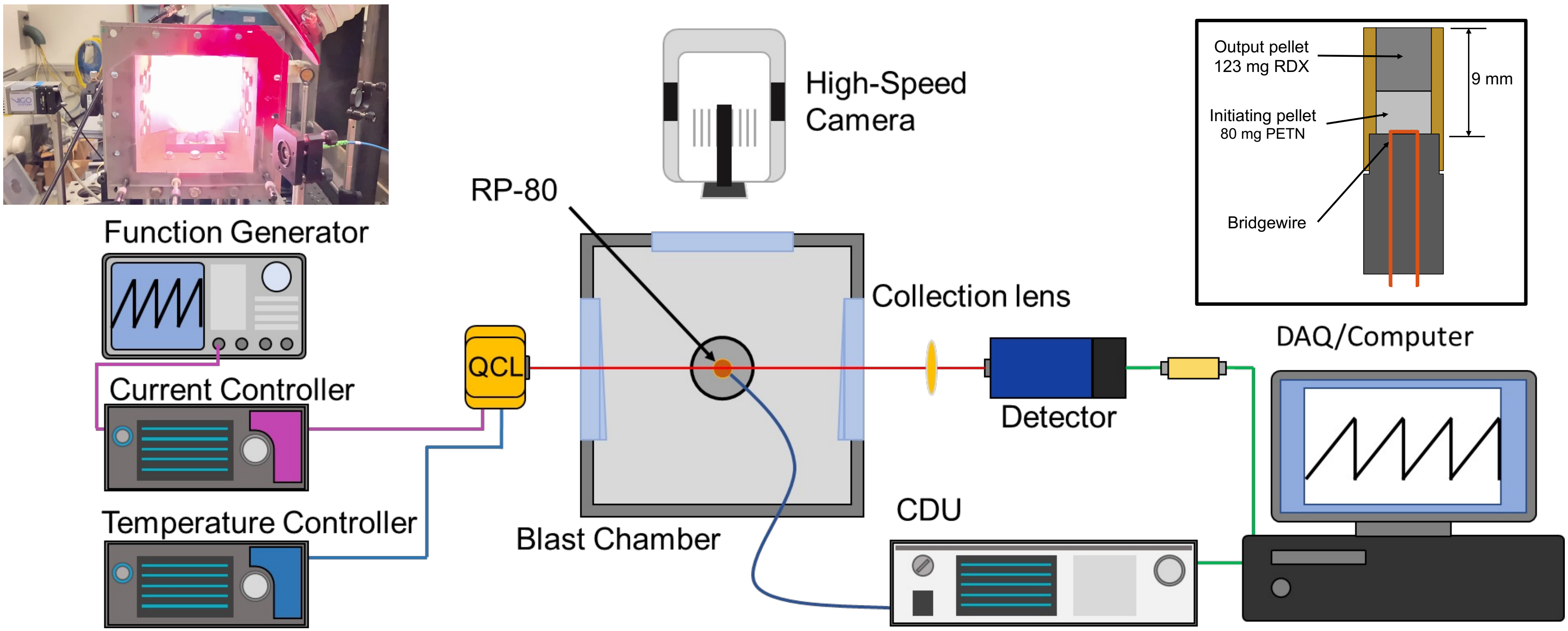
QCL targets CO P(0,31) and P(2,20) transitions near 2008.5 cm^{-1} (~5 μm)

- E" ~1901 and 5052 cm^{-1}, ΔE"=3151 cm^{-1}
    - Measurements are deliberately biased to fireball's hot outer shell!

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



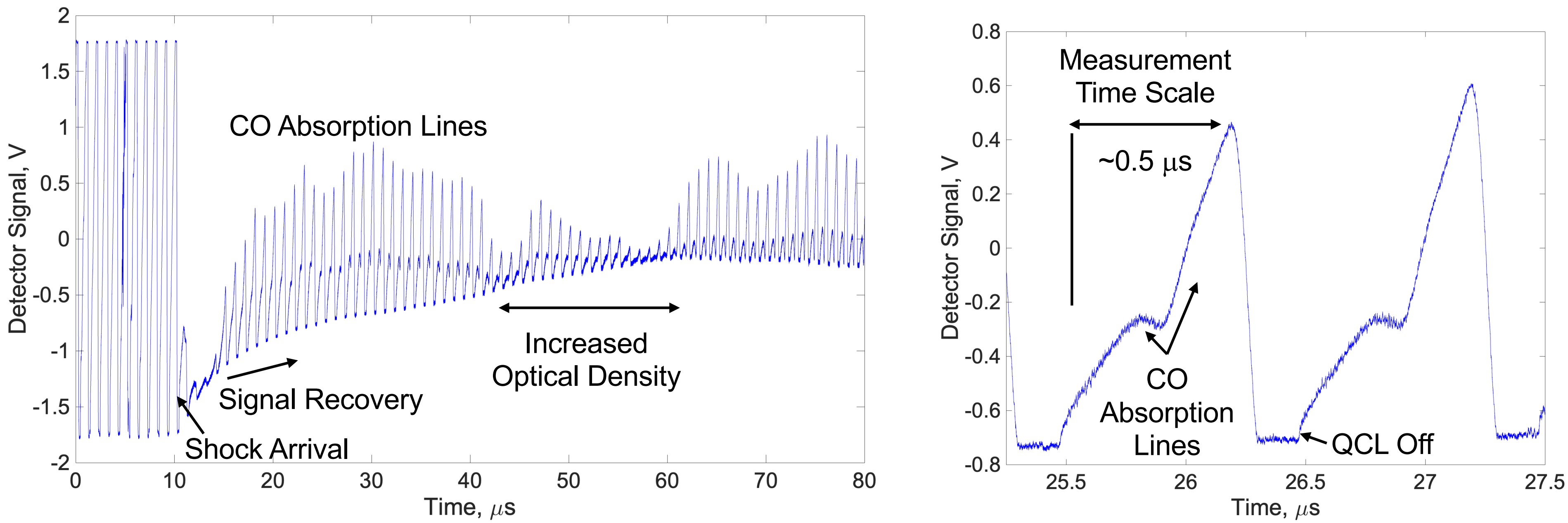
Experimental Setup



Key Details

- QCL scanned across CO transitions at 1 MHz, signal acquired on 200 MHz detector at 3 GS/s

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

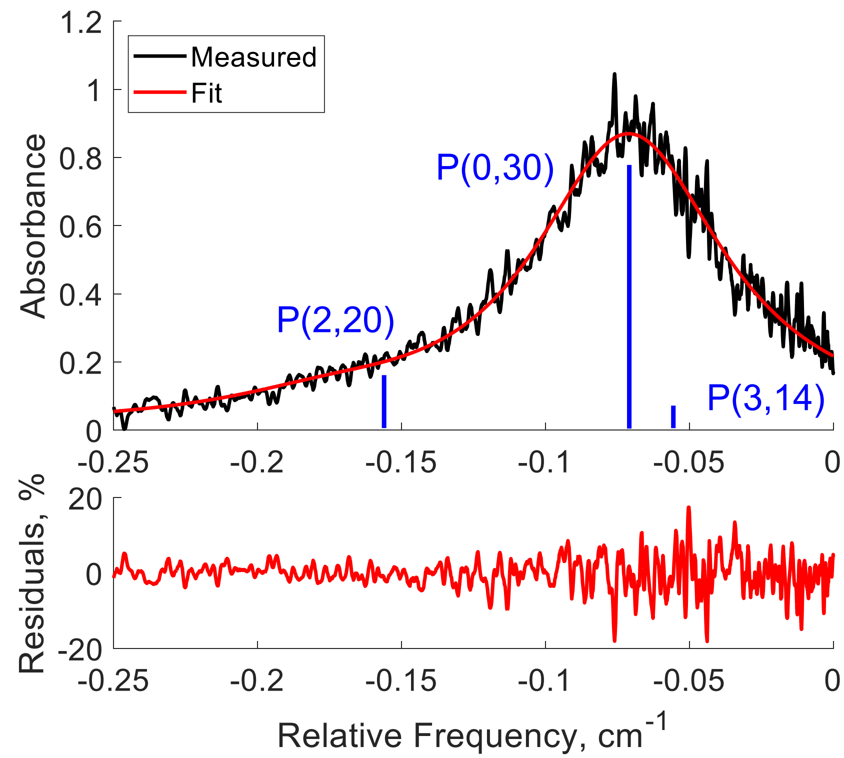
Results: Example Absorbance Spectrum

Key Takeaways

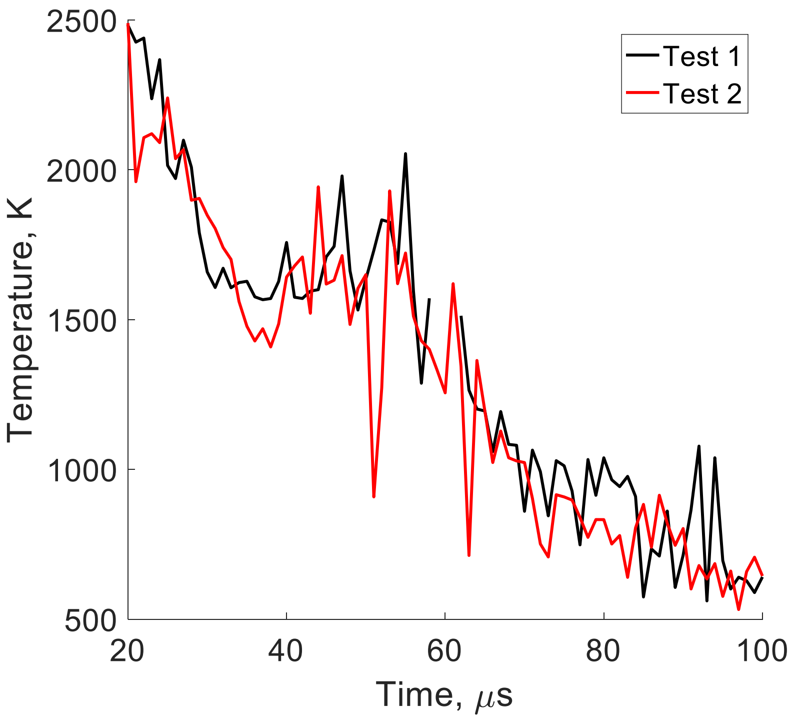
- Large absorbance
  - Relatively high-SNR
- Spectrum dominated by 2 lines
- Spectrum well modeled by uniform LOS absorption model using HITEMP2019
  - Single *T, P, $P_{CO}L$* from each fit

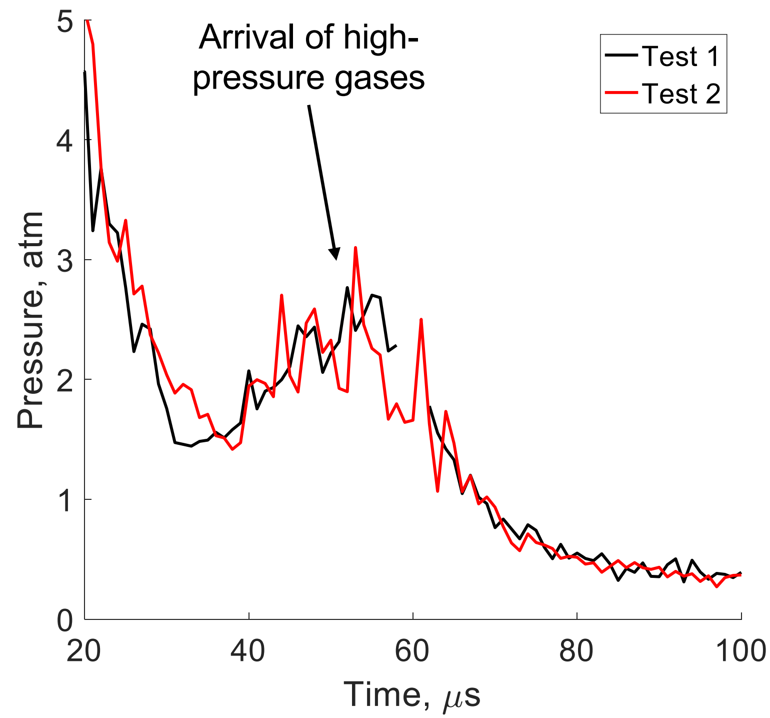
T = 1360 K,
P = 1.63 atm,
$P_{CO}L$ = 0.315 atm-cm

Example Single-Scan Measurement



Results: Time Histories at *y* = 51 mm



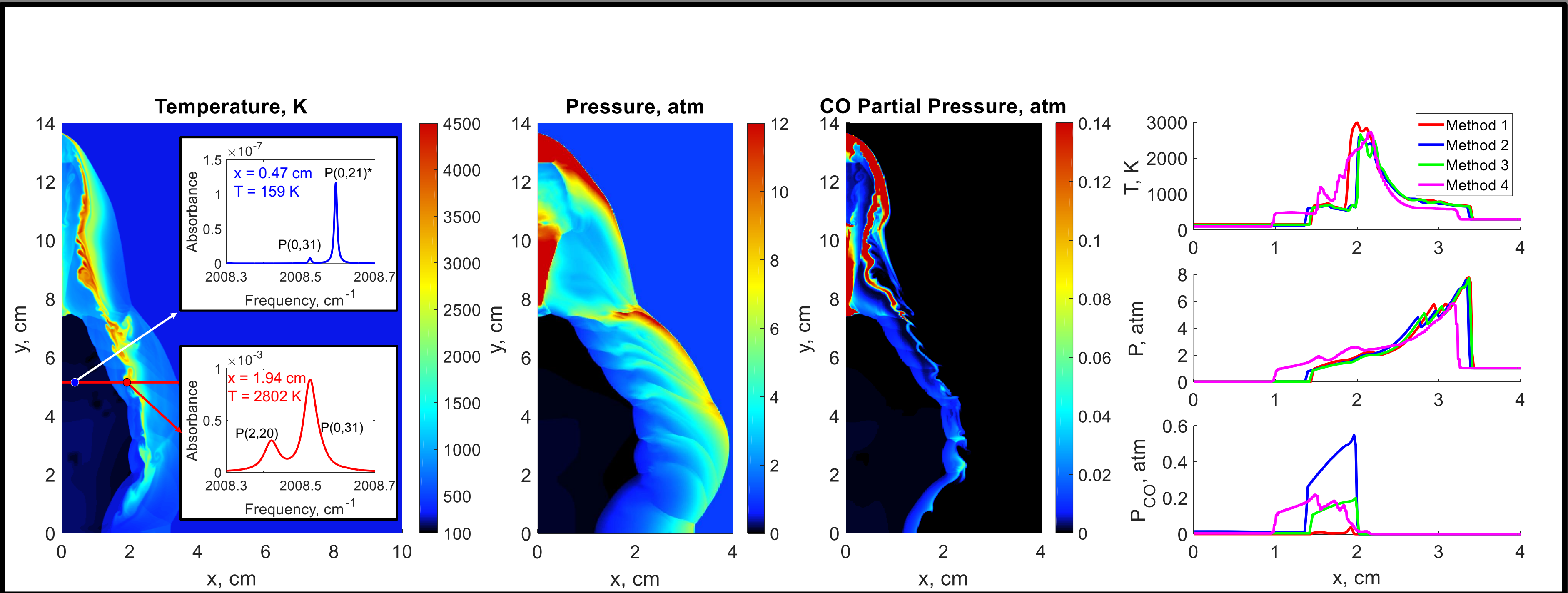


Key Takeaway

- Results are highly time resolved and repeatable

So how can this data be used to evaluate fireball models?

Compare with synthetic LAS measurements from CFD+Spectroscopy!



Fireball Modeling

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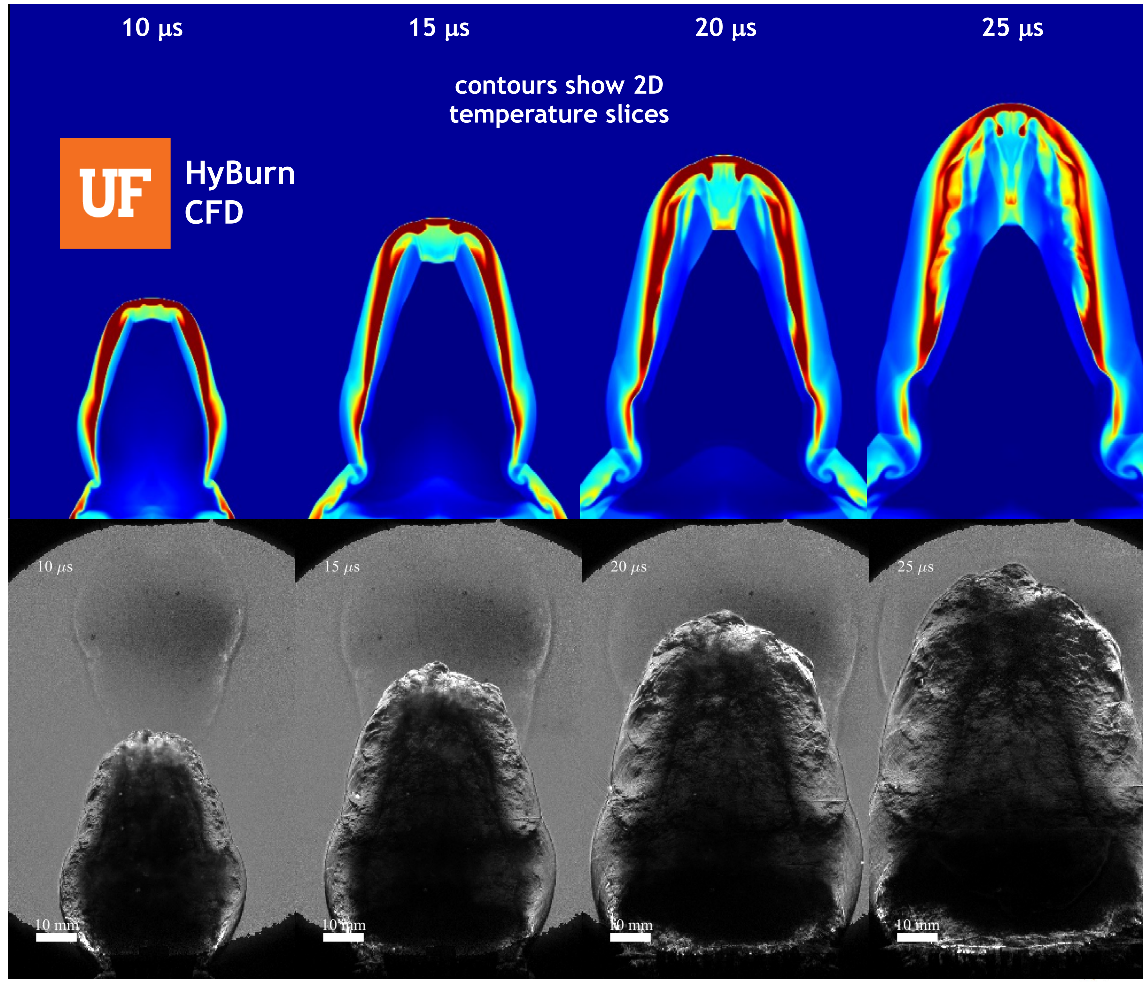
Simulation Framework



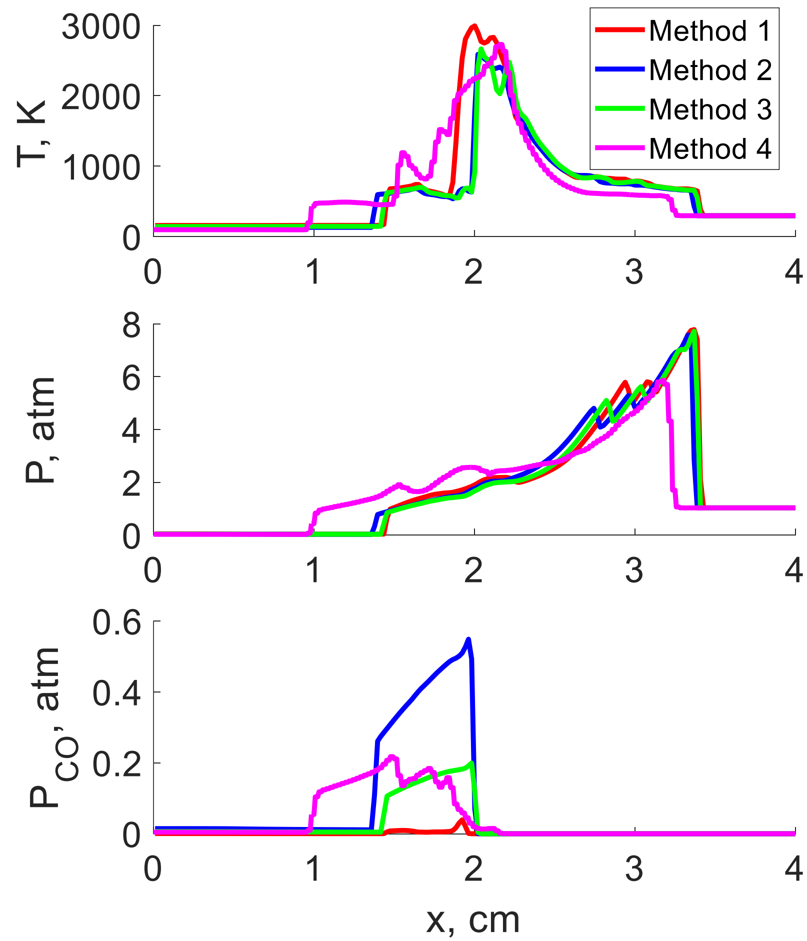
Multi-physics requires several coupled computational tools

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

<u>Evaluated 4 CFD Models</u>

- **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



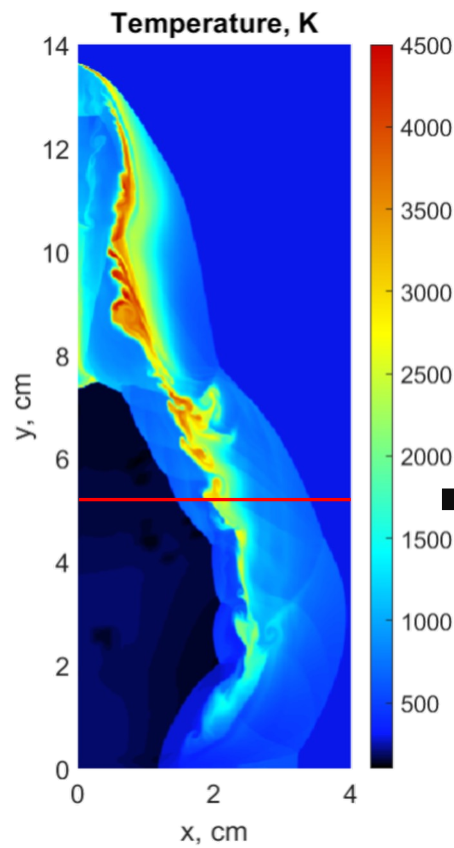
Results: Comparison with Synthetic LAS Measurements

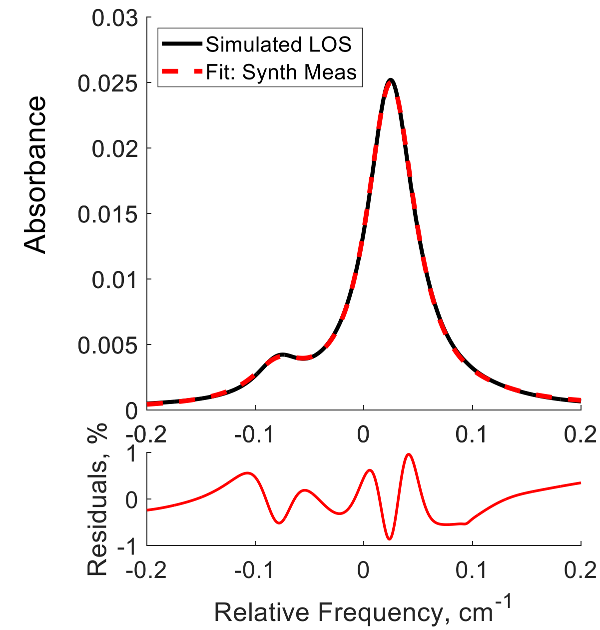
1. CFD provides
   - T, P, X_{CO}, X_{CO2}, X_{H2O}, X_{OH}, X_{NO} as f(x)
2. Used spectroscopic model to calculate path-integrated absorbance spectrum:

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

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

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!***



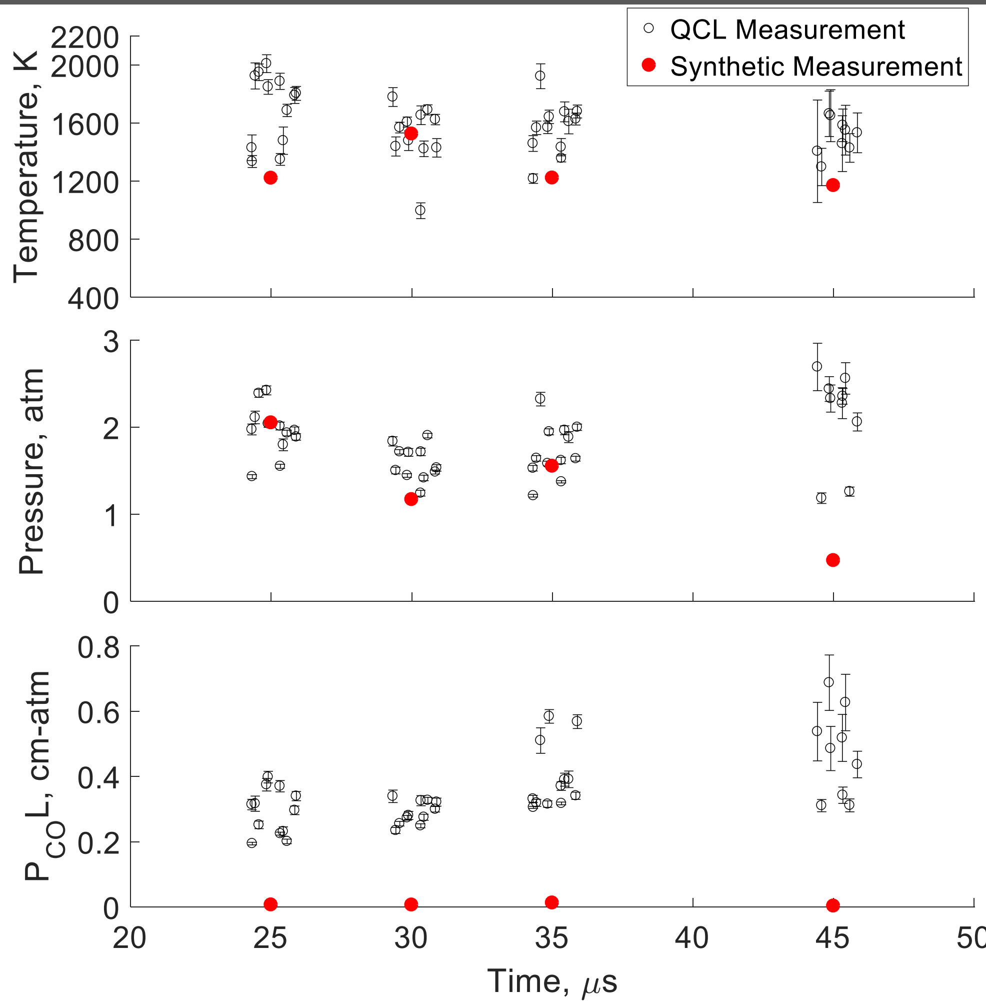


Fitting results:
T = 1593.8 K
P = 1.14 atm
P_{CO} = 0.00044 atm

Results: Comparison with Synthetic LAS Measurements

Key Takeaways for Method 1

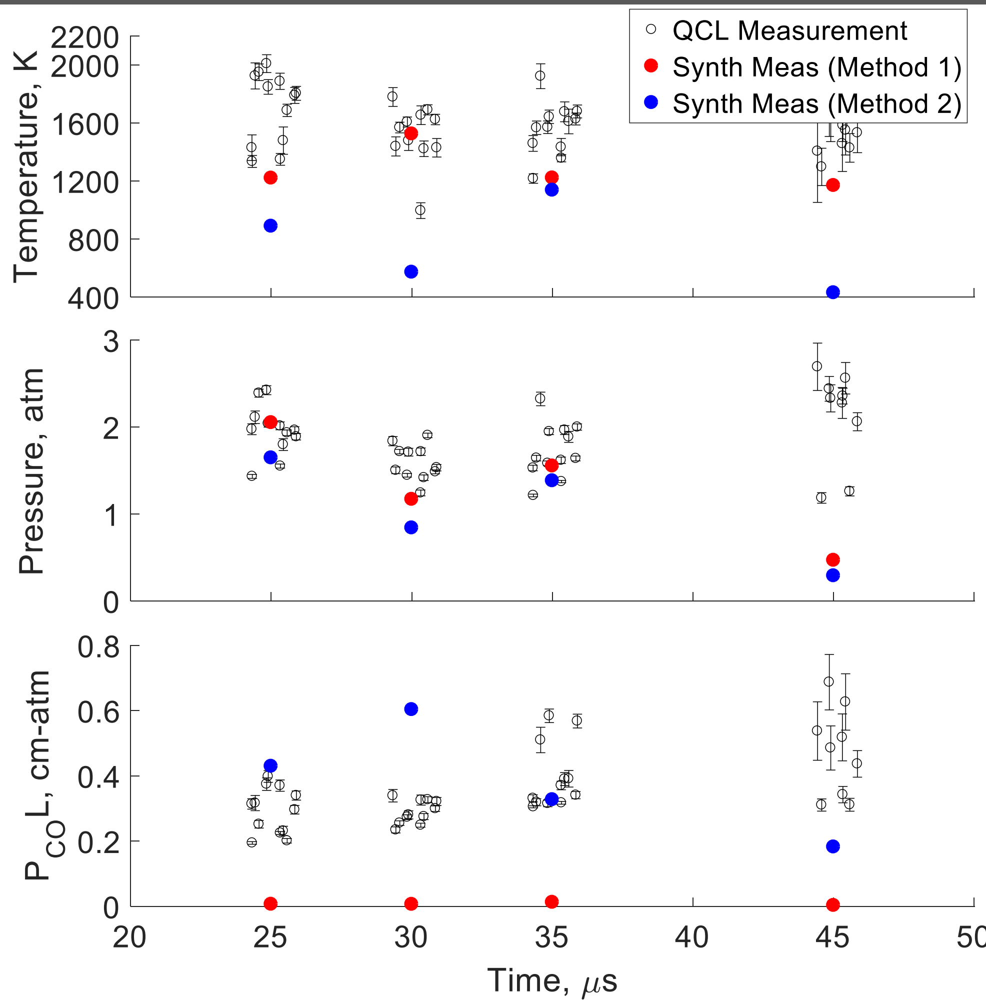
- Measured T in general agreement with synthetic measurement
- Measured P in agreement between 25-35 μs
- *Measured $P_{CO}L$ is order of magnitude larger than synthetic measurement!!!!!*



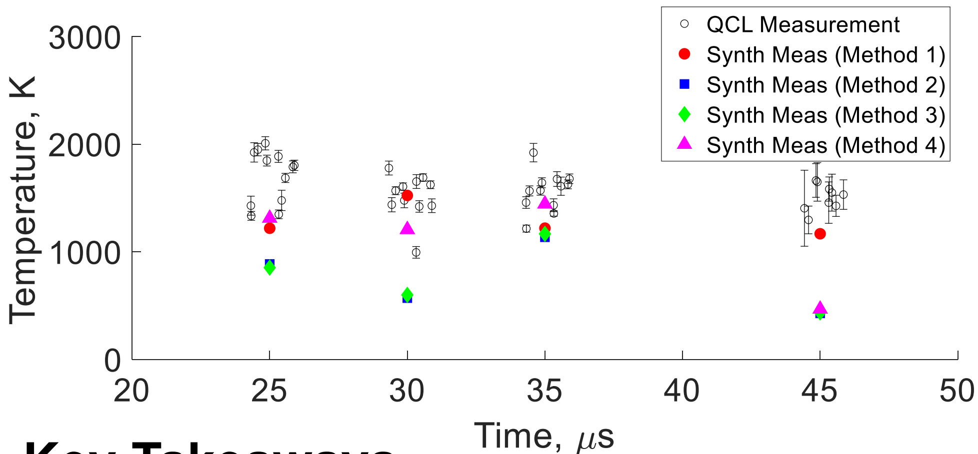
Results: Comparison with Synthetic LAS Measurements

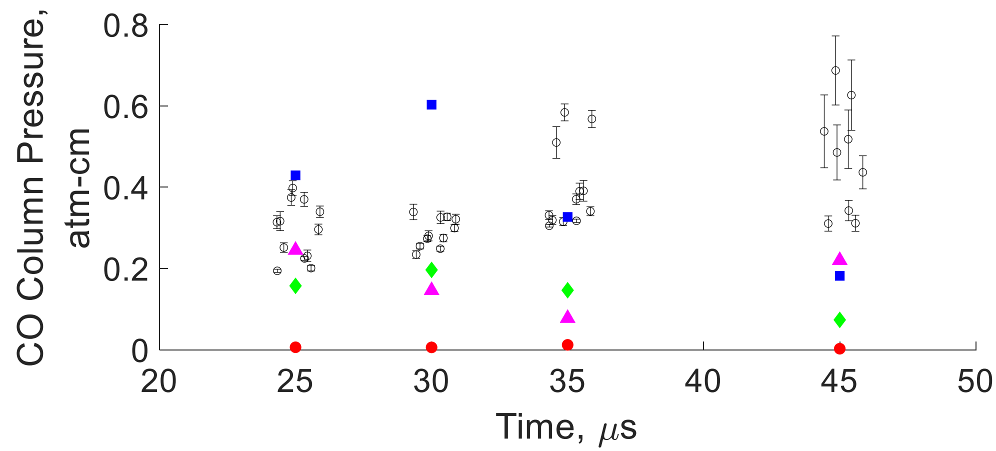
Key Takeaways for Method 2

- Synthetic measurement of $P_{CO}L$ dramatically improved (correct order of magnitude)
  - Illustrates importance of accounting for carbon freeze out!
- But synthetic measurement of T and P exhibit significantly worse agreement with QCL measurement…



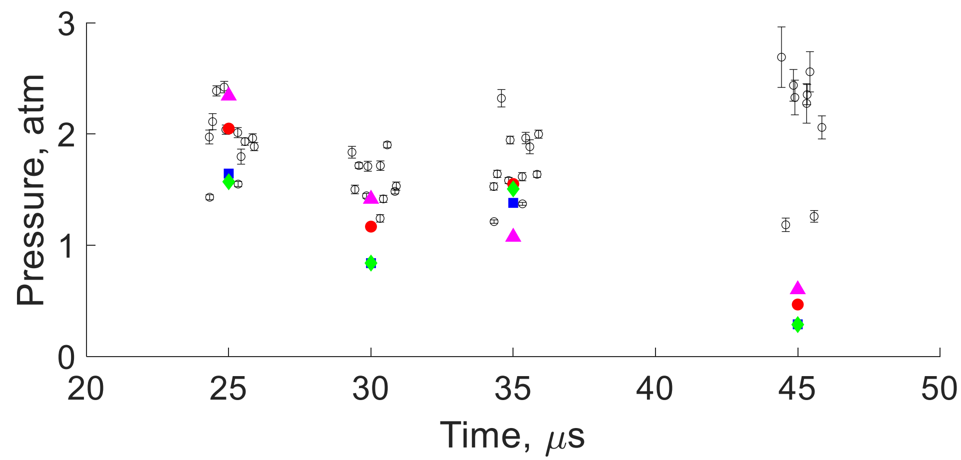
Results: Comparison with Synthetic LAS Measurements





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!***



Conclusions

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

Main Challenges Addressed:

- Optical density

  → Careful alignment + MHz scanning
- Elevated pressures

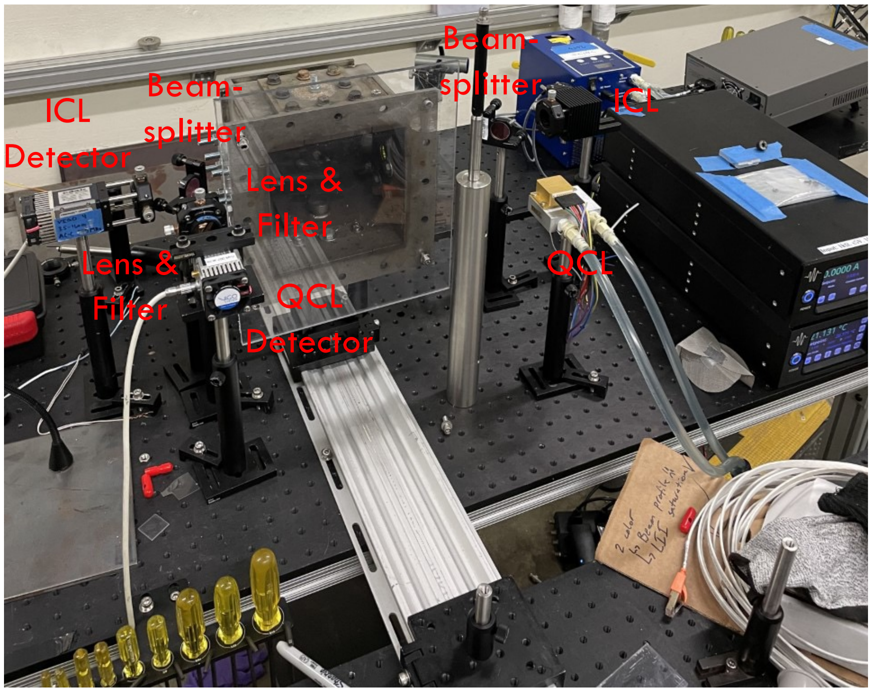
  → Wavelength selection + data processing
- MHz measurements

  →Wavelength selection + modulation through bias-tee
- Extremely Nonuniform LOS

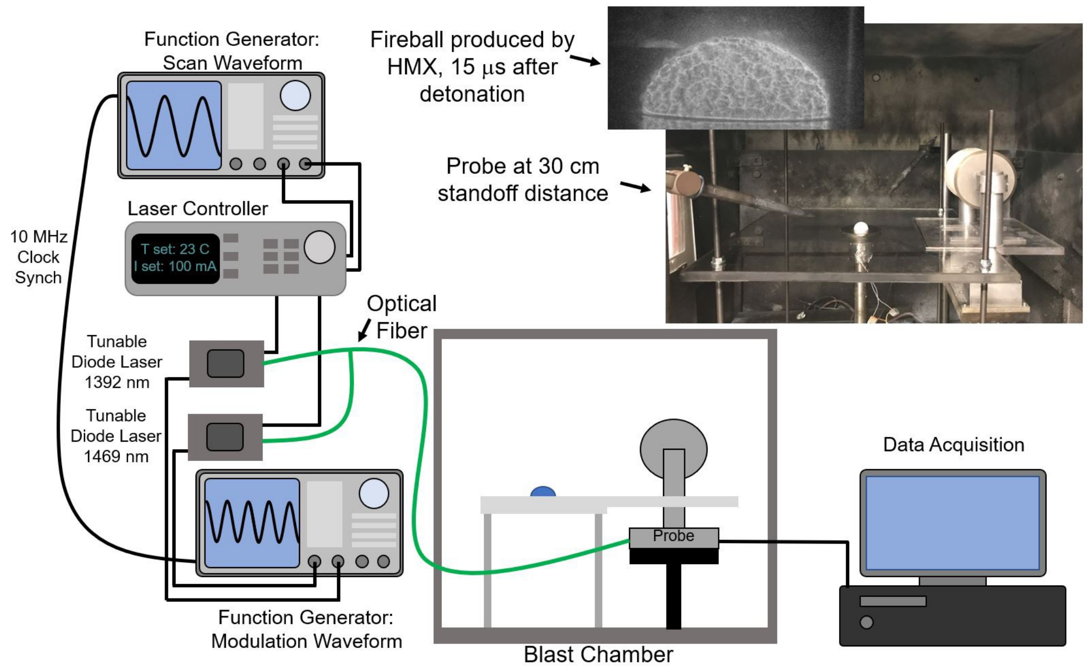
  → Wavelength selection + comparison with synthetic measurements

Future Work

1. Expand to simultaneous CO & CO_2



2. Expand mid-IR diagnostics to larger scale



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Acknowledgements

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  - Dr. Marco Arienti and Andrew Thompson (SNL)

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

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)*

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