Quantitative Laser Diagnostics for Combustion Chemistry and Propulsion

Lecture 10: TDLAS Applications to Energy Conversion

1. Introduction
2. Fuel in IC engines – fuel and T
   - Absorption cross section vs gasoline blend
3. H_2O and T in slagging coal gasifier
4. H_2O in transfer coal gasifier
5. NO and CO in coal-fired boiler exhaust
6. Future trends – energy conversion

Transport coal gasifier at the National Carbon Capture Center Wilsonville, AL

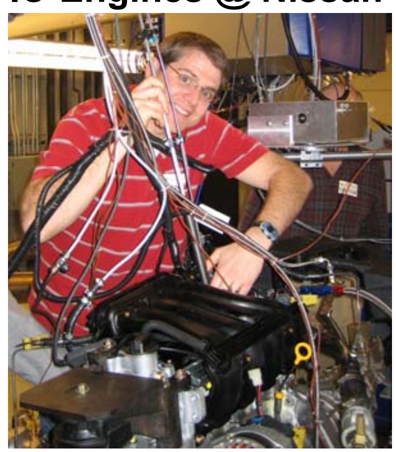
1. Introduction:
TDLAS is Practical in Harsh Environments

- Utilizes economical, robust and portable TDL light sources and fiber optics
- Can yield multiple properties: species, T, P, V, & m in real-time over wide conditions
  - T to 8000K, P to 50 atm, V to 15km/sec, multiphase flows, overcoming strong emission, scattering, vibration, and electrical interference
- Demonstrated in harsh environments and large-scale systems:
  - Aero-engine inlets, scramjets, pulse detonation engines, IC engines, arcjets, gas turbines, shock tunnels, coal-fired combustors, rocket motors, furnaces….
- Potential use in control of practical energy systems

Coal-fired Utility Boiler

Chao, *Proc Comb Inst*, 2011

IC-Engines @ Nissan

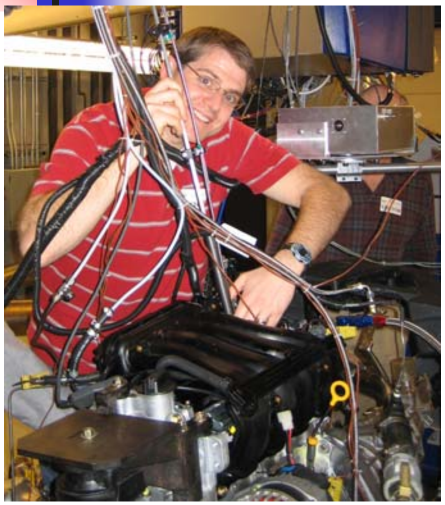


Jeffries, *SAE J. Eng*, 2010

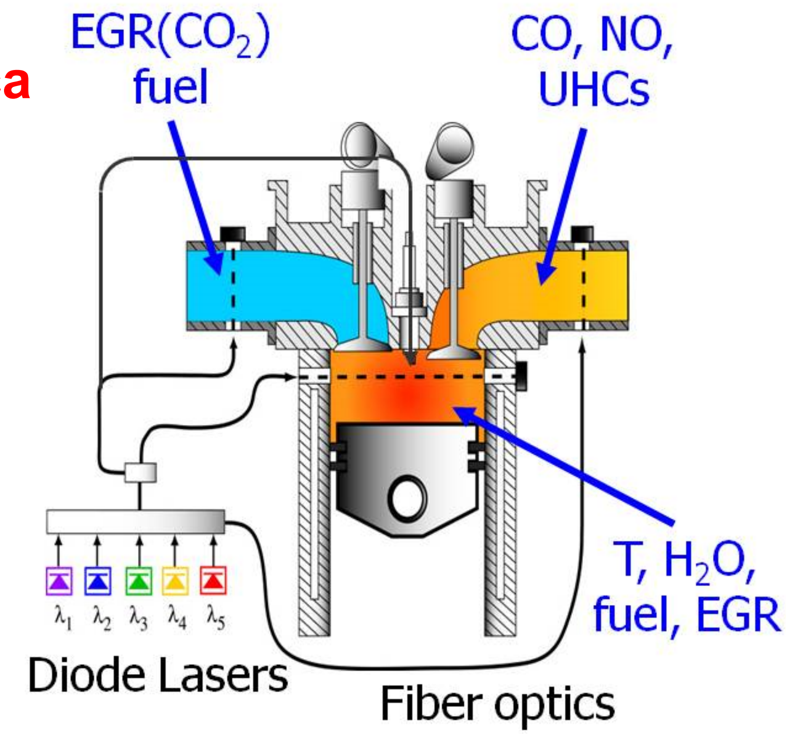
Coal Gasifier @ U of Utah

Jeffries, *Pittsburgh Coal Conf*, 2011

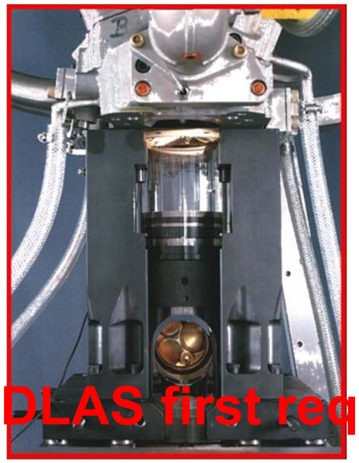
2. Fuel and T Sensing in IC Engines w/ TDLAS



Nissan North America 2007, Fuel & T



Nissan/PSI/SU Sensor @UC Berkeley, 2005 T & H_2O

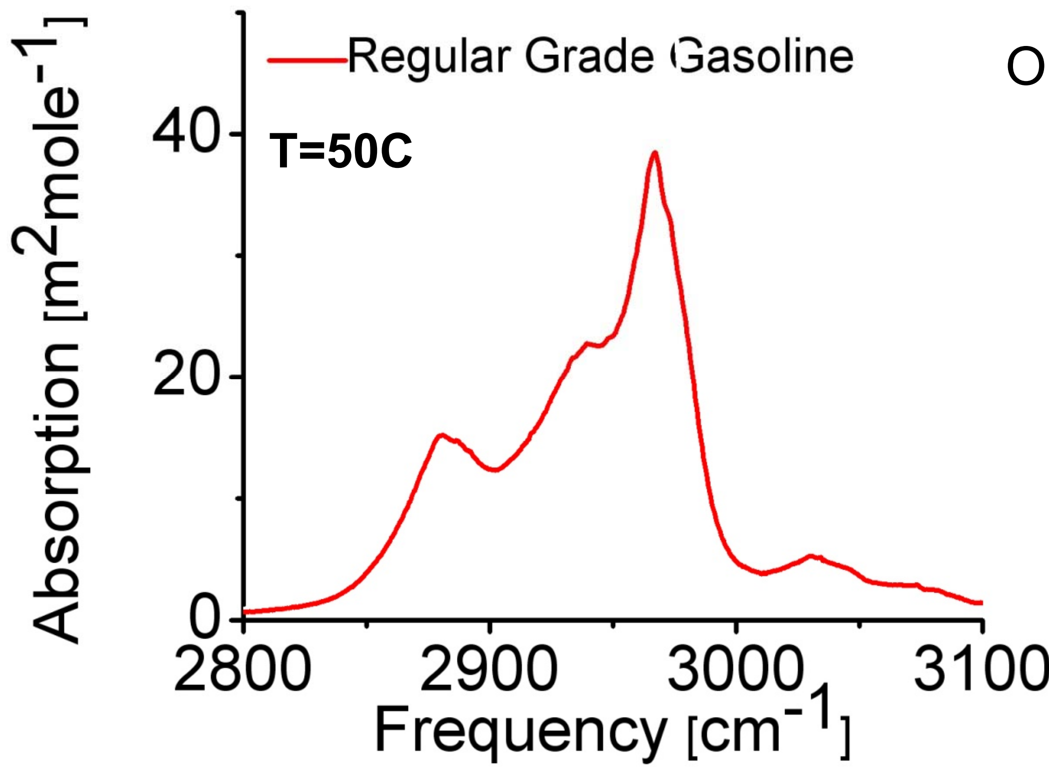


CRF Sandia, 2006 T & H_2O

Quantitative TDLAS first requires cross section data

2. Fuel and T Sensing in IC Engines w/ TDLAS

Gasoline has Unstructured Absorption & Many Blends

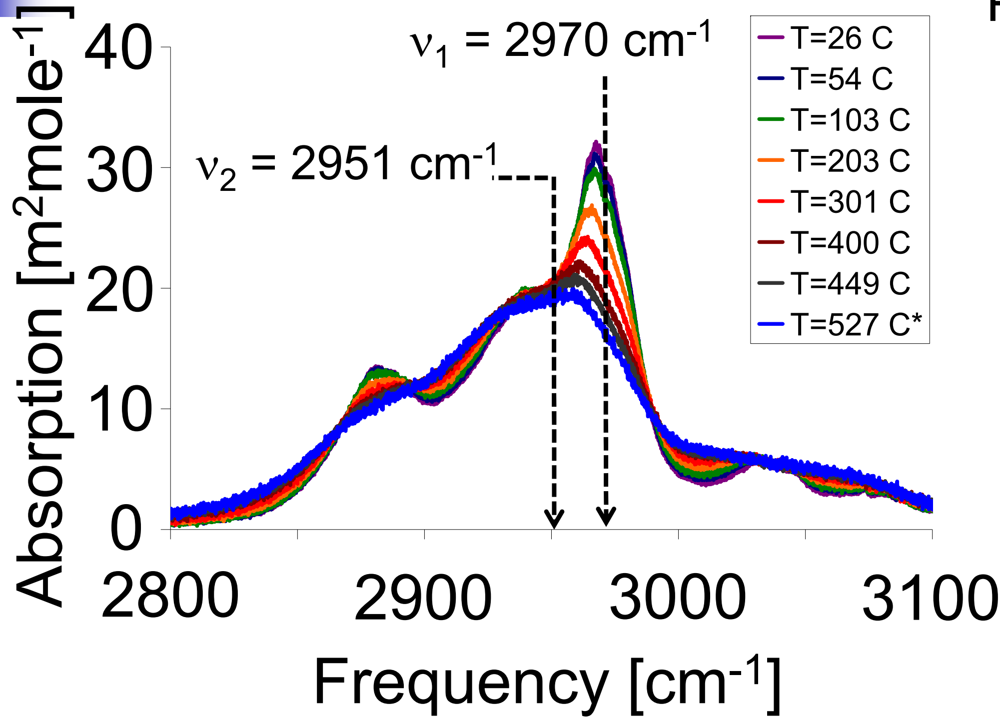


Optical frequency in cm^{-1}
defined: $\nu \equiv 1/\lambda$
where λ is wavelength

- Absorption spectrum measured with FTIR
- Strongest absorption in region of C-H stretching vibration

2. Fuel and T Sensing in IC Engines w/ TDLAS

Gasoline Absorption Varies with Temperature



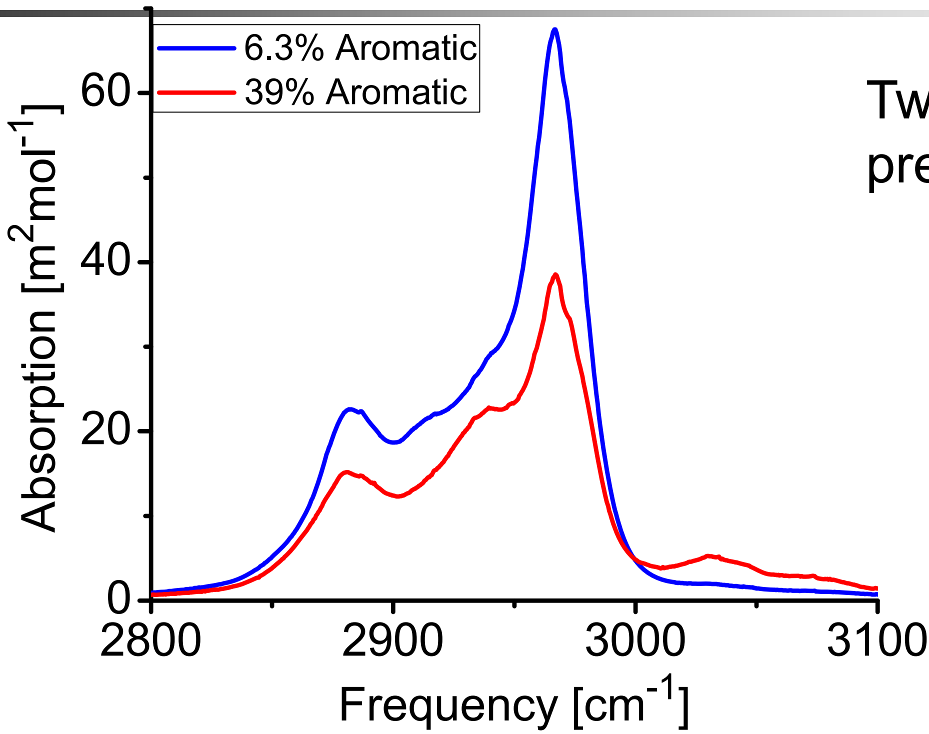
Premium grade gasoline

Optical frequency in cm^{-1}
defined: $\nu \equiv 1/\lambda$
where λ is wavelength

- Absorption cross section versus temperature measured with FTIR
- Strongest absorption in region of C-H stretching vibration
- Pick one laser frequency (ν_1) with large T dependence
- Pick one laser frequency (ν_2) with small T dependence
  - Determine temperature from absorption ratio of selected frequencies

2. Fuel and T Sensing in IC Engines w/ TDLAS

Gasoline Absorption Varies with Blend



Two different blends of premium grade gasoline

- Measured (FTIR) absorption cross section varies with blend

but cross-section model can be assembled with knowledge of gasoline composition

2. Fuel and T Sensing in IC Engines w/ TDLAS

Stanford Model of Gasoline Absorption Cross Section

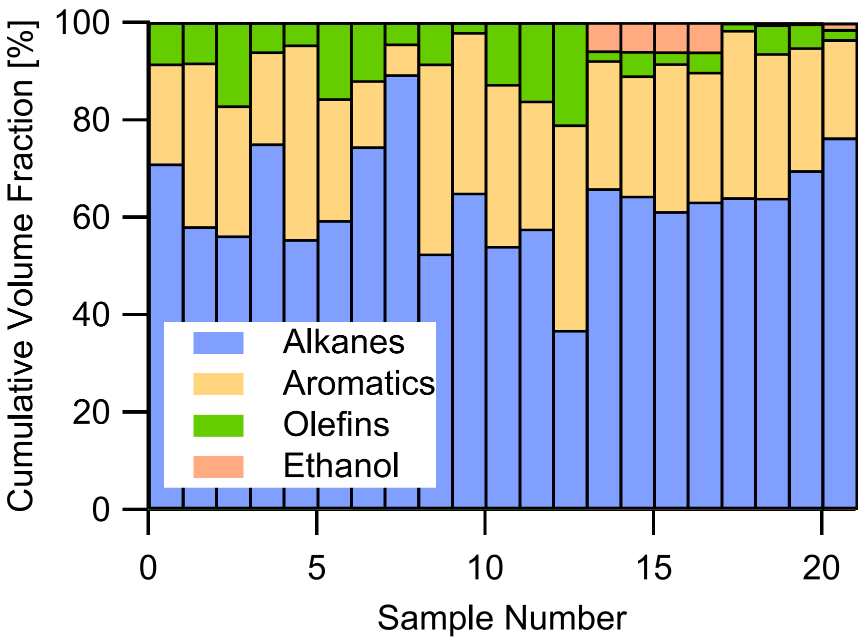
$$\bar{\sigma}_{\text{model}}(\lambda,T)=\sum_{j=1}^{5} X_j \sigma_j(\lambda,T)$$

- Gasoline absorption cross section model:
  - Determine composition of gasoline blend by hydrocarbon class
    - Fractions of paraffin, olefin, aromatics, and oxygenate from standard tests (ASTM D1319 & ASTM D4815)
      - Assume oxygenates are ethanol
      - Normal- and iso-paraffin fraction based on fuel grade
  - Determine absorption cross section $\sigma_j(\lambda,T)$ for hydrocarbon class
    - Empirical database (see Klingbeil et al., Fuel **87**(2008)3600)
  - Weighted sum of σ_j by mole fraction X_j of each hydrocarbon class
- Absolute measurements without calibration using this cross section

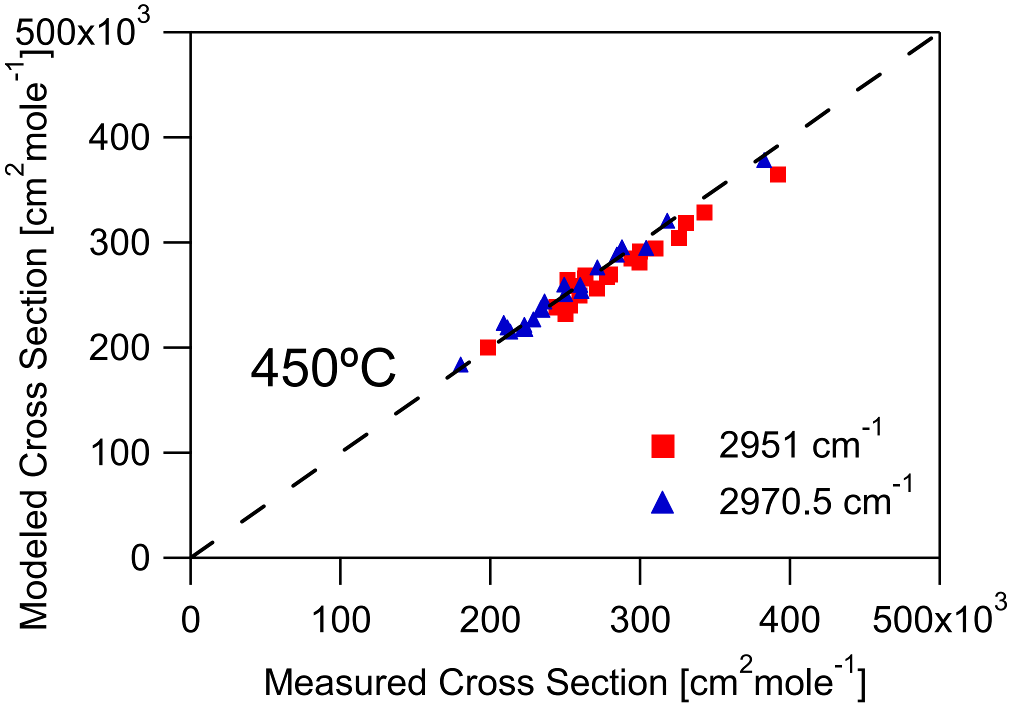
2. Fuel and T Sensing in IC Engines w/ TDLAS

Cross Section Model Validation Experiments

Gasoline Composition



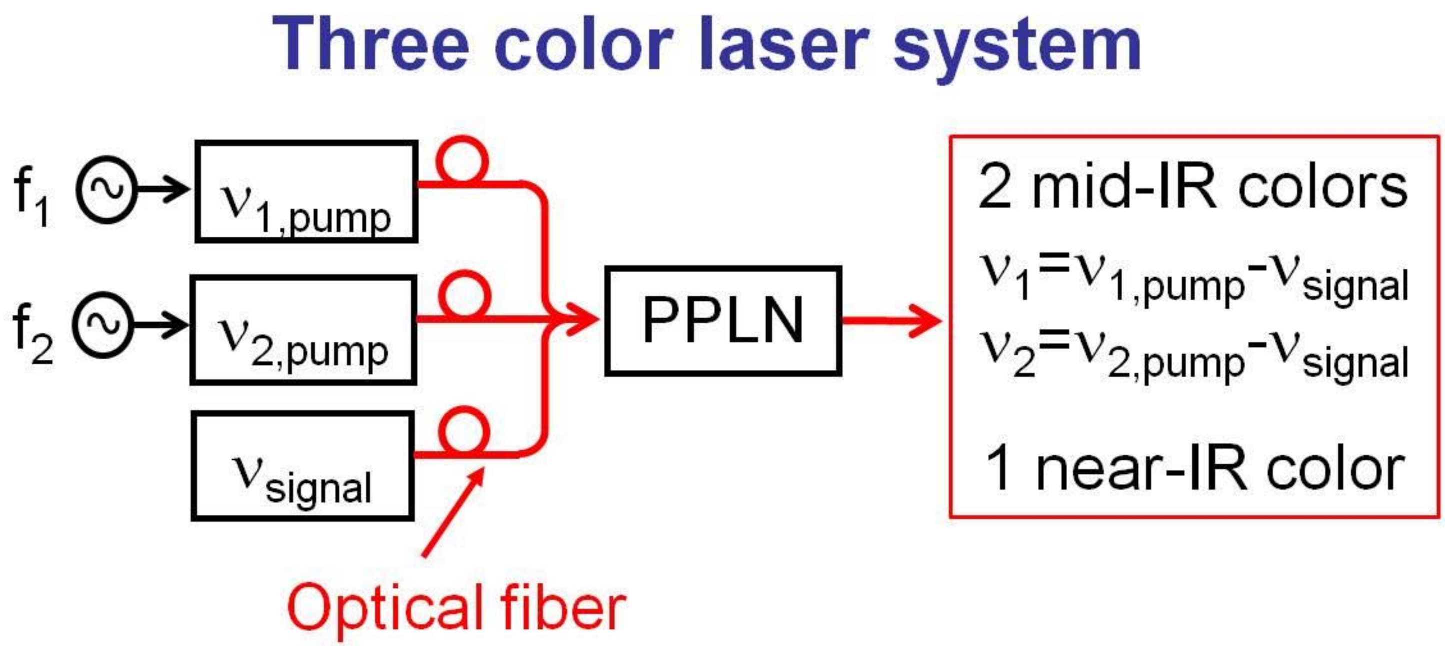
Comparison between model and experiment



- 21 Gasoline samples measured (sample collection augmented by Chevron)
  - Sample pool covers expected range of gasoline compositions
  - Composition variation in cross section larger than x2 at target ν_1 & ν_2
- FTIR measured cross sections in good agreement with model predictions

2. Fuel and T Sensing in IC Engines w/ TDLAS

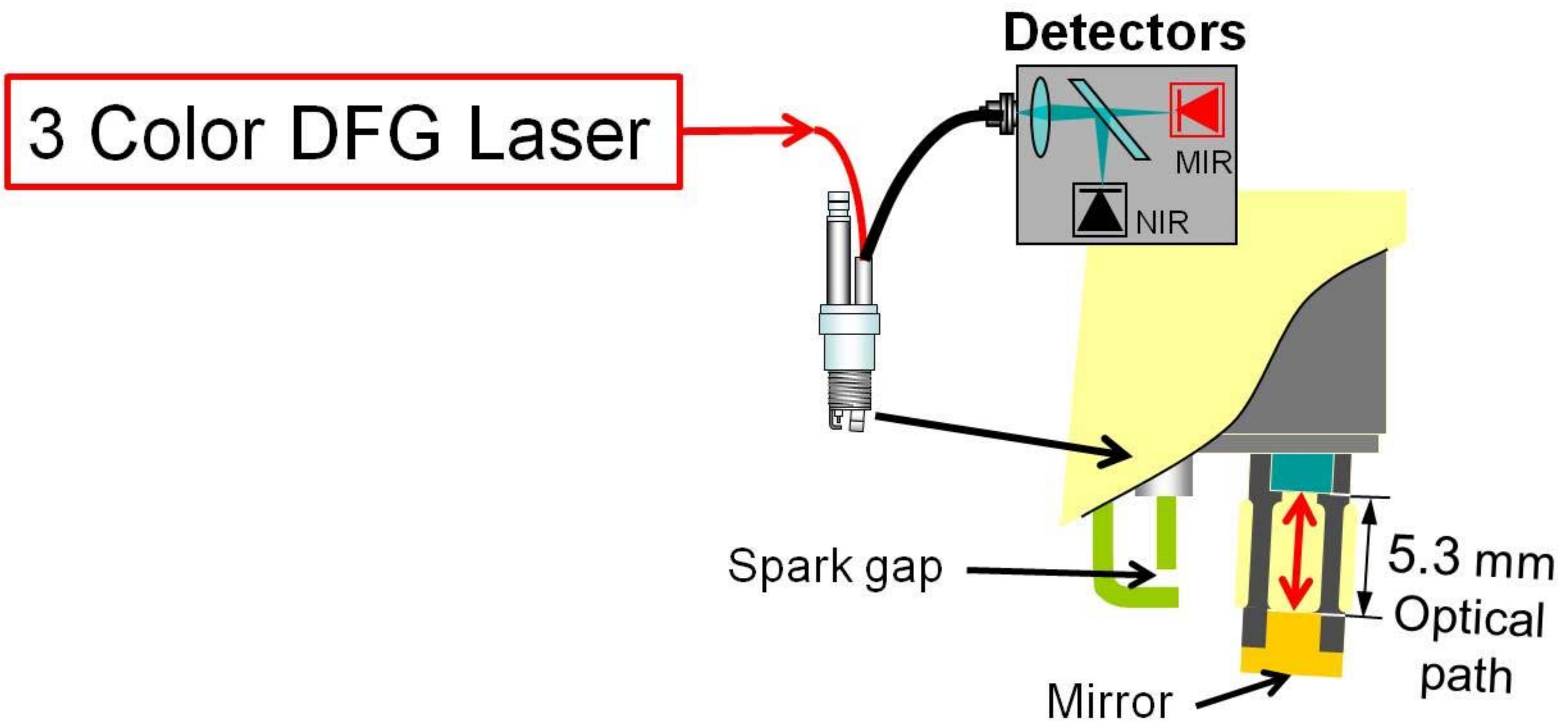
Gasoline Sensor Needs 3-Color Laser



- Difference frequency of two near-IR lasers for mid-IR outputs
  - Third near-IR laser provides two mid-IR outputs
- Two Mid-IR colors for simultaneous fuel and T
- NIR color can be used to exclude effects of fuel droplets

2. Fuel and T Sensing in IC Engines w/ TDLAS
Optical Access Key to In-cylinder Fuel Measurements

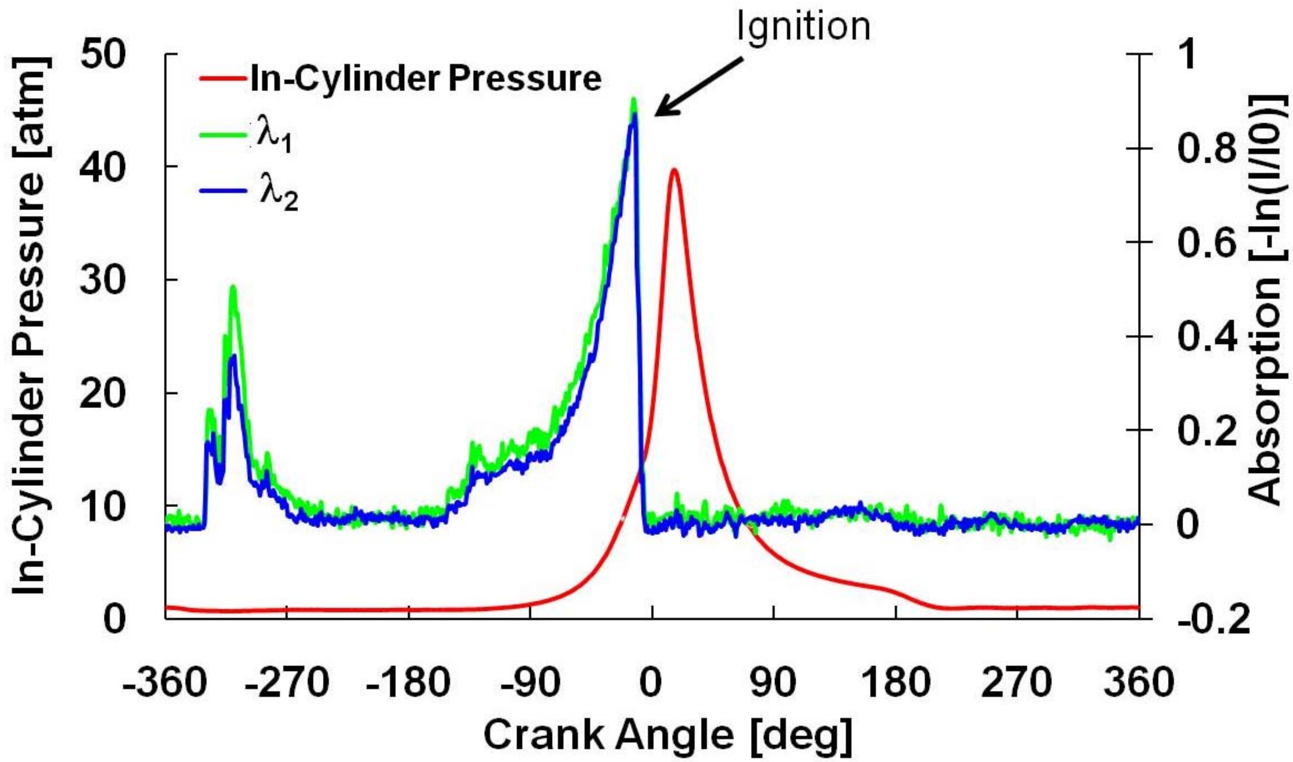
SU, Nissan, PSI collaborative project (2003-2008)



- Measure fuel vs time (CA) close to spark ignition

2. Fuel and T Sensing in IC Engines w/ TDLAS
Crank-Angle-Resolved Gasoline Absorption

- **Single-cycle data from production engine**



Nissan North America (2007)

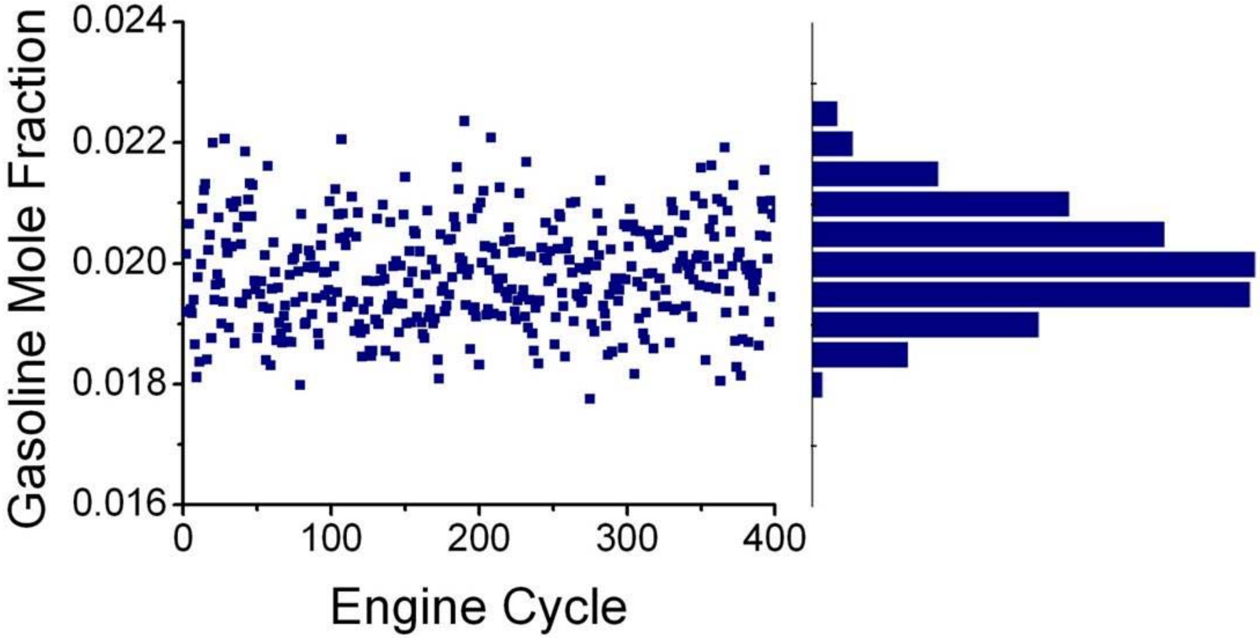
- **High-quality, low-noise data for entire cycle**
- **Sensor provides cycle-by-cycle statistics of F/A ratio**
  - **Critical for understanding/controlling UHC emissions**

Jeffries et al., *SAE International Journal of Engines, 2010*

2. Fuel and T Sensing in IC Engines w/ TDLAS

Cold Start Fluctuations Critical for Emissions Control

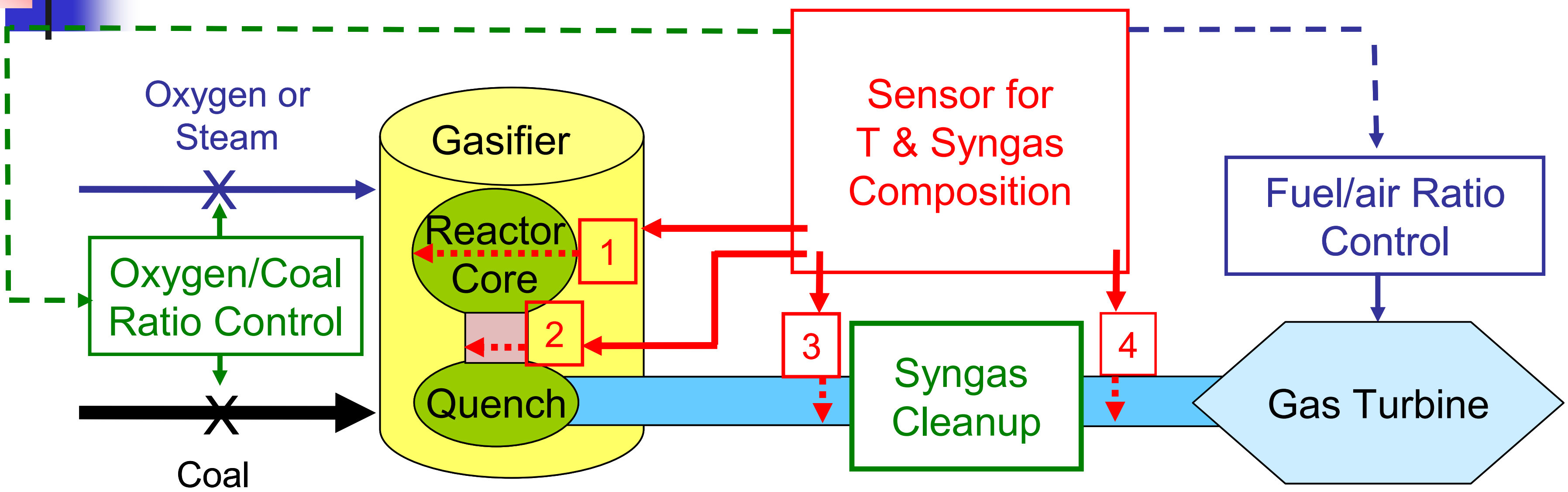
Peak fuel at ignition for 400 cold start cycles



- **High-resolution data quantifies changes in fuel loading**
- **Provides new tool to optimize MPI & DIG engines**

Next: Sensors to optimize coal gasification

3. H_2O & T in Slagging Coal Gasifier @ Utah
Vision for TDLAS Sensing in IGCC

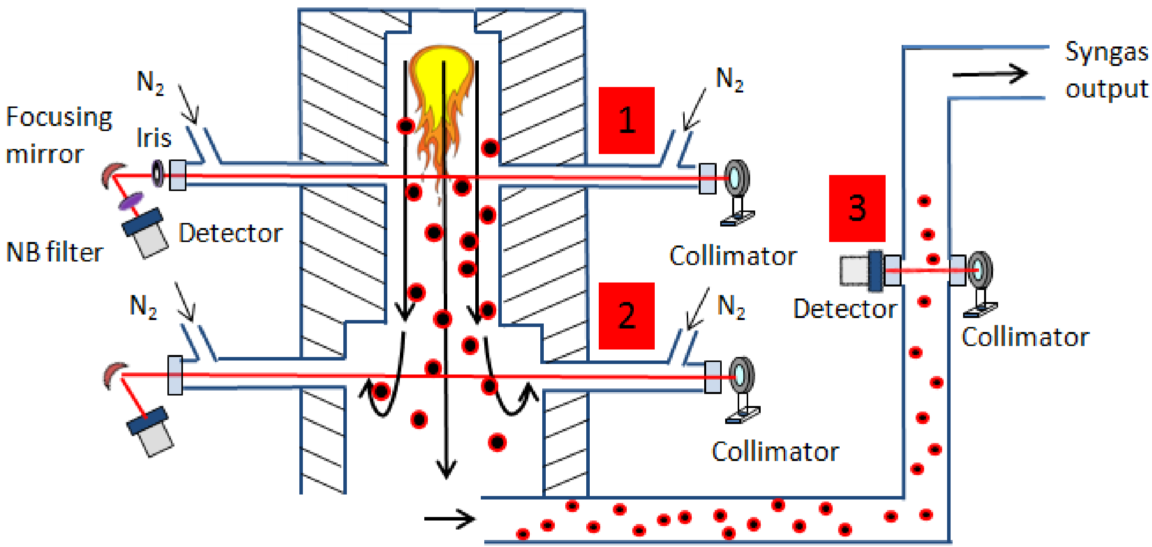


Vision: Sensor for control signals to optimize gasifier output and gas turbine input

- Two flow parameters considered: gas temperature and syngas energy
  - Gas temperature determined by ratio of H_2O measurements
  - For O_2 blown systems CO, CH_4, CO_2, and H_2O provide syngas energy
    - Where H_2 can be determined by gas balance
- Four measurement stations considered: spanning reactor core to products

3. H_2O & T in Slagging Coal Gasifier @ Utah

Entrained flow gasifier @ Utah



Sensor locations
1: Reactor Core
T: 1300K-1700K
2: Quench
T: 600K-1000K
3: Post-quench
T: 330K-400K

Pressure range investigated:
50psig to 200psig

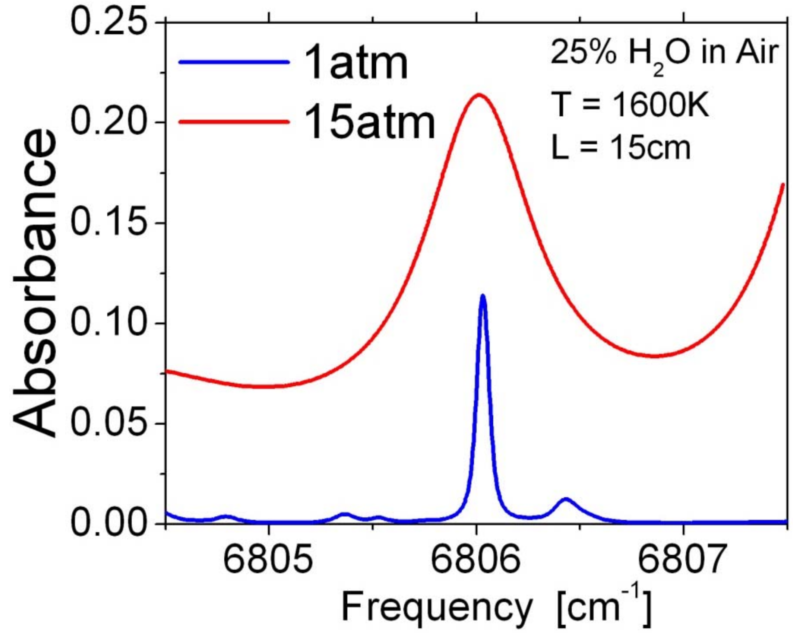
- **Measurement locations 1 and 2 provide opportunity for control**
  - **Temperature sensing by ratio of H_2O absorption lines**
- **Measurement location 3 monitors syngas heating value**
  - **Monitor CO, H_2O, CO_2, CH_4, and assume balance H_2**

Jeffries et al., *Pittsburgh Coal Conf*, 2011

3. H_2O & T in Slagging Coal Gasifier @ Utah

Challenge: Absorption Broadened by Pressure

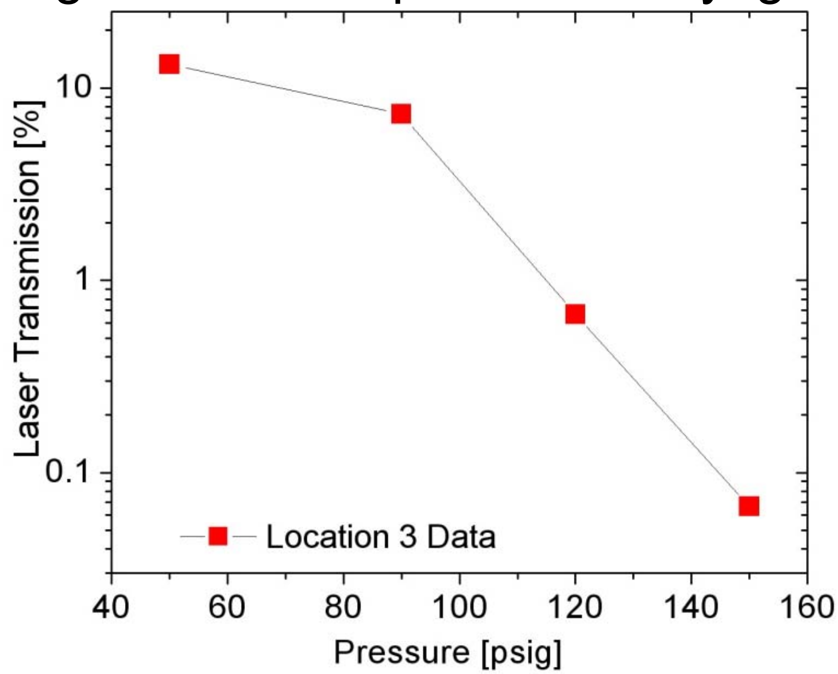
- Practical combustion devices often operate at elevated pressures



- Pressure broadening
  - Blends nearby transitions
  - Eliminates the baseline between transitions
- Particulate in the synthesis gas attenuates laser transmission
- Solution: 1f-normalized WMS: accounts for varying transmission

3. H_2O & T in Slagging Coal Gasifier @ Utah
Transmission loss by particulate scattering

Transmission of laser light at non-absorbing wavelength vs reactor pressure at syngas output

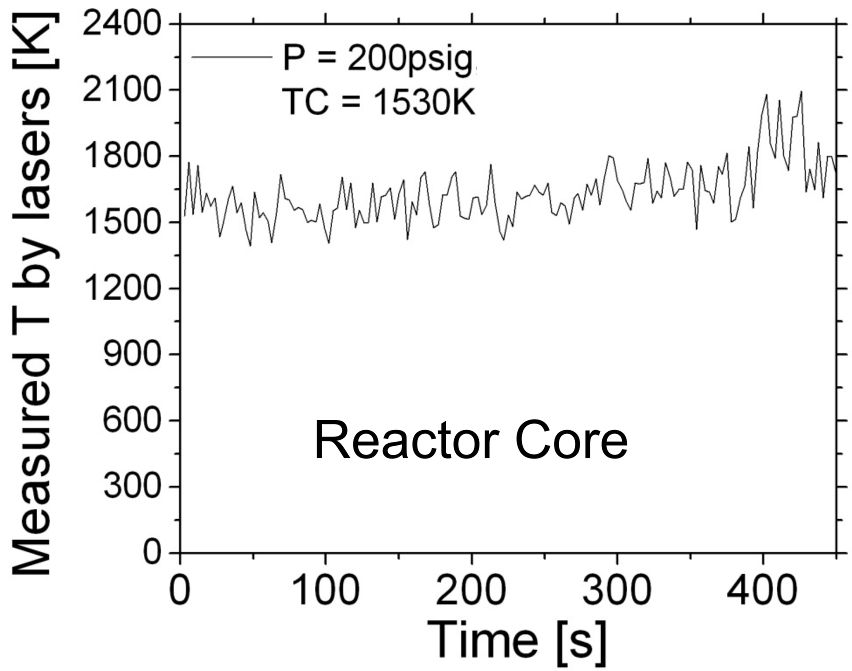


- Reactor loading, throughput, and efficiency increase with pressure
- Particulate loading also increases with pressure
- Scattering losses severely reduce laser transmission

Solution: 1f-normalized wavelength-modulation spectroscopy (WMS *2f/1f*)

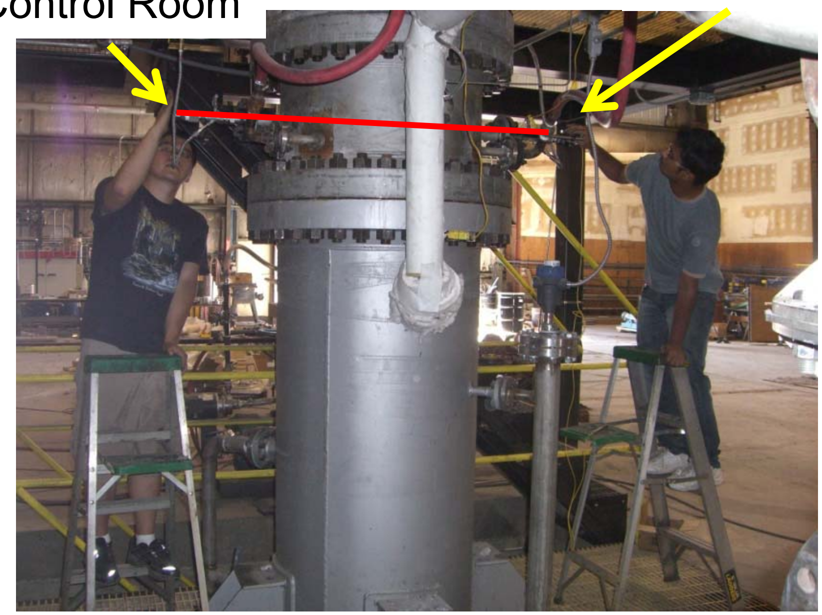
3. H_2O & T in Slagging Coal Gasifier @ Utah
TDLAS Temperature in Reactor Core

Two H_2O transitions: 7426cm^{-1}, E"~1300cm^{-1}, f = 13kHz
7466cm^{-1}, E"~2660cm^{-1}, f = 10kHz



Fiber to Control Room

Detector



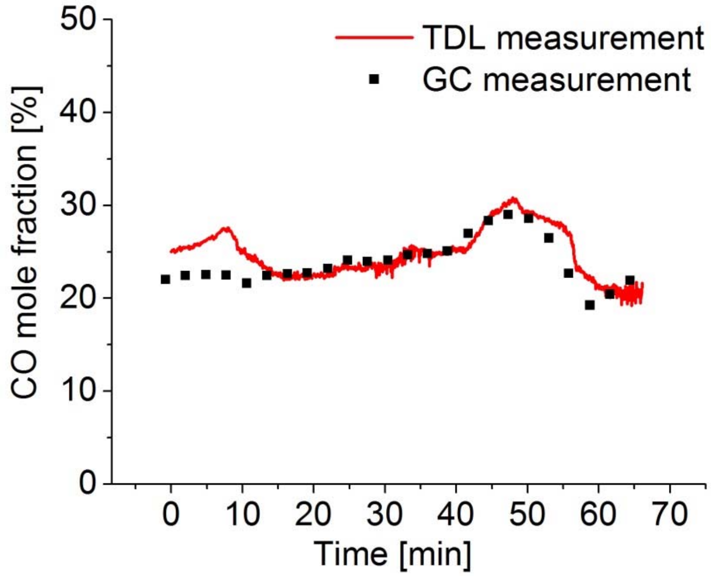
Laser beam alignment @Utah
– no access during experiments

- **Normalization scheme successful with low transmission (< 0.02%)**
- **Fluctuations in T reveal unsteadiness in reactor core**

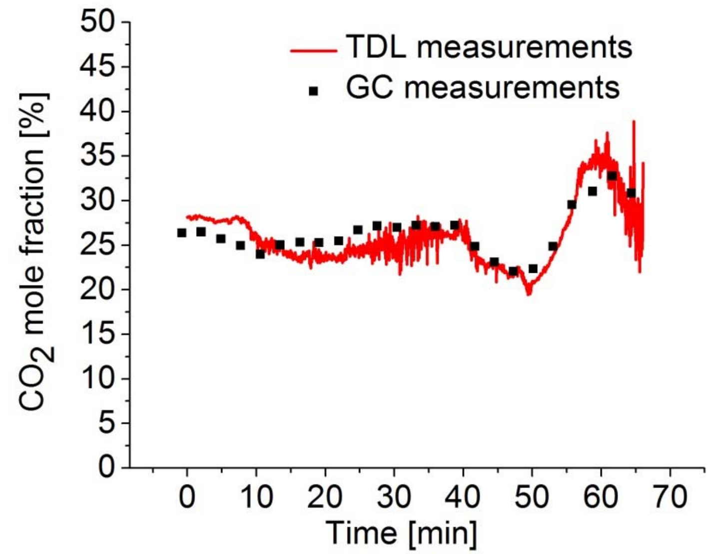
3. H_2O & T in Slagging Coal Gasifier @ Utah

CO and CO_2 vs Time in Syngas Output

CO measurements



CO_2 measurements

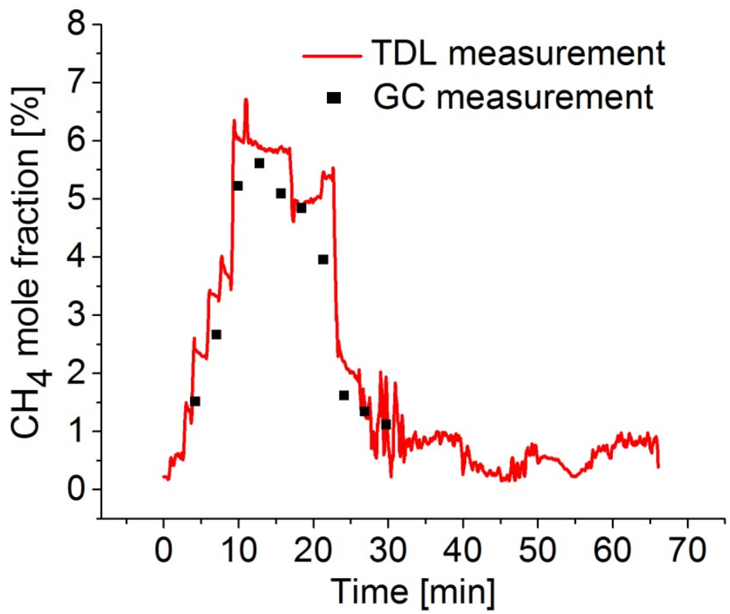


- Monitor composition of syngas output at location 3
  - Simultaneous measurements of CO, CH_4, CO_2, and H_2O
- Coal/O_2 feed rates varied changes CO & CO_2 values during final 30 minutes
- GC data adjusted to account for ~4 min sampling/drying delay
  - TDL data in good agreement with GC

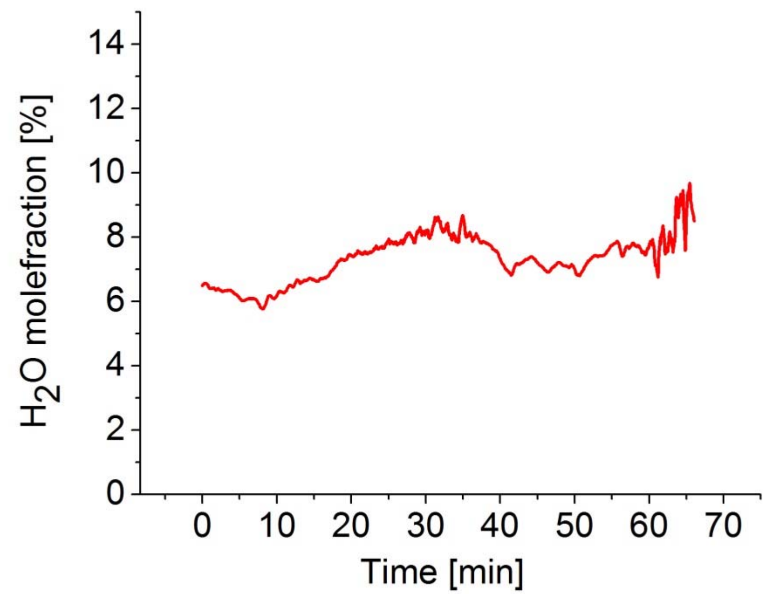
3. H_2O & T in Slagging Coal Gasifier @ Utah

CH_4 and H_2O vs Time in Syngas Output

CH_4 measurements



H_2O measurements



- Monitor composition of syngas output at location 3
  - Simultaneous measurements of CO, CH_4, CO_2, and H_2O
- CH_4 added to syngas to test sensor response during first 30 minutes
- GC data adjusted to account for ~4 min sampling/drying delay
  - TDL data in good agreement with GC

Part 4: Extend to industrial-scale gasifier

4. H_2O in Transfer Coal Gasifier @NCCC
Large-Scale DoE Demonstration Facility

Instrumentation shelter

Note man-sized figure

- NCCC transport gasifier based on a circulating fluidized bed concept

Goal:

Laser absorption *in situ* measurements of moisture and temperature of syngas

4. H_2O in Transfer Coal Gasifier @NCCC

TDL Sensor Located Downstream of PCD

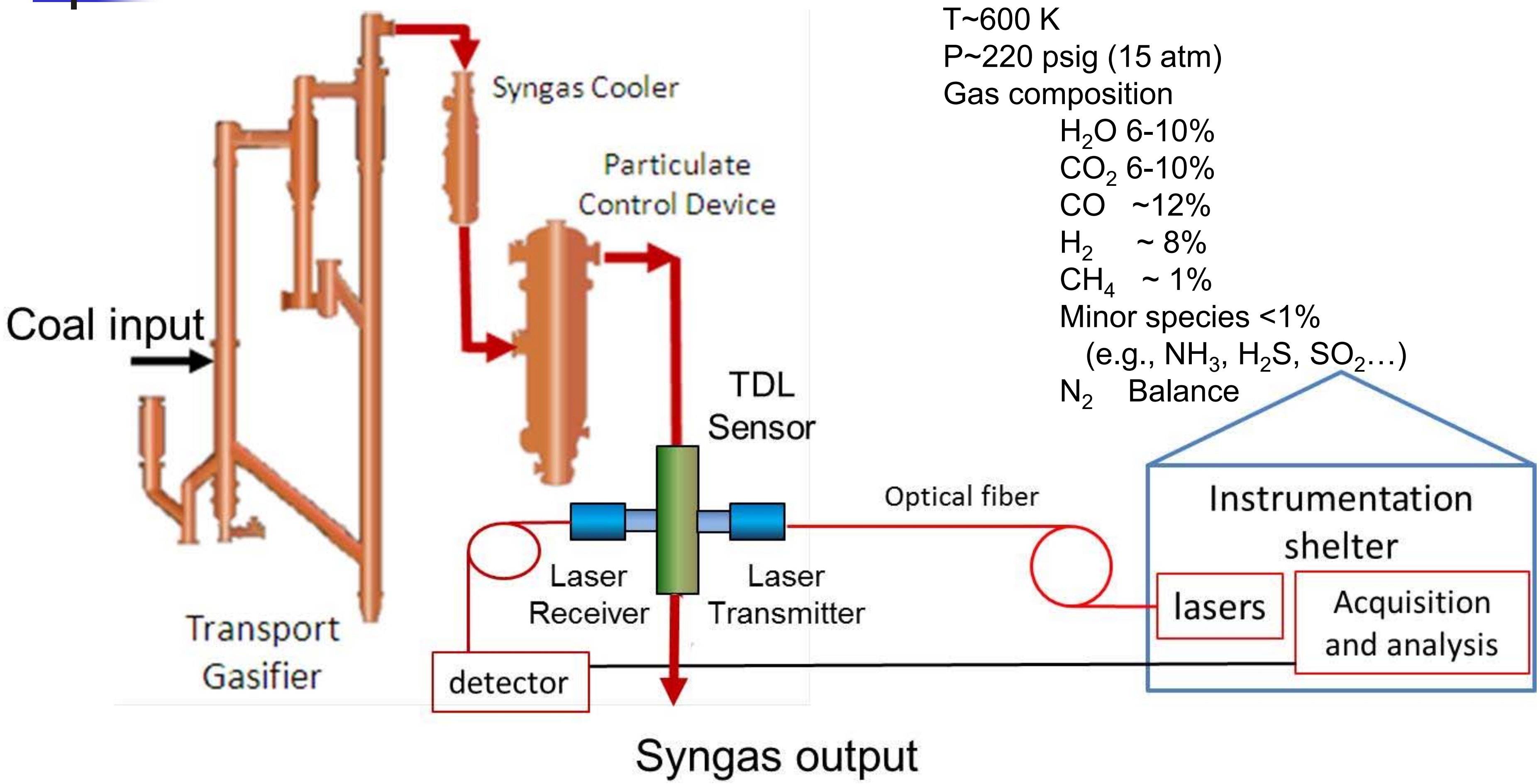
Nominal conditions at TDL sensor

T~600 K

P~220 psig (15 atm)

Gas composition

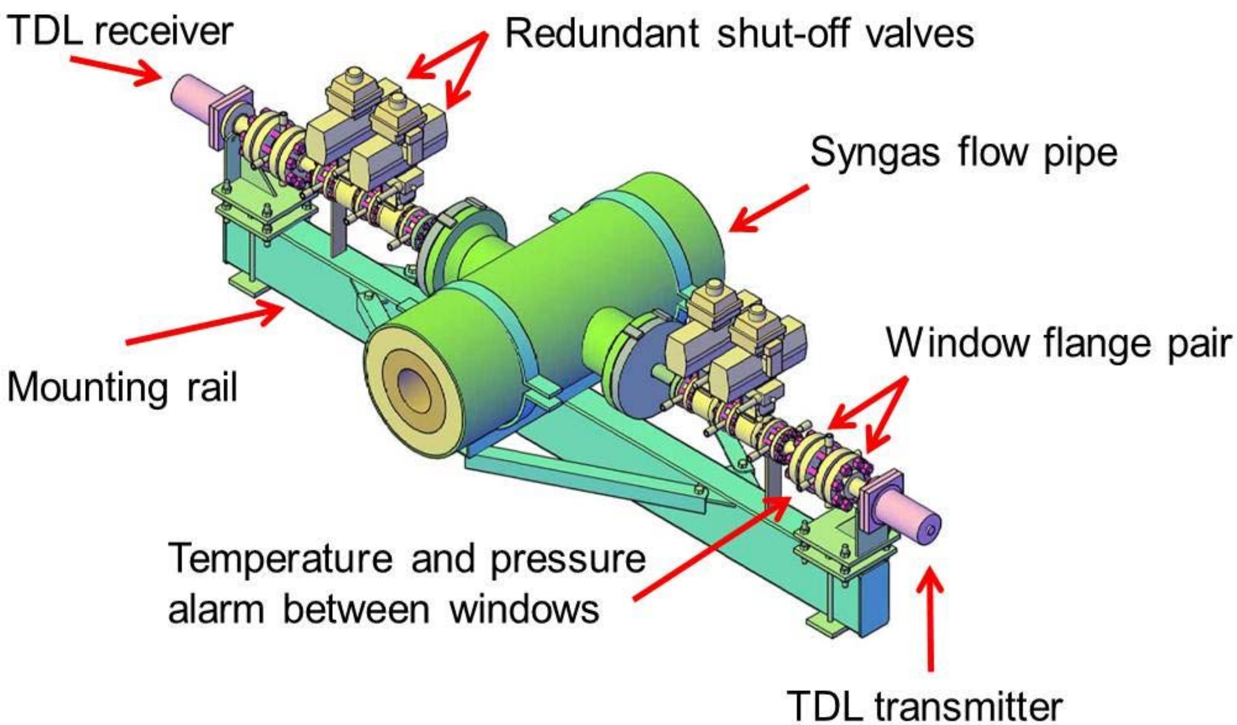
- H_2O 6-10%
- CO_2 6-10%
- CO ~12%
- H_2 ~ 8%
- CH_4 ~ 1%
- Minor species <1% (e.g., NH_3, H_2S, SO_2…)
- N_2 Balance



- TDL sensor monitors syngas flow 99 feet downstream of the PCD
- Small (0.01%) transmission due to beam steering & scattering from ash

4. H_2O in Transfer Coal Gasifier @NCCC

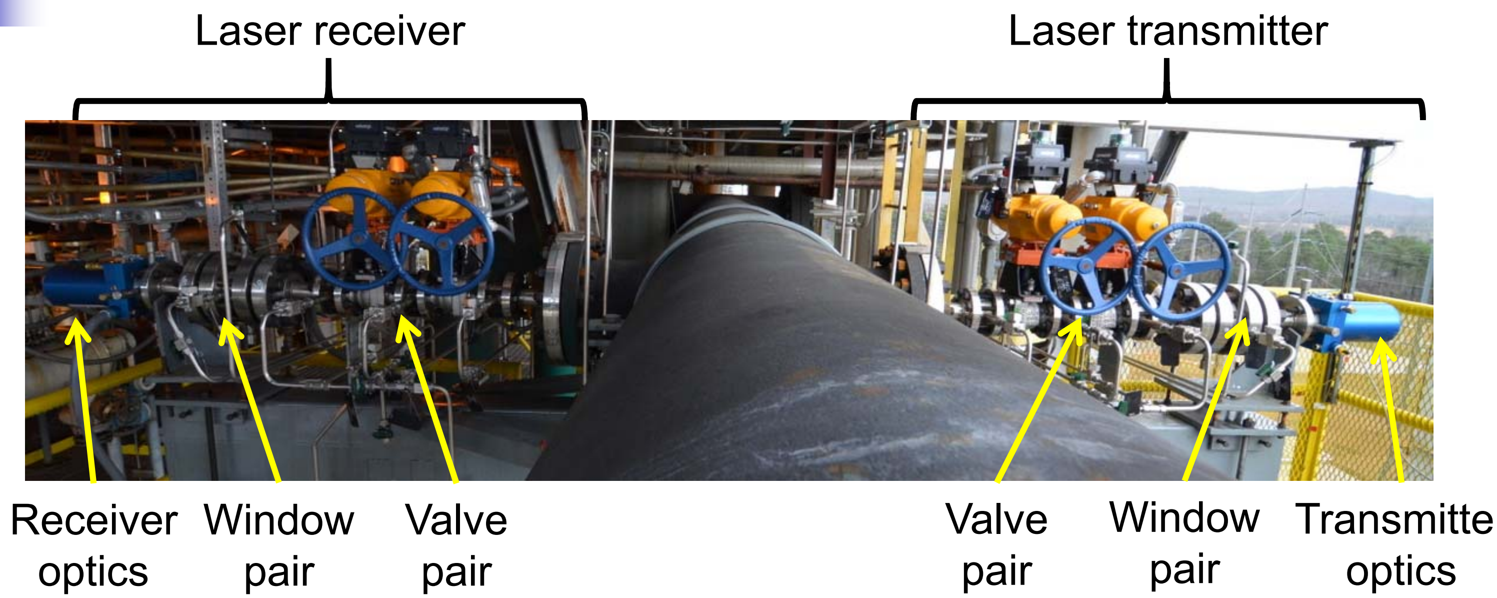
Laser Sensor Installed on Syngas Output Flow



- Safety a paramount element of engineering design
  - Redundant shut-off valves to isolate laser sensor
  - Redundant sapphire windows with P/T failure sensor
- Transmitter and receiver mounted on rail hung from process pipe to minimize thermal motion from process/weather

4. H_2O in Transfer Coal Gasifier @NCCC

Laser Sensor Installed on Syngas Output Flow

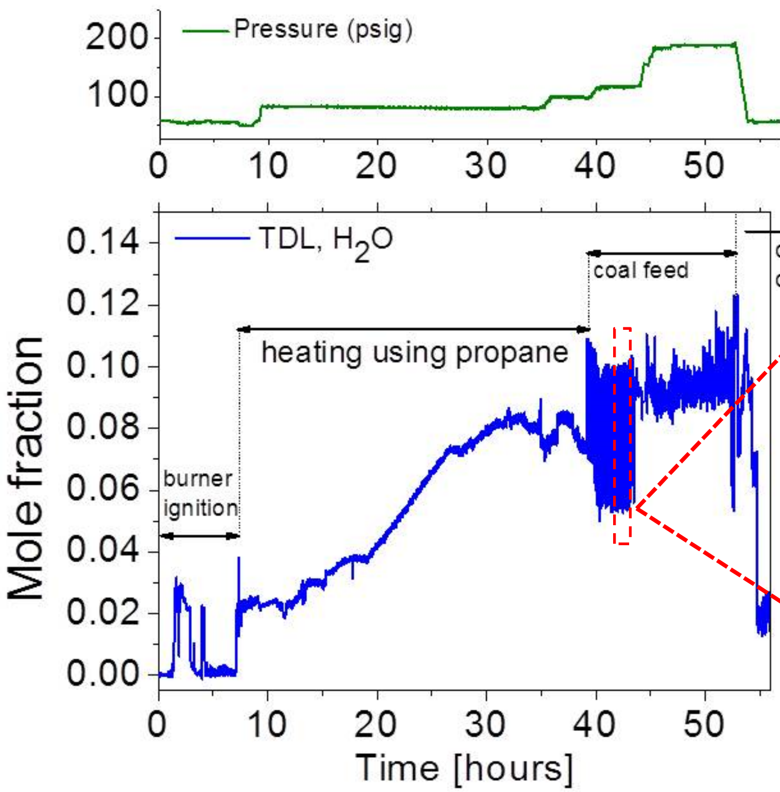


- Photo illustrates the large-scale of this commercial size system

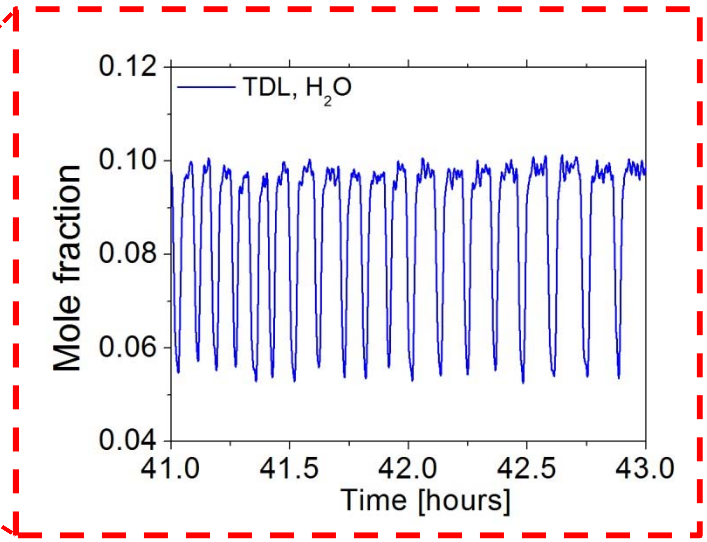
Now let's look at sensor measurements during start-up

4. H_2O in Transfer Coal Gasifier @NCCC

Time-Resolved TDLAS During Gasifier Start-up



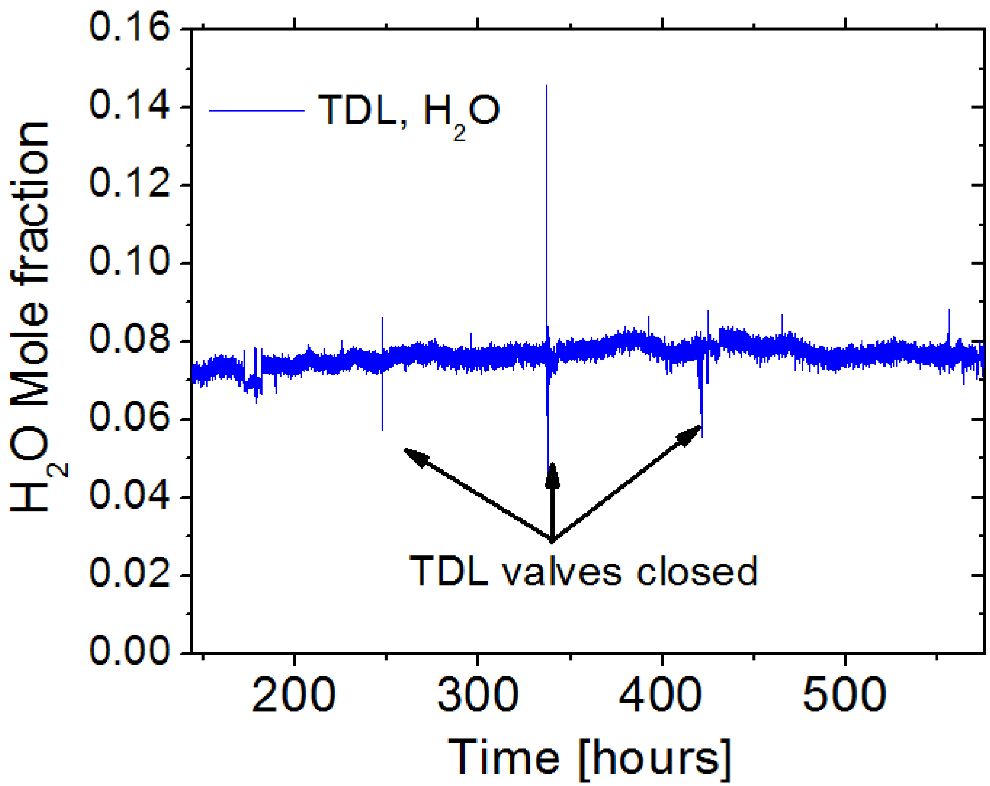
TDL shown @ 2s resolution



H_2O% fluctuations from pulsed coal feed for controlled gasifier warm-up

- *In situ* measurements of syngas moisture content capture start-up events
  - Propane heater ignition (H_2O combustion products) and warm-up
  - TDLAS of H_2O captures pulsing of coal feeder to control warm-up rate of the rig
  - Transition to gasification
- TDL sensor captures a shut-down at 54 hours

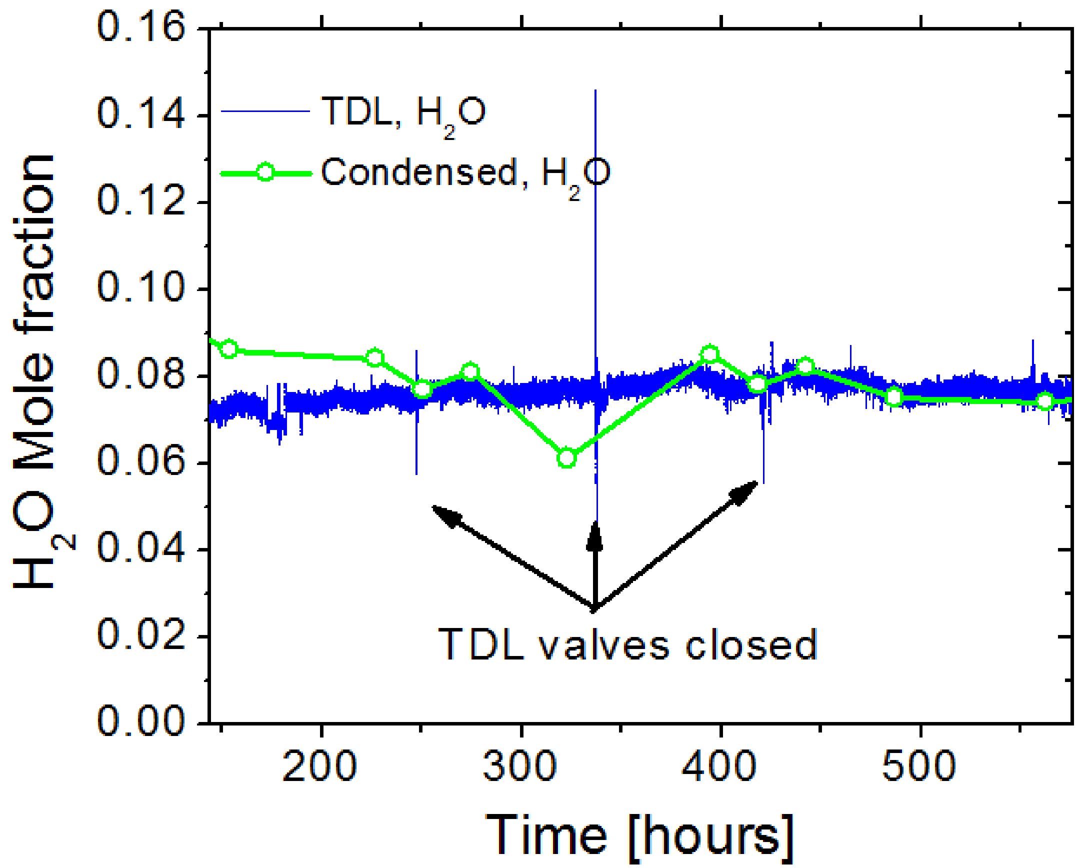
4. H_2O in Transfer Coal Gasifier @NCCC
Continuous Time-Resolved Unattended TDLAS



- Unattended operation yields continuous record of H_2O
- Valves closed 3 times during run due to reactor upset not related to TDL
- Light transmission stable over entire campaign (depends on P)
  - No degradation of window transmission or laser performance

4. H_2O in Transfer Coal Gasifier @NCCC

TDL H_2O Compared to Liquid H_2O Samples

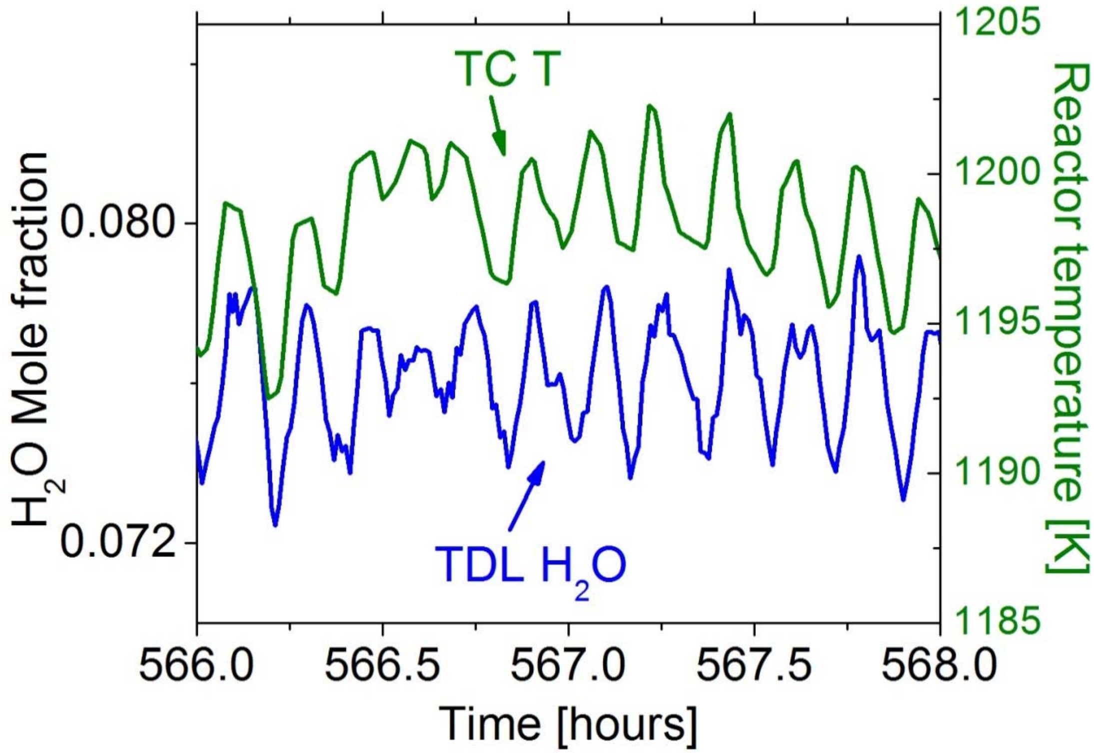


- Liquid H_2O samples taken from syngas every day or two
- TDLAS data in good agreement with samples

Can Sensor reveal real-time moisture fluctuations?

4. H_2O in Transfer Coal Gasifier @NCCC

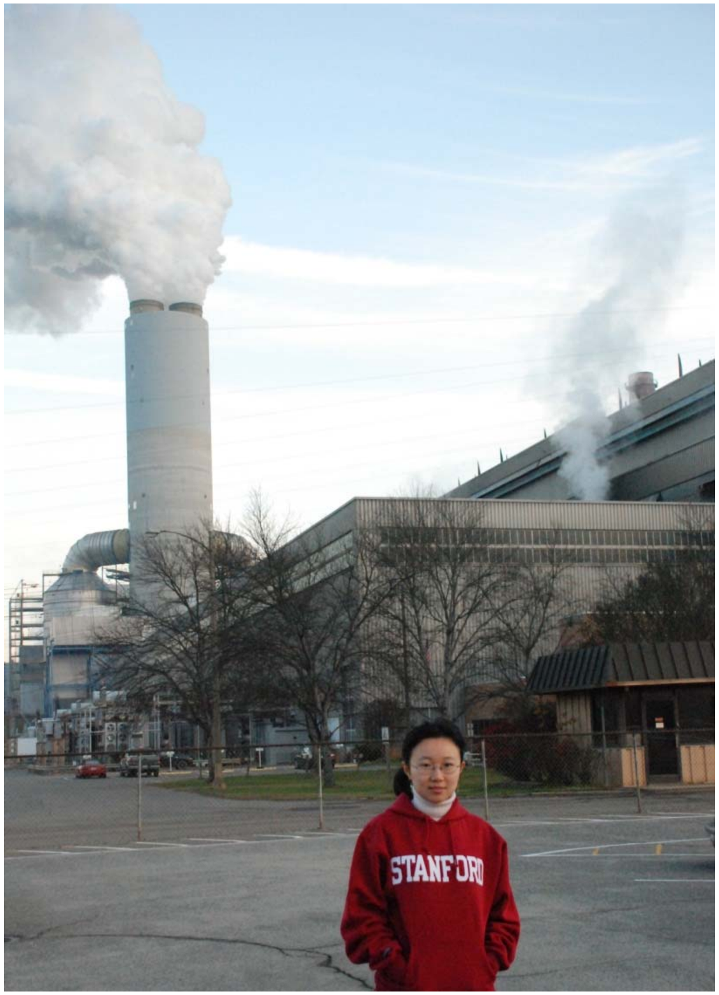
Syngas H_2O Fluctuations Capture Reactor Conditions



- H_2O fluctuation tracks the reactor thermocouple (note small ΔT)

Part 5: Measurements of NO and CO at exit of powerplant boiler

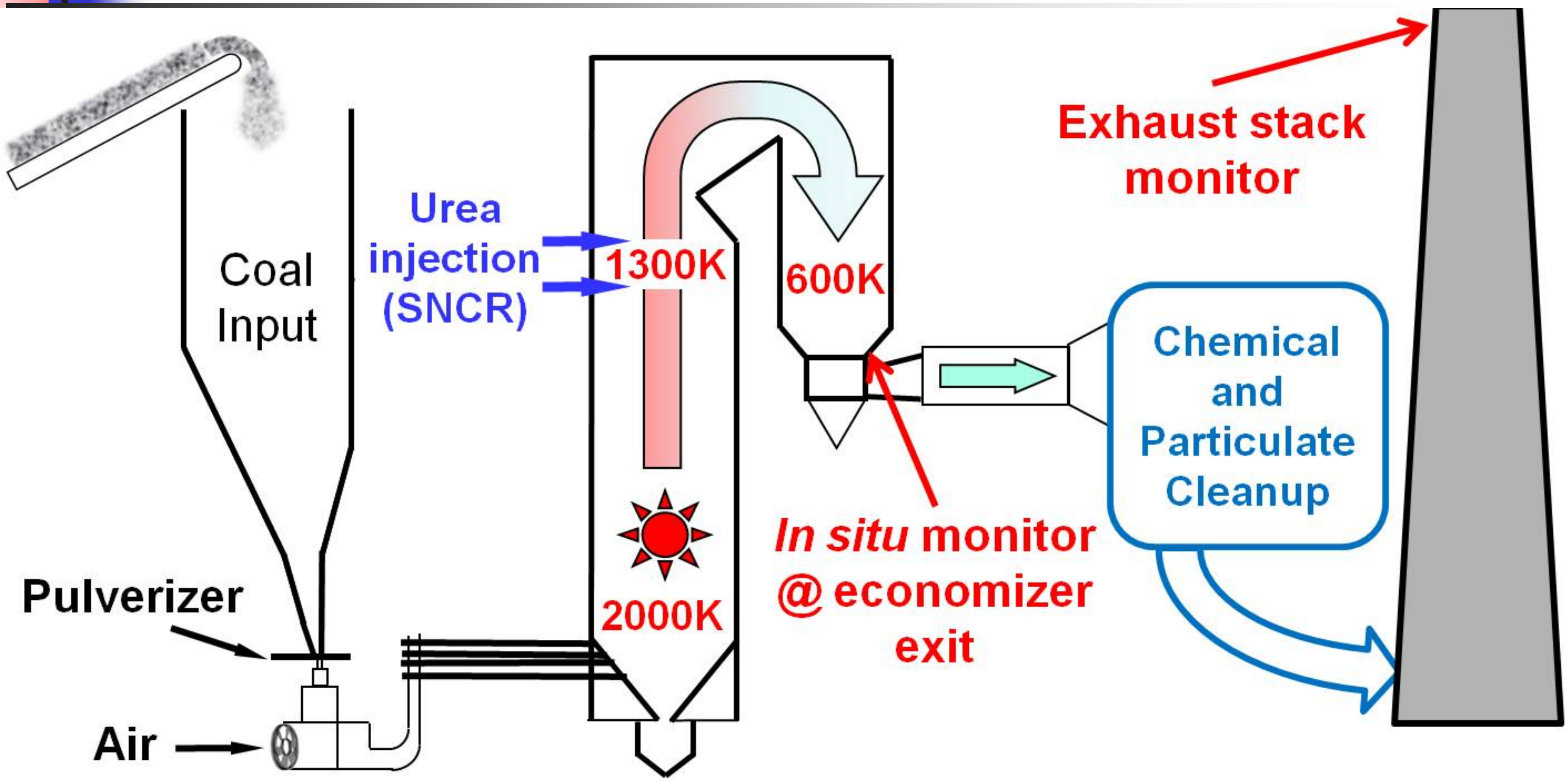
5. NO and CO in Coal-Fired Boiler Exhaust



Xing Chao, 2009/10

5. NO and CO in Coal-Fired Boiler Exhaust

Emissions Sensing in Coal-Fired Powerplants



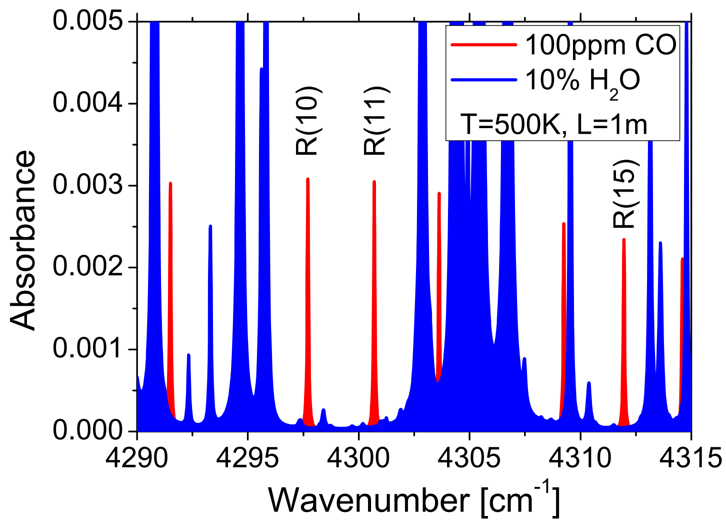
- ***In situ*** **CO and NO measurements at economizer exit of pulverized coal boiler for characterization of SNCR**

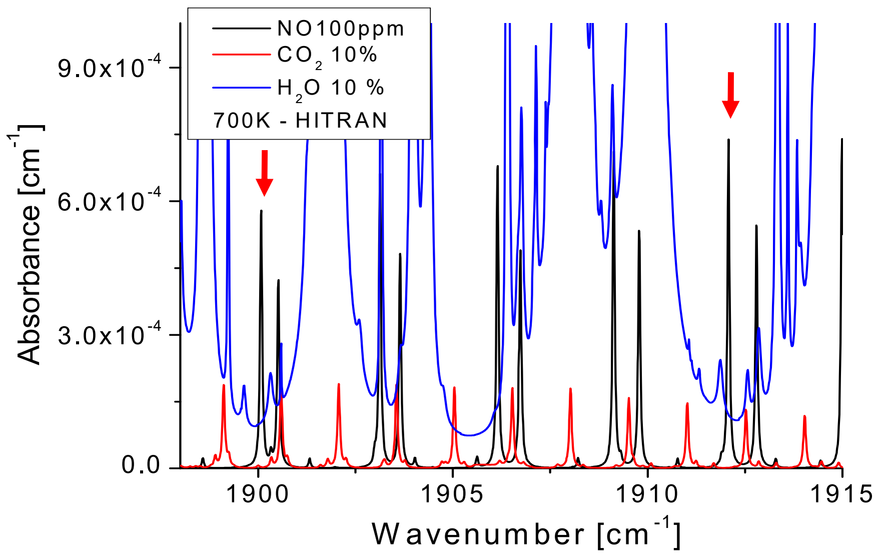
5. NO and CO in Coal-Fired Boiler Exhaust

Interference Absorption and Scattering Attenuation

- Measurement of other species must consider H_2O interference

CO





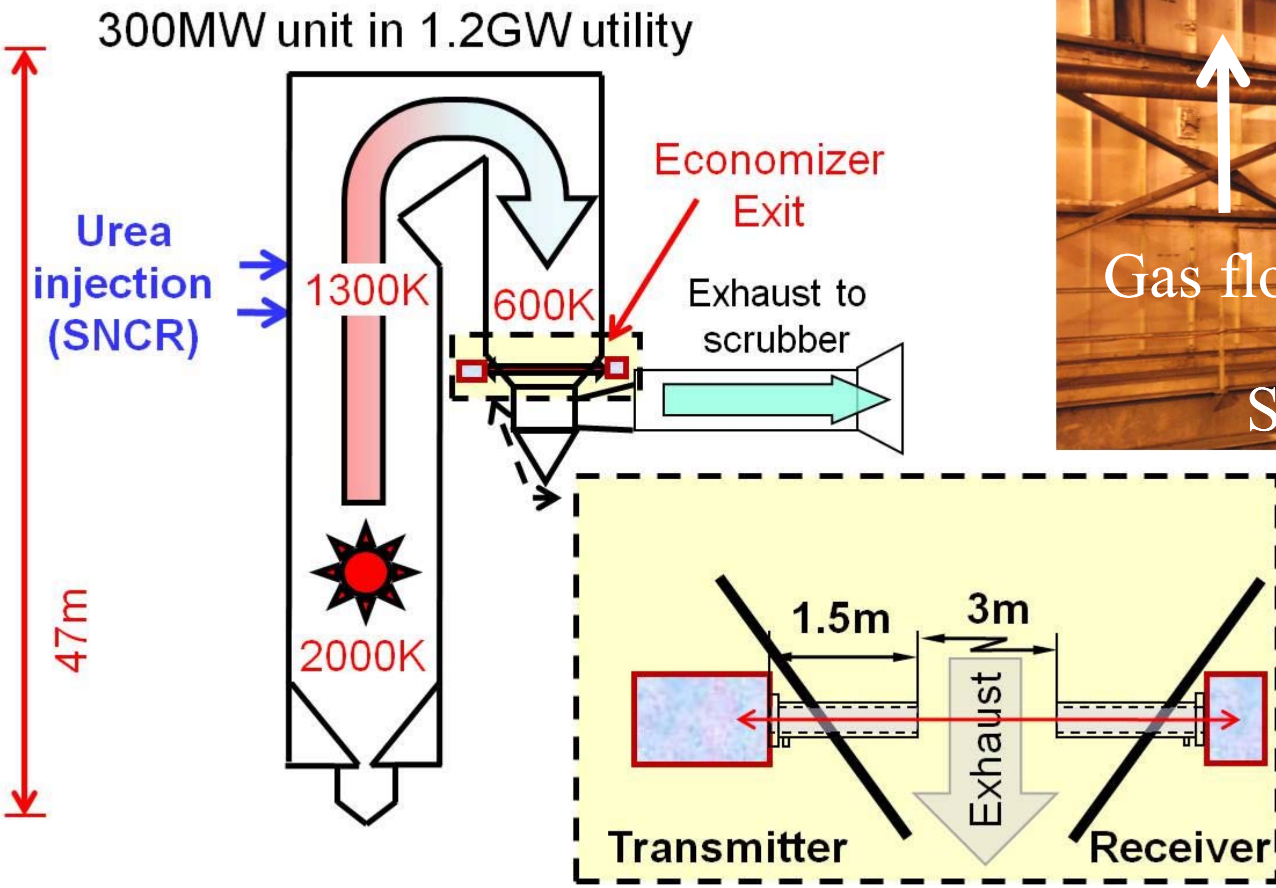
NO

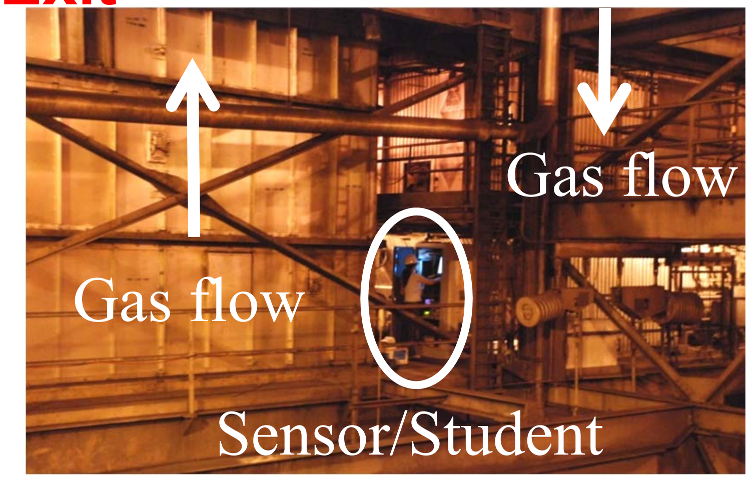
- Several candidate CO lines found that are free of H_2O interference
- Two good candidate NO lines are found relatively free of interference

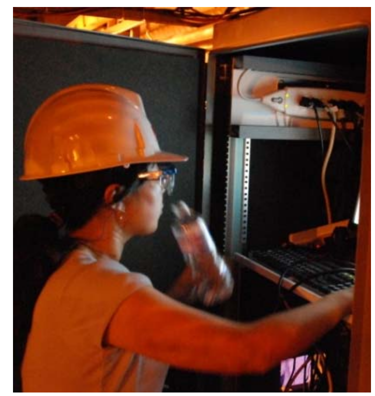
- Particulate in the flow (flyash, soot, etc) attenuates the beam, but Stanford's 2f/1f approach resolves the problem

5. NO and CO in Coal-Fired Boiler Exhaust

Sensing at the Economizer Exit





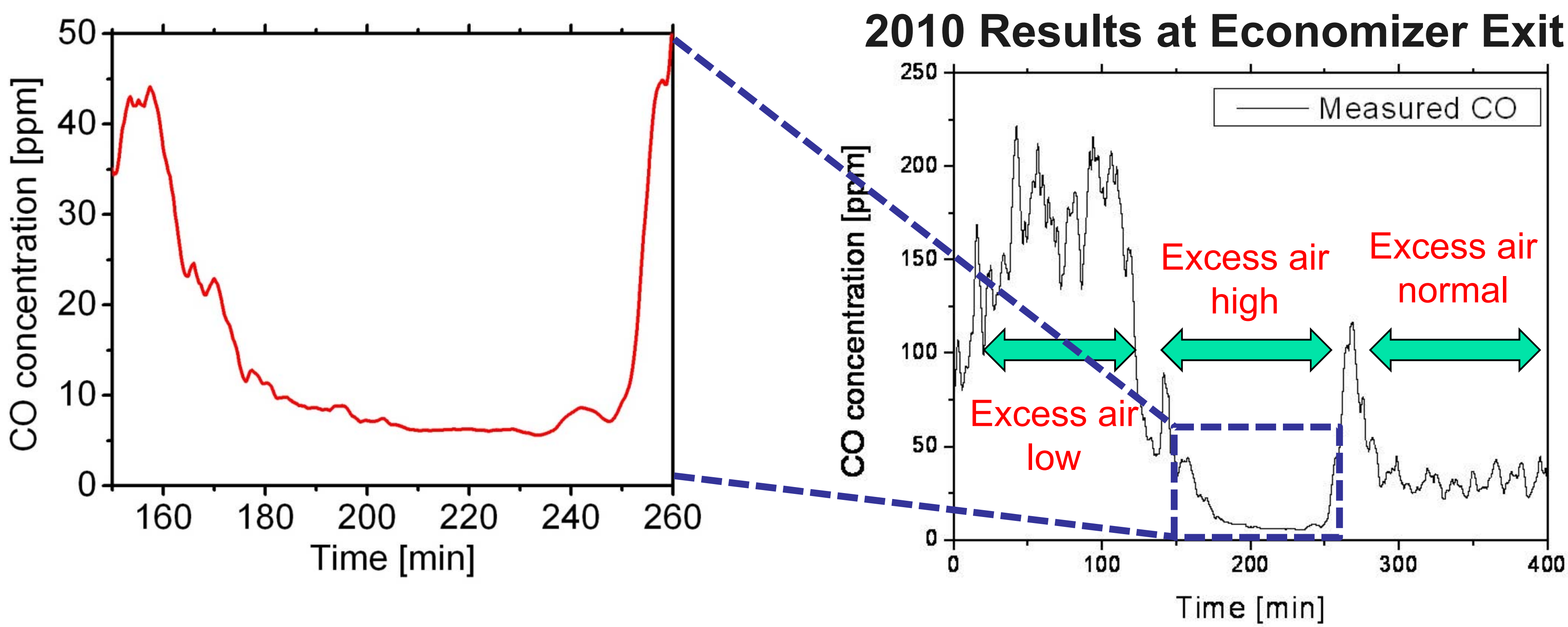


- **Utilizes 5.2μm QC for NO and 2.3μm TDL for CO**
- **Dusty environment results in large scattering losses**
  - **50-90% of incident light scattered**

5. NO and CO in Coal-Fired Boiler Exhaust

CO Sensing with 2.3 μm DFB Laser

- **Continuous monitoring of CO with varying excess air**

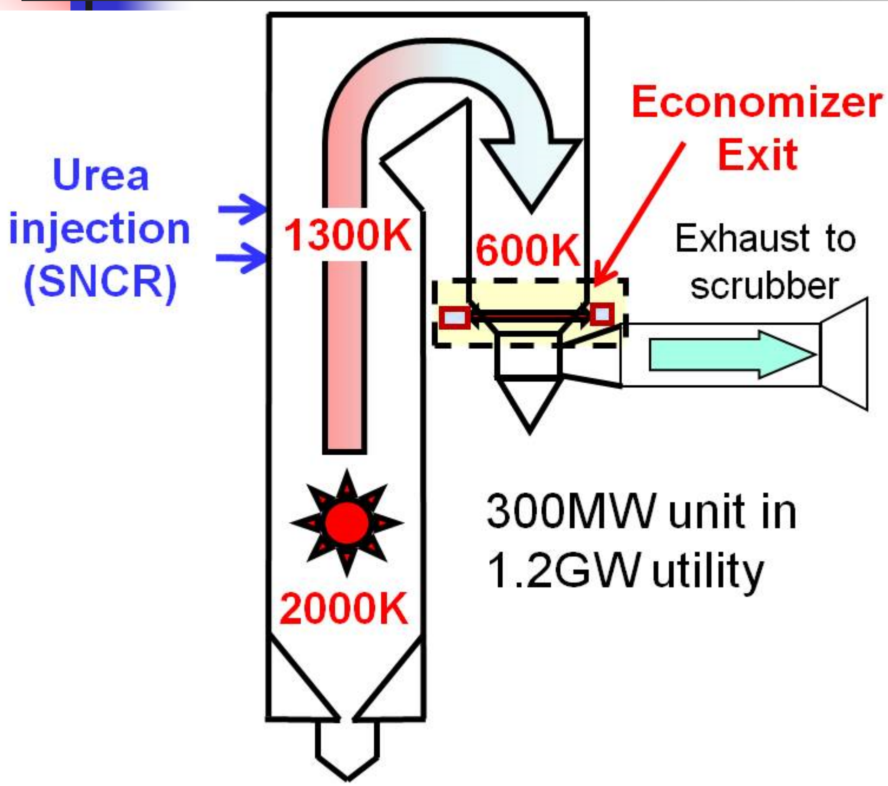


- **Correlates with excess air as expected**
- **Sensitive (ppm) time-resolved CO detection**
- ***In situ* sensor avoids delay/mixing of stack CEM**

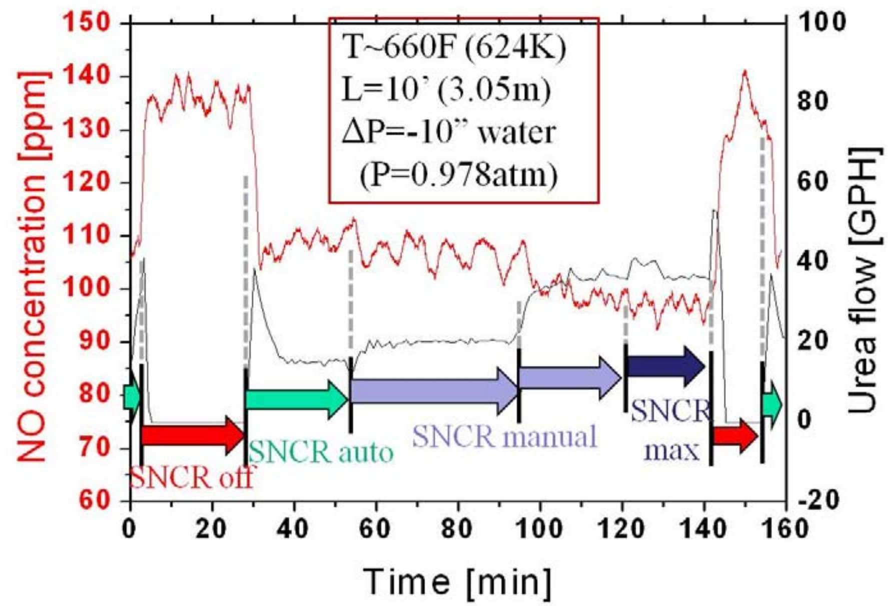
Chao et al., *Proc Combustion Institute*, 2011

5. NO and CO in Coal-Fired Boiler Exhaust

NO Sensing with 5.2 μm QC Laser



2010 Results at Economizer Exit of Pulverized Coal-Fired Plant



- **Sensitive (ppm) time-resolved NO detection**
- ***In situ* sensor avoids delay/mixing of stack CEM**
- **Potential for control of individual boilers**

6. TDLAS for Energy Conversion – Future Trends

- Portable TDL-based sensors useful for T, V, species and mass flux over wide range of conditions, industries
- Potential use as control variables for combustion emissions/efficiency
- Potential use for compliance monitoring of pollutant emissions

- Current and future topics:
  - Extension to UV and mid-IR to access new species
    → CO, CO_2, HC's, radicals, NO, NO_2
  - Advanced energy utilization: bio-fuels, gasification, liquifying natural gas

Next Lecture

Shock tubes and applications to combustion kinetics