Understanding Soot Development and Thermal Stratification in Combustion Engines through Hyperspectral Non-linear Optical Diagnostics

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Outline of Presentation:

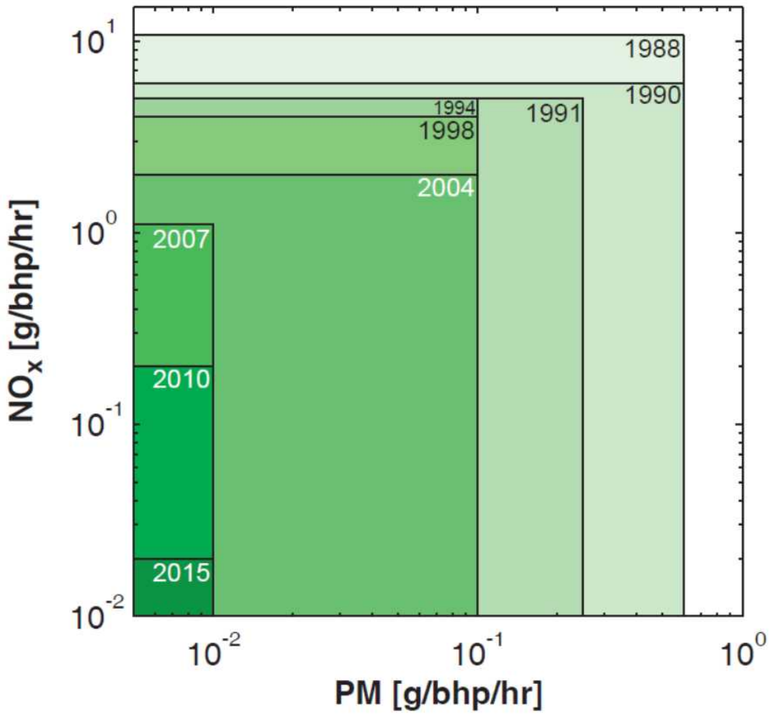
1. Brief (Re)introduction to the Project

2. High Level Progress Report (Milestone Completion) for FY17

3. Discussion of Technical Progress

4. Looking to the Future
   - FY18 Milestones
   - Strategy for Future Funding

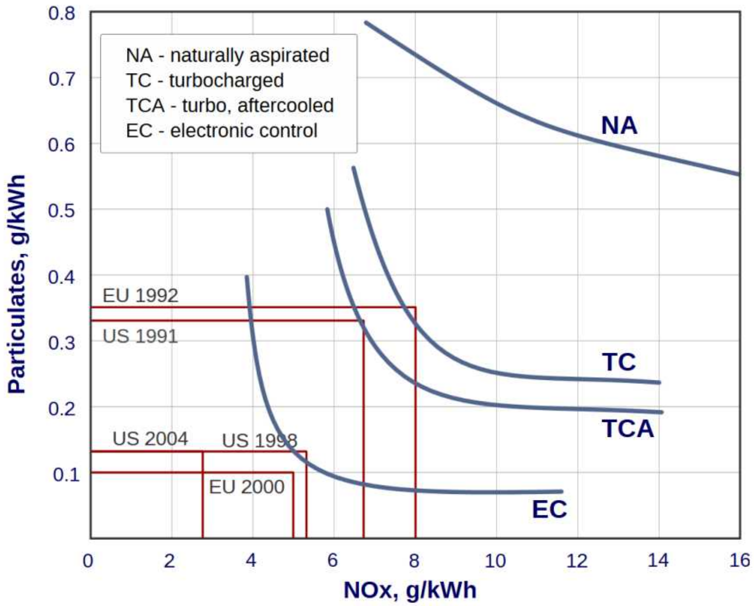
Basic Motivation: DOE Goal for High Efficiency with Low Emissions



- Historical NO_x and particulate emission regulations for heavy-duty on-road diesel engines

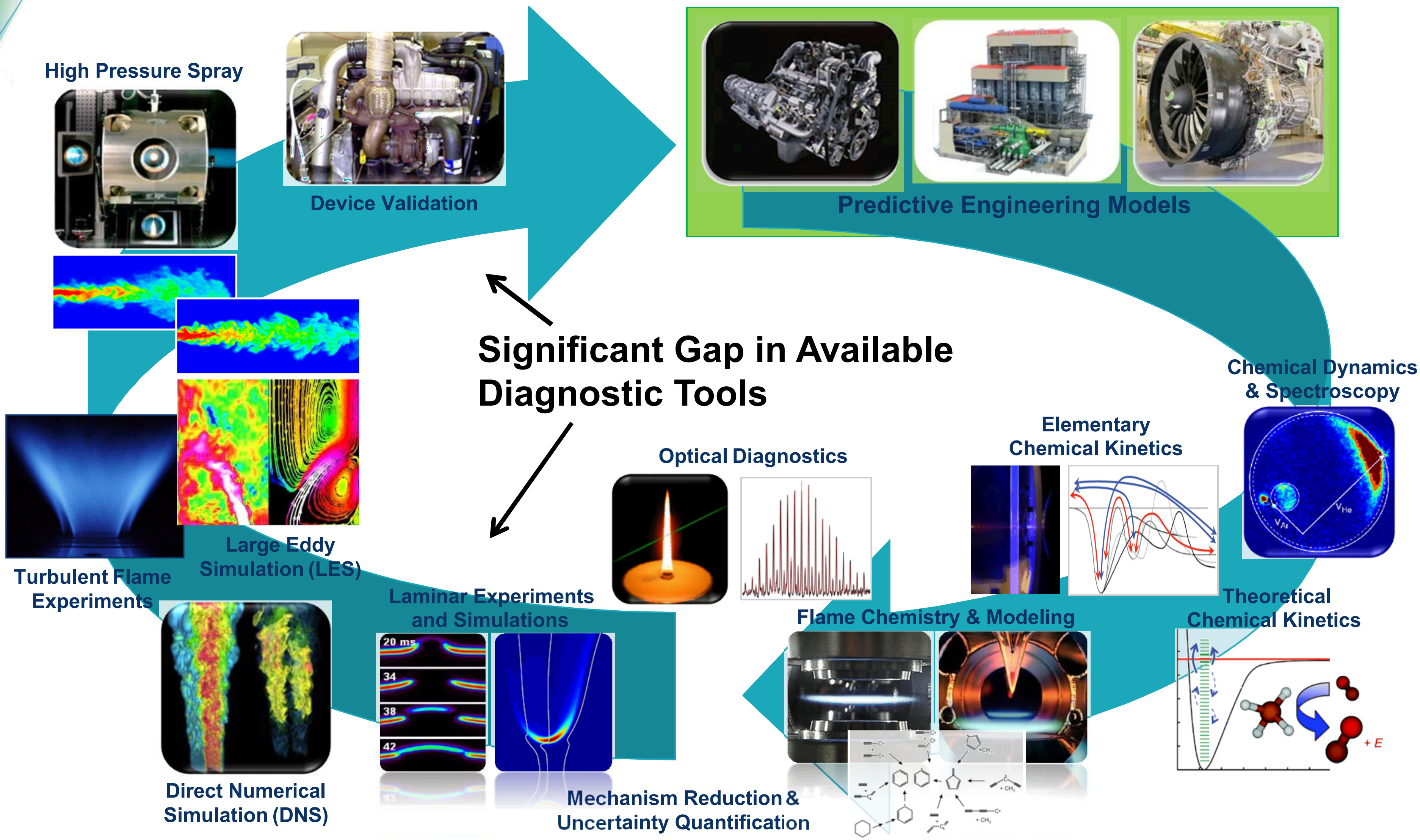
We cannot meet these regulations yet without costly particulate filters.

- Governmental Standards for pollutants, such as NO_x and particulate emissions for IC engines, are rapidly decreasing caused by human health and environmental climate change concerns.



- Major technological changes are needed

Basic Science Foundation for Predictive Combustion Models: The CRF Mission



Next Generation Engines Require New Tools for Model Development and Validation

What are the hurdles that have limited the available *in-operando* optical diagnostics?

- High pressure (complex spectroscopy)
- High turbulence with long path lengths, unsteady combustion
- Significant interference to optical signals (soot, luminosity, fluorescence, nonresonant interference, surface scattering)

✓ **In this project we are developing diagnostic capabilities that conquer these limitations to probe advanced concept engines.**

Next Generation Engines Require New Tools for Model Development and Validation

What are the major questions yet to be answered for next generation engines?

- How does soot form in diesel engines, and how can we avoid it?
  - We need experimental validation for soot formation models *at the relevant conditions for engine operation (high pressure, high temperature, high turbulence)*
- What mechanisms govern thermal stratification in the low emissions low temperature gas combustion (LTGC) engine concept?
  - We need a robust thermal imaging capability to directly probe thermal stratification during real engine conditions

Project Outline:

Experiment (Year 1-3)

- Optical diagnostics development and optimization for high pressure engine combustion application and creation of a mobile cart system
- Application of coherent imaging capabilities to directly measure thermal stratification in the high efficiency low-emission low temperature gasoline combustion (LTGC) engine concept
- Application of optical diagnostic capabilities to study joint temperature / soot volume fraction / major speciation in the LLFC heavy-duty diesel engine concept.

Theory (Year 2-3)

- ODT/LES modeling to provide detailed comparison to the statistics measured experimentally on the thermochemical state associated with soot formation jointly with soot volume fraction

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FY16 Milestones

Develop High Pressure fs/ps CARS Model

✓ Perform 60 bar / 1000K CARS measurements in a high pressure cell 6/1/2016

- Finished Cell Construction, Pressure Safety Testing 1/2016
- Obtained highest pressure CARS data on supercritical N_2 molecules in literature 3/2016

✓ Develop a high pressure fs/ps CARS model and validate against cell data 10/1/2016

- Added high pressure physics to Sandia's time-domain CARS model 2/2016
- Validated N_2 CARS data up to 75 bar 4/2016

Progress towards FY17 Milestones

Diagnostic Development

1. High pressure (> 60 atmosphere) measurements of engine-relevant mixtures of molecules
   11/1/2016 ✓ New spectral model for O_2 has been developed. Iteration expected.
2. Tailor the structure of the picosecond probe pulse, optimized for high pressure experiments
   12/1/2016 ✓ Breadboard device for high efficiency fs -> ps conversion
3. Develop an active femtosecond pulse-shaping strategy to pre-compensate for engine windows
   2/1/2017 ✓ Demonstrated correction of high order dispersion from engine windows.

Measurements in Optical Engines

4. Set up mobile cart for femtosecond/picosecond coherent Raman in Dec's Engine Lab
   3/1/2017 ✓ Designed and built vibrationally damped mobilization cart.
5. Collect thermal stratification data from the homogenous charge compression ignition engine
   7/1/2017 Some equipment setbacks… but still on track to complete these measurements this FY.

Combustion Simulation

6. Simulate lift off length vs spray injection momentum/kinetic energy. 3/1/2017

John Hewson working on methods to speed up calculation time.
Initial results on soot f_v / temperature in atm combustion.

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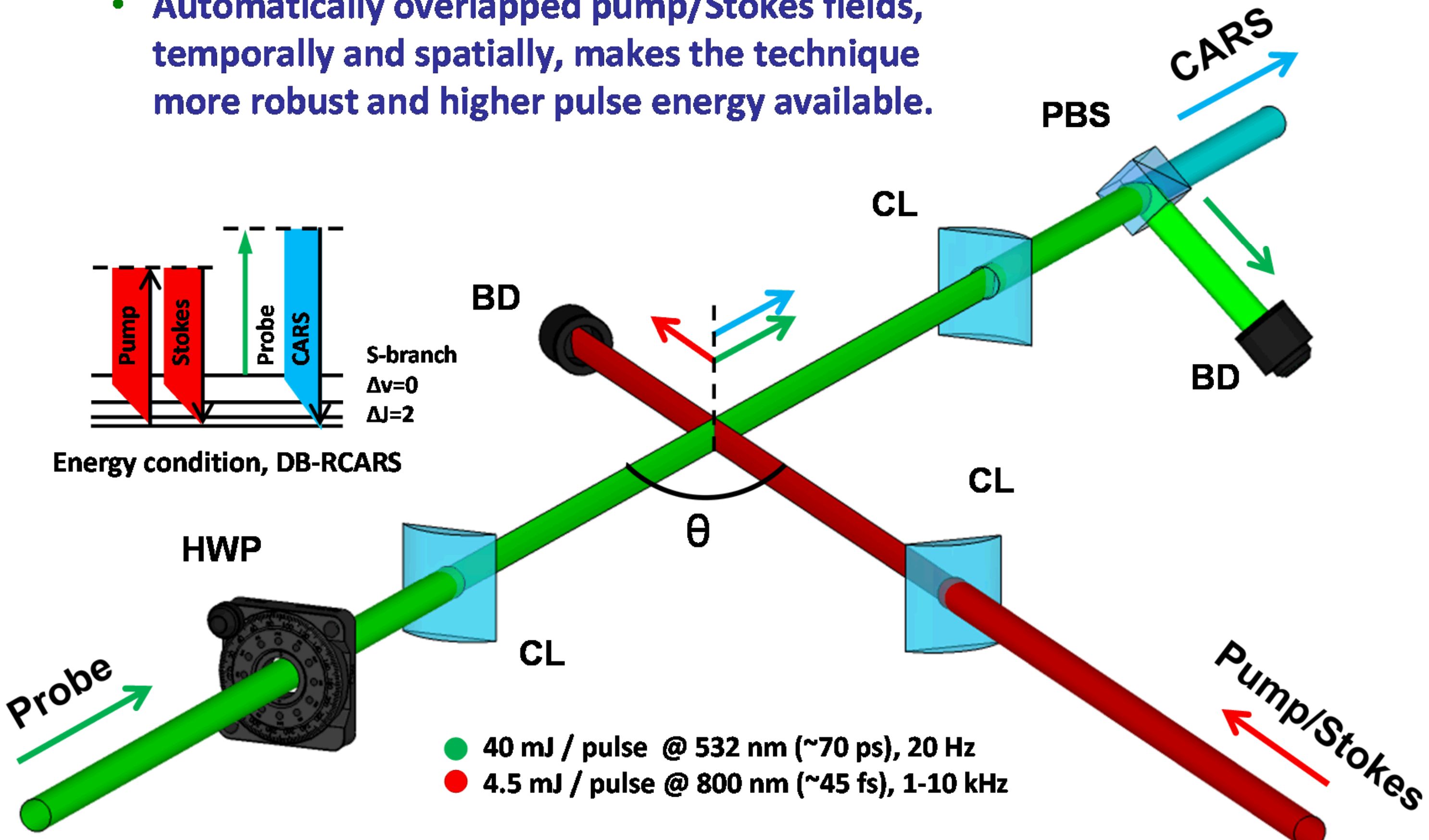
Two-Beam Coherent anti-Stokes Raman Spectroscopy (CARS): Advantages for Engine Research

Better Spatial Resolution, Reduced Sensitivity to Turbulence

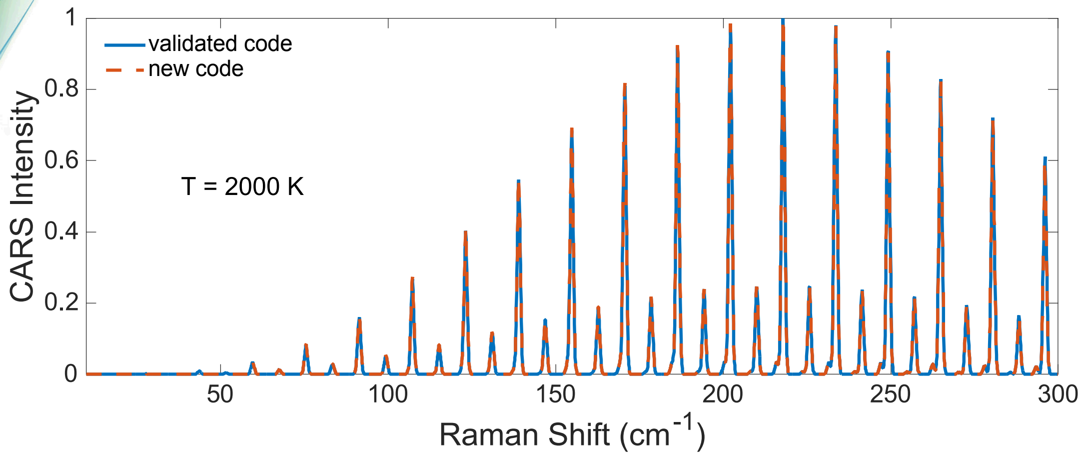
- **Improved spatial resolution (< 50 µm).**
- **Automatically overlapped pump/Stokes fields, temporally and spatially, makes the technique more robust and higher pulse energy available.**



- 40 mJ / pulse @ 532 nm (~70 ps), 20 Hz
- 4.5 mJ / pulse @ 800 nm (~45 fs), 1-10 kHz

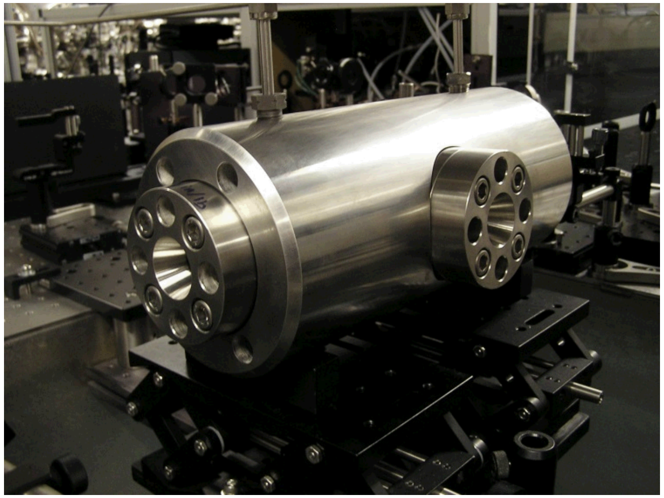
Time synchronized femtosecond (fs) and picosecond (ps) laser system, phase locked to an external 100 MHz RF source

High pressure rotational CARS experiments and simulation



- We have built upon our existing time-domain CARS code, which has been benchmarked at atmospheric pressure, to now include high pressure effects such as pressure broadening, coherent line-mixing and Dicke narrowing.

- Completed constructed of experimental high pressure cell for spectroscopy model validation measurements from 1-150 atm and 300-1000K.



We need $[O_2]$, but there are problems even at 1 atmosphere!

$$\frac{x}{N_2}=\sqrt{\frac{S_{K,x}}{S_{J,N_2}}}\left(\frac{\sigma_{J,N_2}}{\sigma_{K,x}}\right)\left(\frac{\Delta\rho^{(N_2)}_{J,J'}}{\Delta\rho^{(x)}_{K,K'}}\right)\exp\left[\frac{(\Delta t)^2}{16\log 2}\left(\Gamma^2_{J,N_2}-\Gamma^2_{K,x}\right)\right]\exp\left[-\frac{\tau}{2}\left(\Gamma_{J,N_2}-\Gamma_{K,x}\right)\right]$$

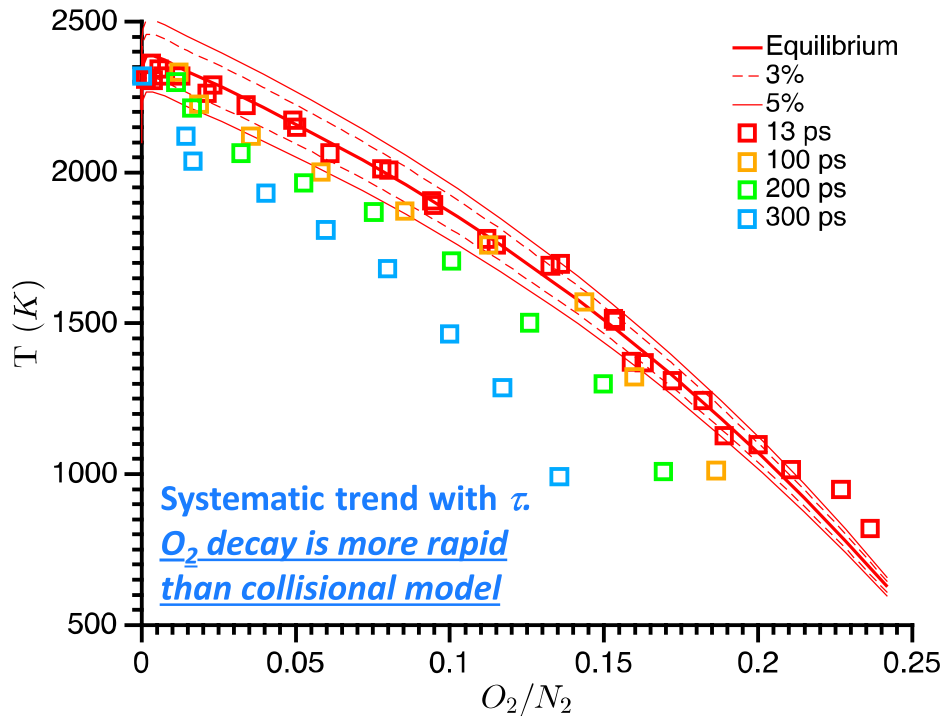
CARS signal for isolated J line

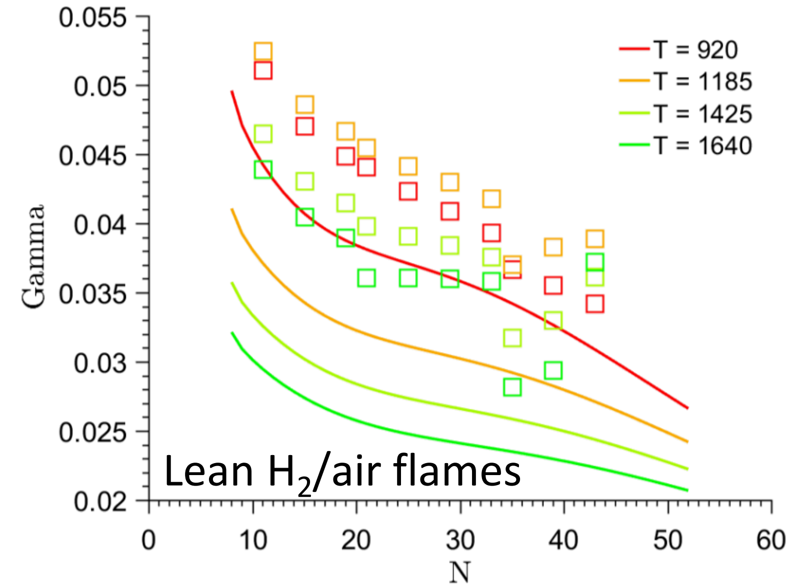
Raman cross sections

Boltzmann populations

Probe pulse duration, Δt

Collisional decay times





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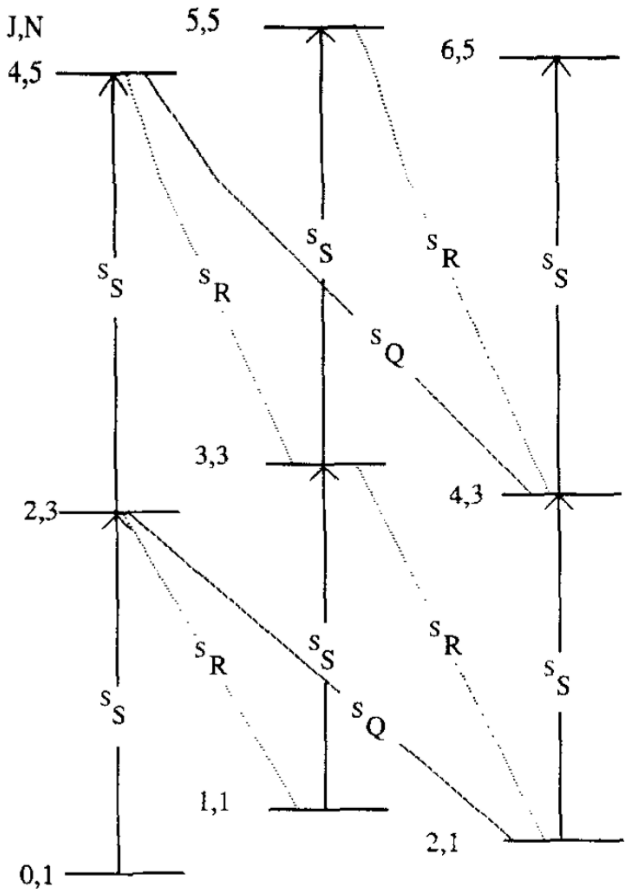
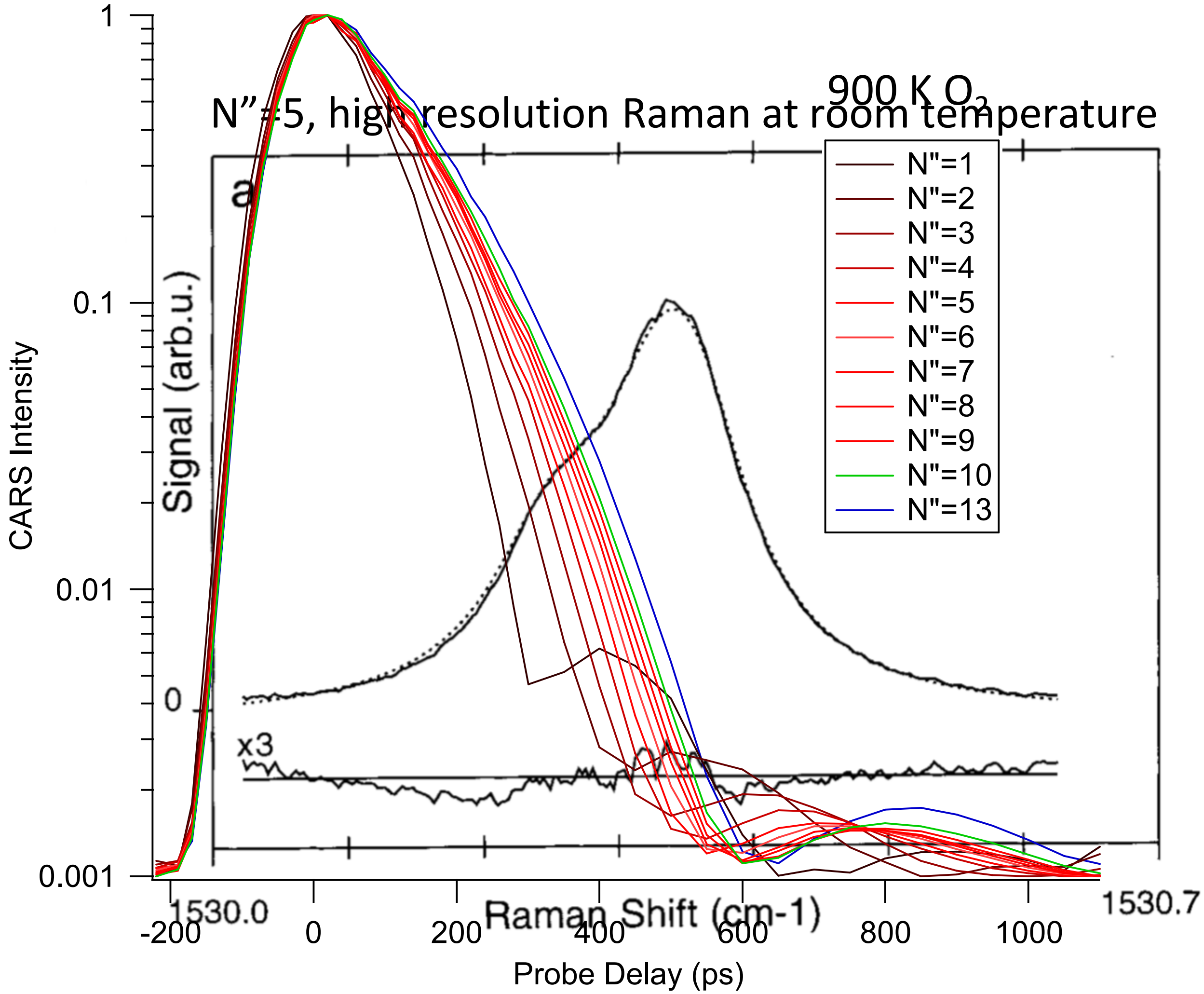


O_2 is treated as a singlet ground state in previous CARS models, but the ground state of O_2 is a triplet.

Nearly perfect Hunds case (b), with a small amount of coupling between nuclear motion and electronic spin angular momentum.

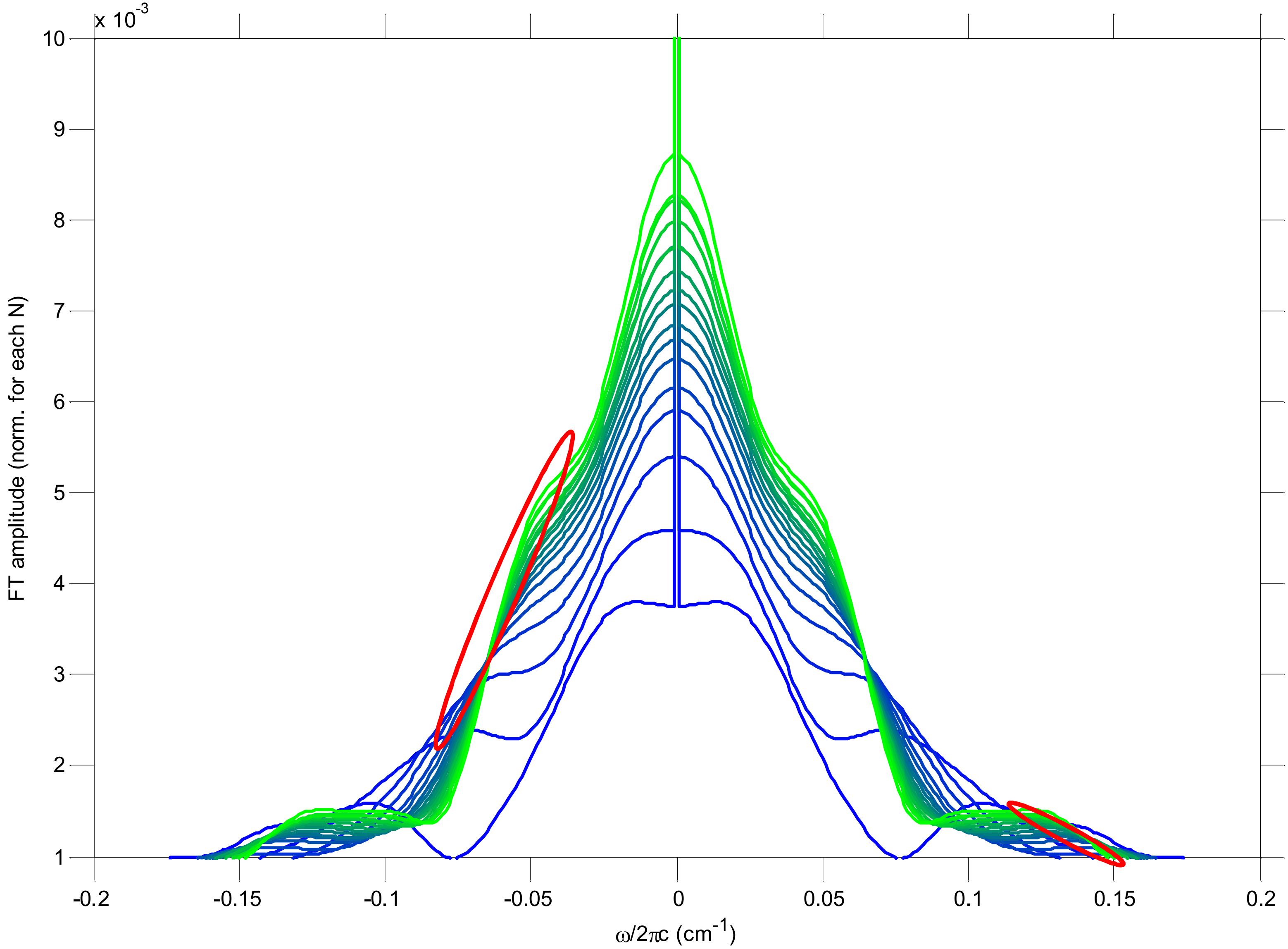
Every Raman-allowed (ΔN=2) transition should result in 3 ΔJ=2 transitions, ~~2 ΔJ=1~~ transitions, and ~~1 ΔJ=0~~ transition.

Time-domain coherence meausrements reveal J-dependent beating of the three electronic spin states

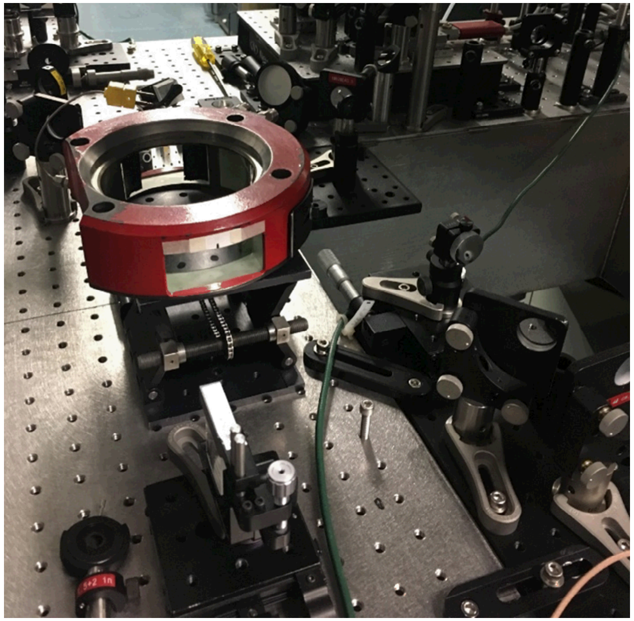


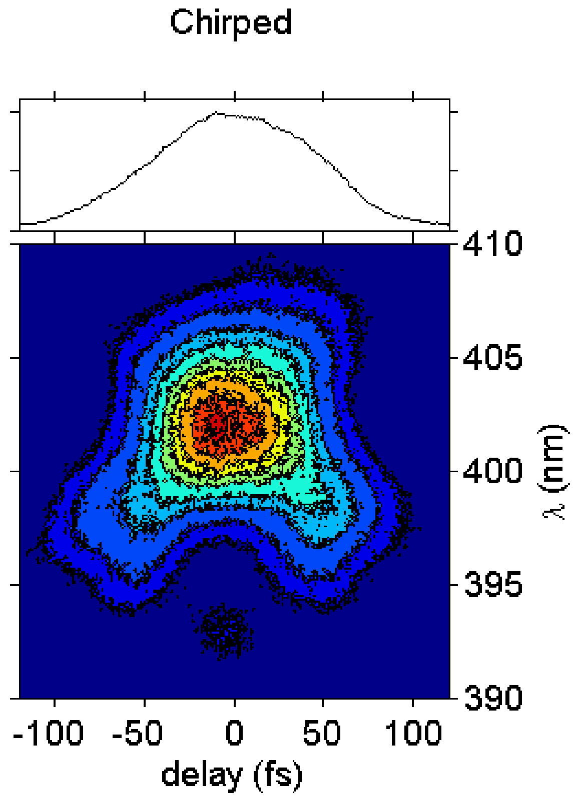
For a normal singlet ground state these decays would be linear.

The discreet Fourier transform yields the N-dependent splittings



Active pulse-shaping was utilized to yield transform limited pulses through optical engine windows





Commercial pulse shaper (FemtoJock). Apply half the correction factor function to the AOM to compensate for the fact that the pulse is measured after two windows.

Mobile cart created for femtosecond laser system transport between engine labs

Rolling cart constructed from 80/20 aluminum chassis.

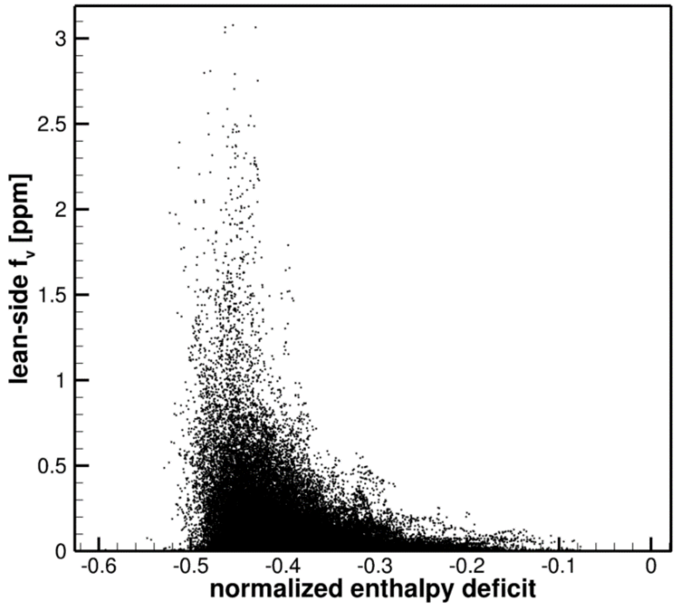
Lifts entire laser table from floor with pneumatic bellows, which dampen vibrations as the laser is moved from one lab to the next.

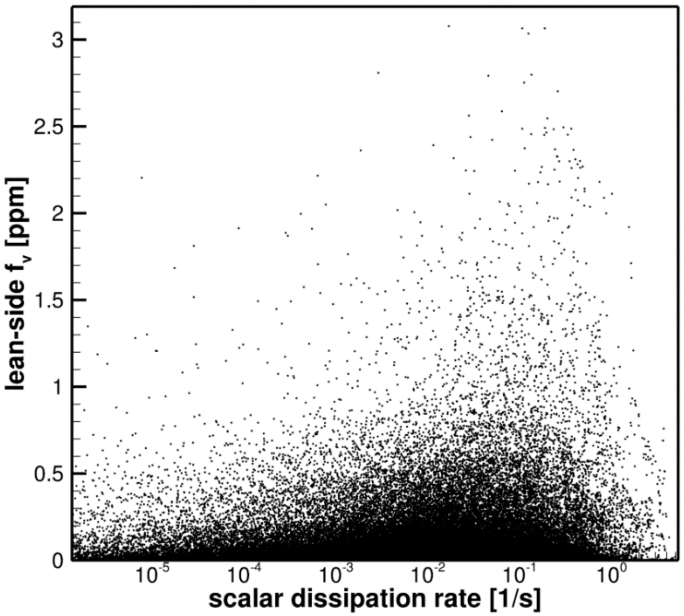
The bellows are deflated and the laser is again supported on high-end vibrationally damped table.

ODT—Lean-side soot emissions

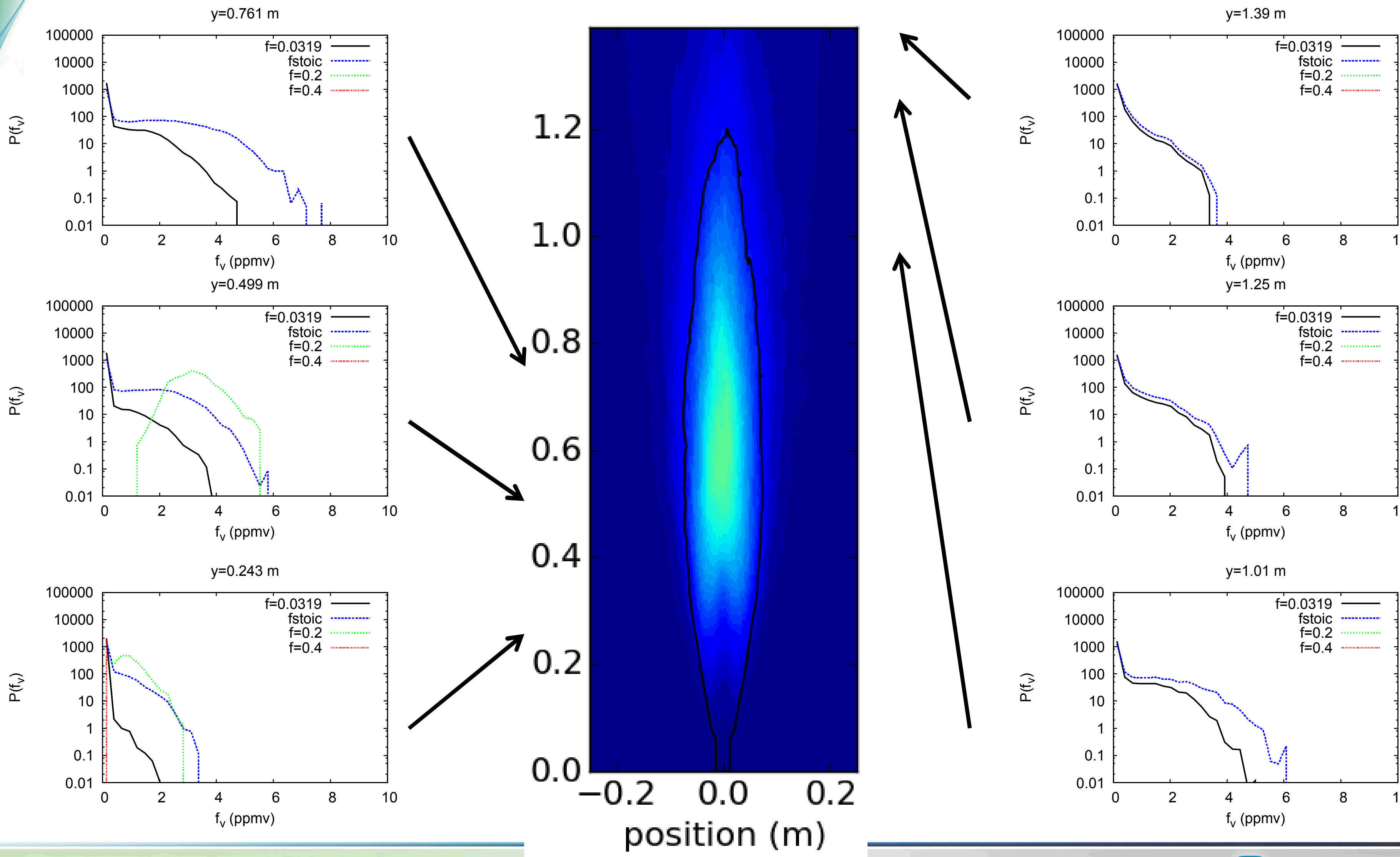
Soot emissions: positive correlation with rapid mixing and enthalpy losses.

- Enthalpy losses reduce kinetic rates
  - can be related to O2/N2 and temperature.
- Fast mixing (large dissipation rates) reduces time available for chemistry.

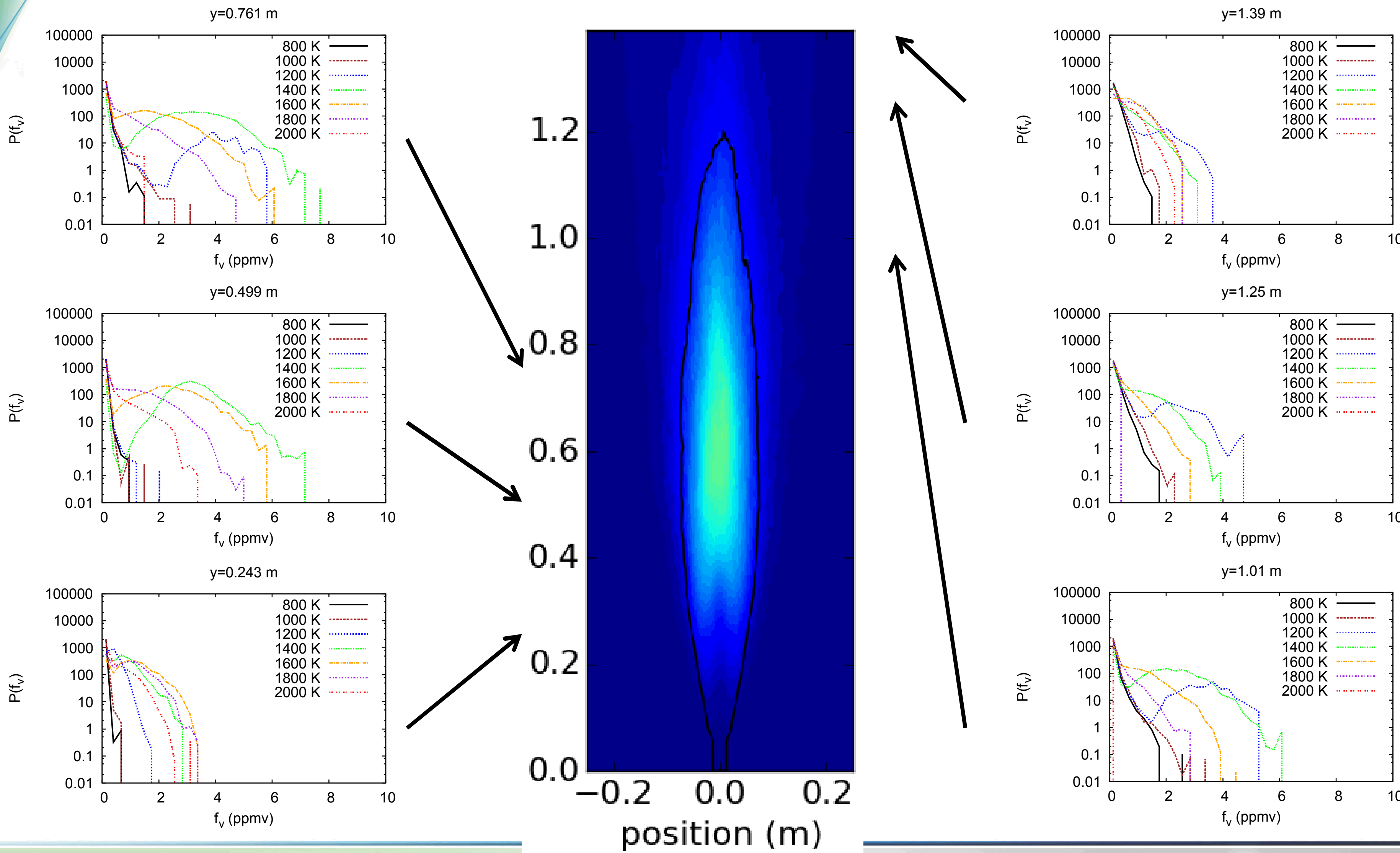




PDF(f_v|Z)—ODT results



PDF(f_v|T)—ODT results



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Fiscal Year 2018 Milestones

Diagnostic Development

1. Verify the effect of combustion products on high P N_2 thermometry 12/1/2017

Measurements in Optical Engines

2. Move mobile fs/ps CARS table to the heavy-duty diesel engine lab 1/1/2018
3. Collect 1D-CARS and PLII joint data from the diesel engine 5/1/2018

Combustion Simulation

4. Simulate lift off length vs spray injection momentum/kinetic energy. 3/1/2017
5. Simulate soot production and burnout as a function of flame lift off 1/1/2018
6. Simulate soot production and burnout as a function of spray and cylinder conditions 6/1/2018

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Possible Future Funding Strategies

Department of Energy, Office of Basic Energy Sciences

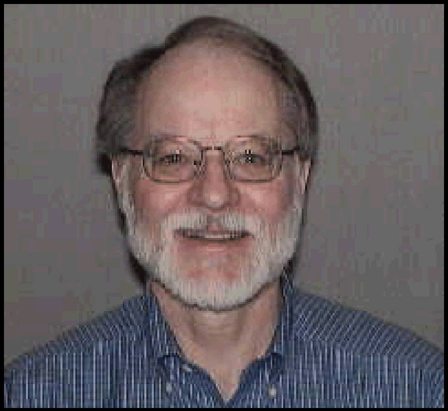
- High level of interest in high pressure molecular physics – collisional processes.
- We have submitted a proposal for fundamental high pressure diagnostics development utilizing the tools developed under this LDRD.

Department of Energy, Office of Vehicle Technologies

- Significant funding portfolio in the CRF for studies of next generation engine operation
- Do *not* fund fundamental diagnostic development work
- Do fund Sandia because of our state-of-the-art techniques and facility
- Requires management assistance to engage program managers

Private Sector Funding

- Discussions between Chuck Mueller and Caterpillar have been very positive, and they are particularly interested in new diagnostic capabilities (the capability to resolve single-engine cycle thermal images, joint temperature/soot imaging)



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