

# Infrared Spectroscopy for High Temperature Estimation in Gases

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# Outline

- **Background**
- **Laminar Flow Results**
- **Turbulent Flow Issues**
- **Applications to Turbulent Flow**

## Measurement Methods (High Temperature Gas)

<b>Contact</b>	<b>Non-contact</b>
Thermocouples (thin film, bead)	Absorption Spectroscopy
Resistance Temperature Devices	Raleigh Scattering
Optical Fiber	Spontaneous Raman Scattering
Semiconductor sensors	Coherent Anti-Stokes Raman
Thin Filament Pyrometers	Laser Induced Fluorescence
Phosphor Thermometry	Ultrasonic thermometry
Noise thermometry	Emission spectroscopy (UV, NIR, IR)
Spectroscopy using probes	Tomography

## Sample Studies: Laminar Flows

- **Infrared Emission/Absorption Spectroscopy for major gas species concentrations and temperature (Hanson et al., 1980; Best et al., 1991)**
- **Ultraviolet Emission/Absorption Spectroscopy for temperatures, OH concentrations (Vaidya et al., 1984)**
- **Coherent Raman Anti-stokes Spectroscopy (CARS) for radical concentrations and temperatures (Eckbreth et al., 1981, Durao et al., 1992)**
- **Laser Induced Fluorescence for pollutant concentrations and temperature (Dec and Keller, 1986)**
- **Infrared emission spectroscopy for major gas species concentrations and temperature (Zhu et al., 1997)**

## Sample Studies: Turbulent Flame

- **Two wavelength Near Infrared Emission Spectroscopy for temperatures and soot concentrations (Sivathanu and Faeth, 1990; Sivathanu et al., 1991, Hamins et al., 1995; Gritzso et al., 1998)**
- **Four Wavelength Infrared Temperature Sensor for Gas Turbine Applications (Glasheen et al., 1998)**
- **Intrusive Infrared/NIR for temperatures, gas and soot concentrations (Sivathanu and Gore, 1991)**
- **CARS and Thin Filament Pyrometer for Temperature Measurements (Kelkar et al., 1997)**

# IR Emission Spectroscopy

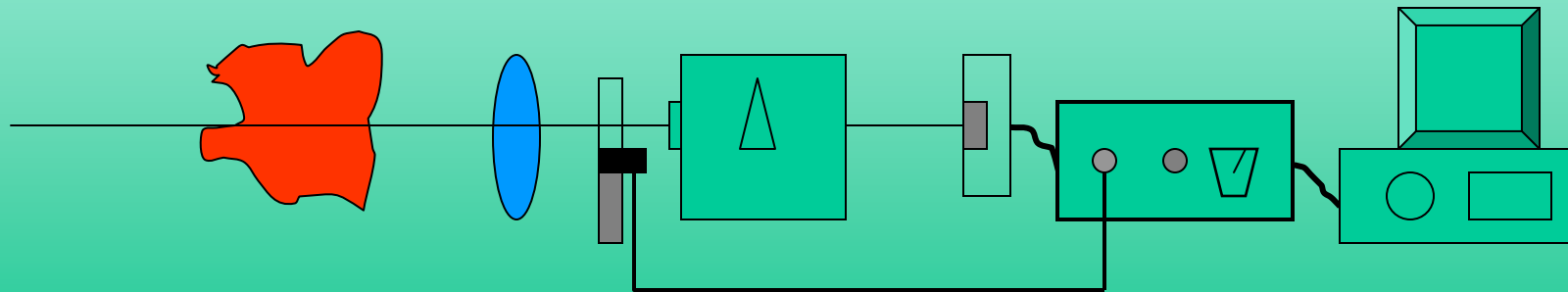
- *Basic method is to obtain multi-wavelength spectral radiation intensity measurements*
- *Utilize these measurements to obtain structure information*
- *Measurement technology is well developed.*
- *Data reduction methods require additional development.*

## Issues in Laminar Flows

- Steady state systems (low frequency)
- Spatial resolution critical
- Absolute accuracy critical
- Relatively well established methods

*Principally used for validating chemical kinetics  
and flow models*

## Experimental Arrangement



- Lens
- Chopper
- Spectrometer
- Detector
- Data acquisition system



## Calibration and Measurement Procedure

Voltages ( $V_\lambda$ ) obtained from a standard blackbody at temperature  $T$  for different wavelengths ( $\lambda$ )

$$V_\lambda = K_\lambda I_{\lambda b}$$

$I_{\lambda b}$  is the Blackbody intensity,  $K_\lambda$  is a calibration constant

$$I_{\lambda b} = \frac{C_1}{\lambda^5 (\exp(C_2 / \lambda T) - 1)}$$

$C_1$  and  $C_2$  are known first and second radiation constants

For unknown signal:

$$I_\lambda = V_\lambda / K_\lambda$$

*Note:  $K_\lambda$  can be a function of  $I_\lambda$  requiring a more extensive calibration procedure.*

## Data Analysis Requirements

- Spectral radiation intensities measured from a path in the hot gas.
- Obtain structure information from the measurements
- For laminar flames, different system specific methods of data reduction available

## Inversion Method

- **Guess temperature and concentration**
- **Utilize narrow band calculations to obtain intensities**
- **Compare with measured intensities**
- **Update guess of temperature and concentration**
- **Iterative program needed**
- **Difficulty is that emissivity depends on both concentration and temperature**
- **Convergence problems for some iterative schemes**
- **Simultaneous absorption measurement allows easier methods**

# HOMOGENEOUS PATHS

*Spectral Radiation Intensity ( $I_\lambda$ ) for homogeneous path*

$$I_\lambda = \varepsilon_\lambda (X_i, P_i, T) I_{\lambda b}$$

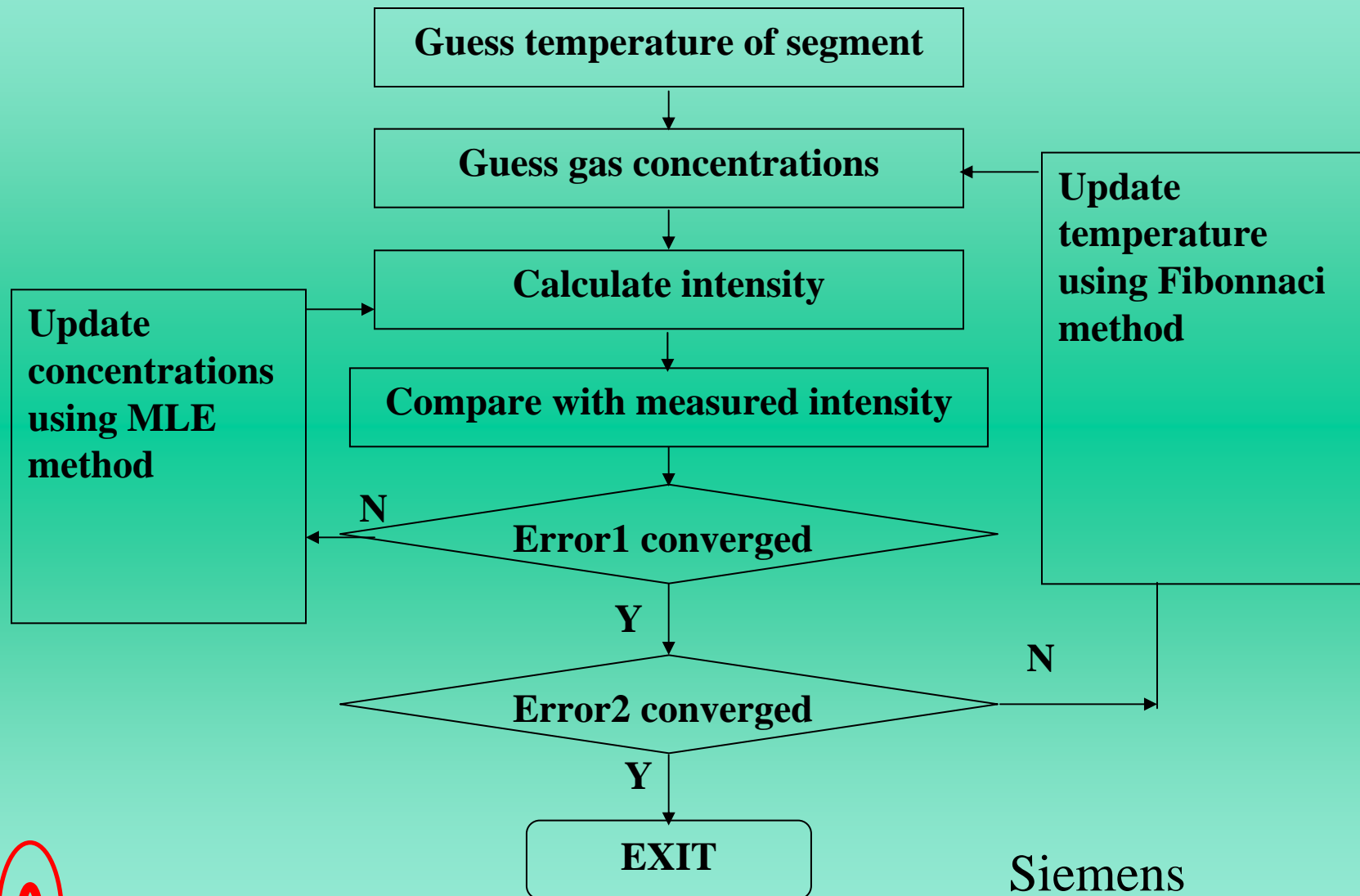
**Emissivity ( $\varepsilon_\lambda$ ) depends on mole fraction ( $X_i$ ), partial pressures ( $P_i$ ) and thermodynamic temperature ( $T$ ).**

- **Gas species of interest: CO<sub>2</sub>, H<sub>2</sub>O, CO and CH<sub>4</sub>**
- **Emissivity: Narrow band model (RADCAL, Hitran)**
- **Amplitude uncertainty: 10%**
- **Wavelength uncertainty: 40 to 50 nm at 4.5 microns**
- **Maximum pressure range: 10 atmospheres**

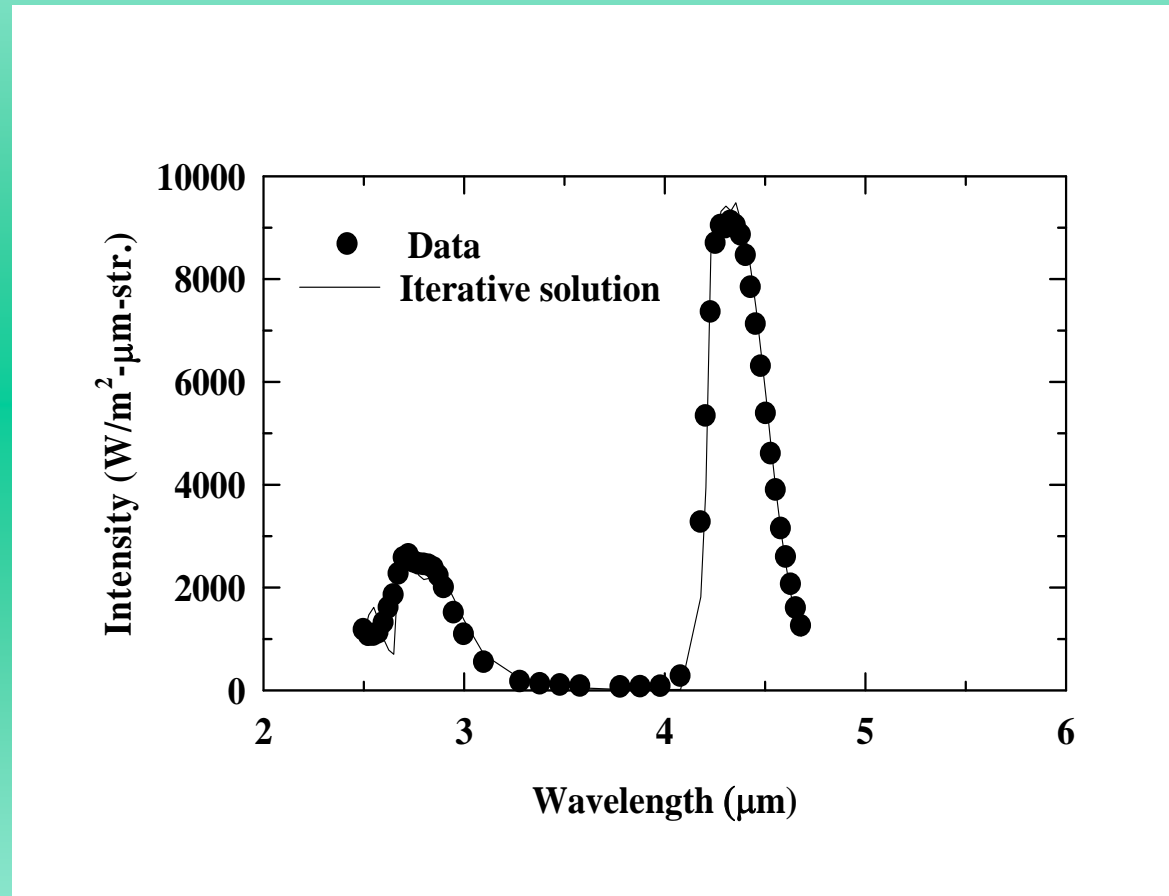
## NARROW BAND MODEL (RADCAL)

Species	Band	Method
<b>CO<sub>2</sub></b>	2.0 μm	modeled
	2.7 μm	modeled
	4.3 μm	modeled
	10.0 μm	modeled
	15.0 μm	tabulated
<b>H<sub>2</sub>O</b>	1.38 μm	tabulated
	1.88 μm	
	2.70 μm	
	6.30 μm	
	20 to 200 μm	
<b>CO</b>	4.6 μm	modeled
<b>CH<sub>4</sub></b>	2.4 μm	tabulated
	3.3 μm	
	7.7 μm	
<b>soot</b>	0.4 to 2000 μm	modeled

## Flow Chart for Iterative Program



# Evaluation in Laminar Flame

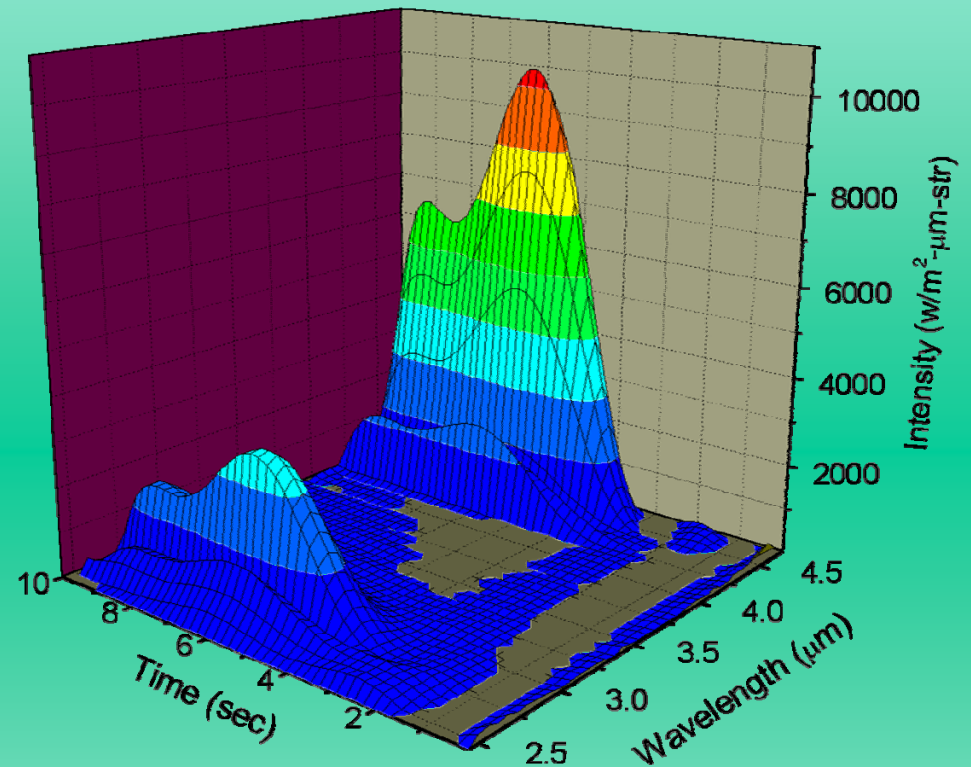
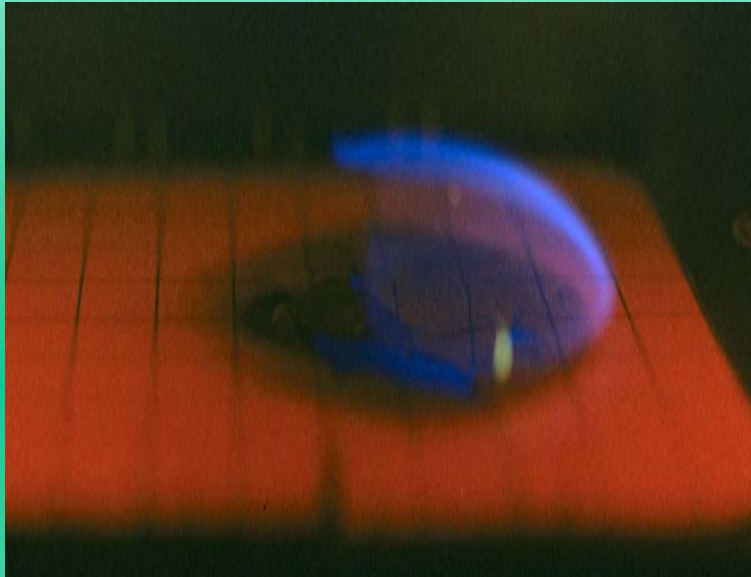


## Deconvolution Results

Quantity	Emission spectroscopy	Thermocouple/GC	Theoretical (Adiabatic)
CO <sub>2</sub> ( $\Phi = 0.81$ )	0.070	.078	-----
H <sub>2</sub> O ( $\Phi = 0.81$ )	0.158	-----	0.157
T(K) ( $\Phi = 0.81$ )	1940	1840	2034
CO <sub>2</sub> ( $\Phi = 0.86$ )	0.074	0.083	-----
H <sub>2</sub> O( $\Phi = 0.86$ )	0.168	-----	0.166
T(K) ( $\Phi = 0.86$ )	2011	1840	2112



# Intensity Data from Microgravity Experiment

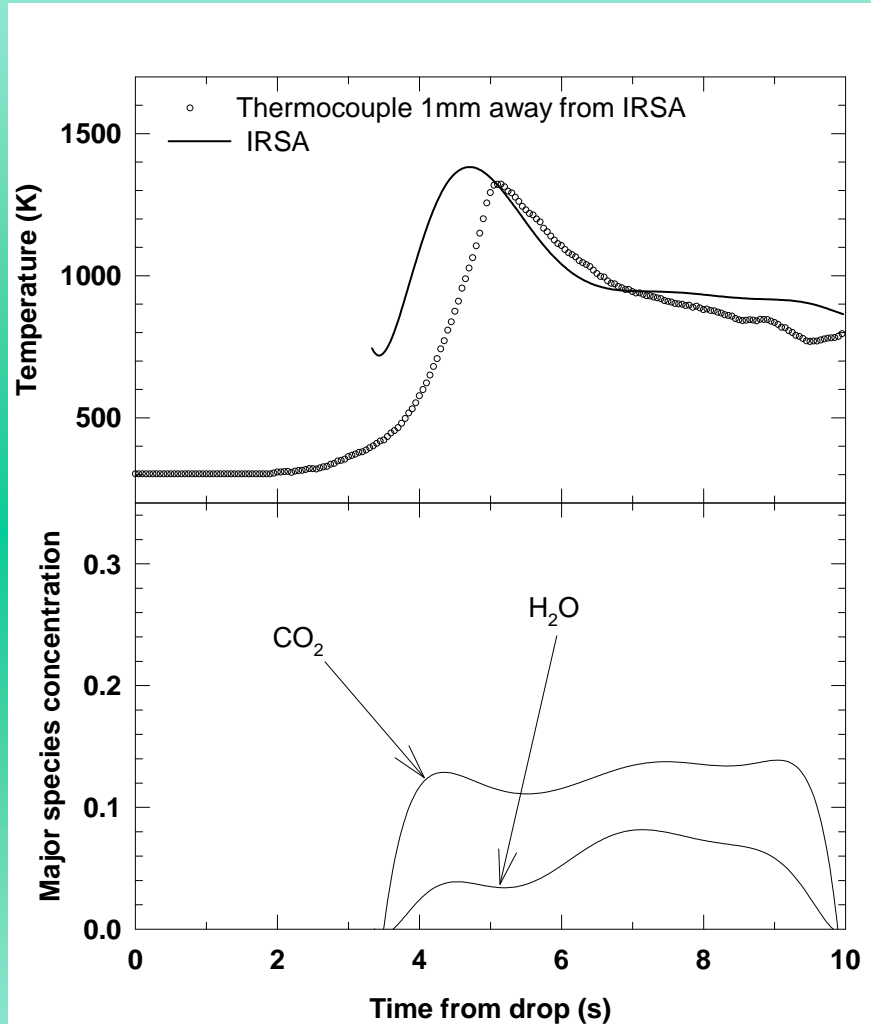


**Sample Radiation Intensities from a Transient Flame  
Experiment at the Japanese Microgravity Facility**



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## Deconvolution Results



- Spectral intensity data collected using a stand alone data logger
- Ten seconds of data collected at a scan rate of 300 Hz
- Temperature and gas concentrations obtained assuming homogeneous paths

## Issues in Turbulent Flow

- Intrusive probes – effect on structure
- Tomography – turbulence/radiation interactions
- Temporal resolution – sufficiently fast
- Spatial resolution – small scales

*Principally used for validating turbulent flow models. Most industrial high temperature flows are turbulent.*

# Issues faced by Industry

*Control of the combustion process: reduce pollutants, increase efficiency, product lifetime*

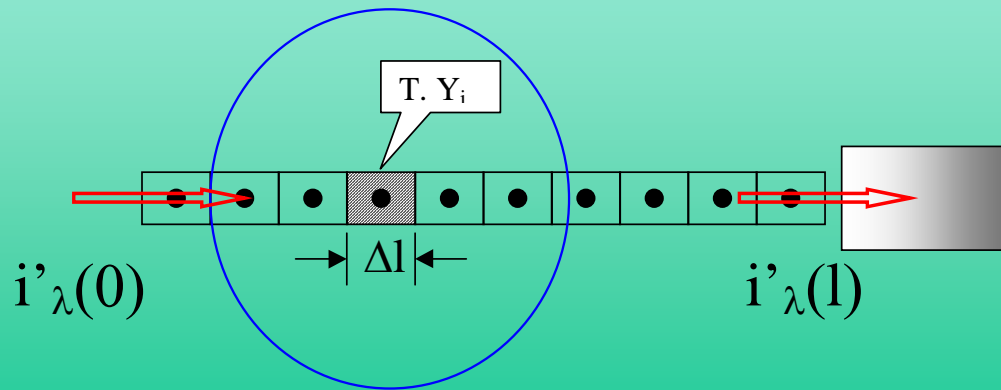
- **What temperature and where?**  
Instantaneous/average temperature  
At all locations/highest temperature location
- **Control signals?**  
Absolute values/trends?  
Correlated with pollutants, efficiency, thermal stress

*Ideal situation is to have a single control variable that is “indicative” of the parameter being monitored. Eg. Total pollutant emitted, Stability index*



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## Equation of Radiative Transfer (Non-homogeneous Paths)

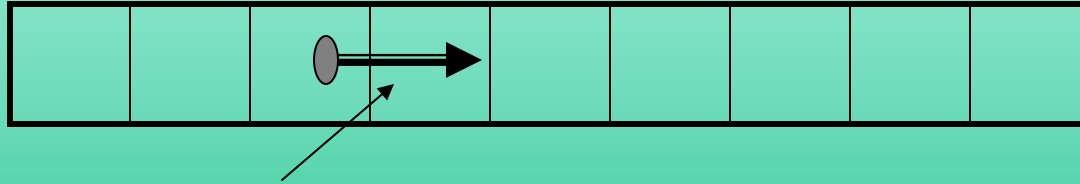


$$\frac{di'_\lambda}{dl} = -\alpha_\lambda i'_\lambda + \alpha_\lambda i'_{\lambda,b}$$

$$i'_\lambda(l) = i'_\lambda(0)e^{-\kappa_\lambda(l)} + \int_0^{\kappa_\lambda(l)} i'_{\lambda,b}(l^*)e^{-[\kappa_\lambda(l) - \kappa_\lambda(l^*)]} d\kappa_\lambda(l^*)$$

$$\kappa_\lambda(l) \equiv \int_0^l \alpha_\lambda(l^*) dl^*$$

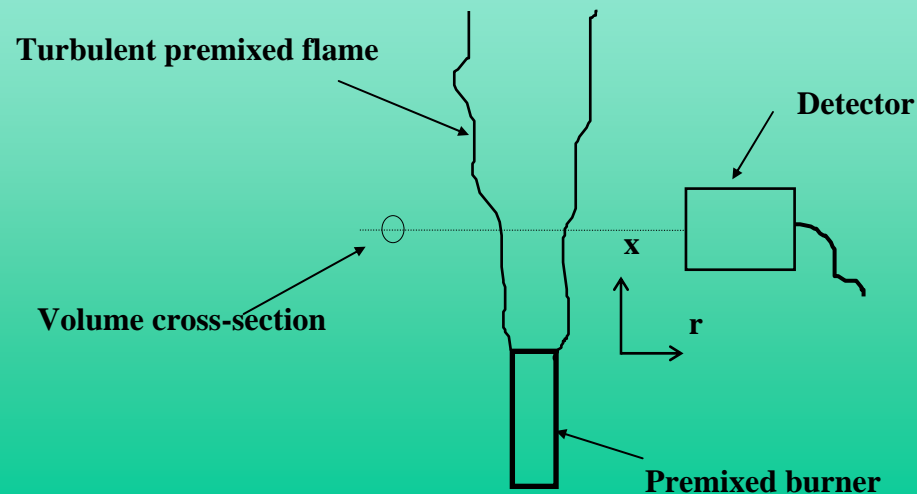
# Intensity Calculations for Turbulent Flows



$$I(J) = I(J-1)\tau_J + \varepsilon_J I_{\lambda b}(J)$$

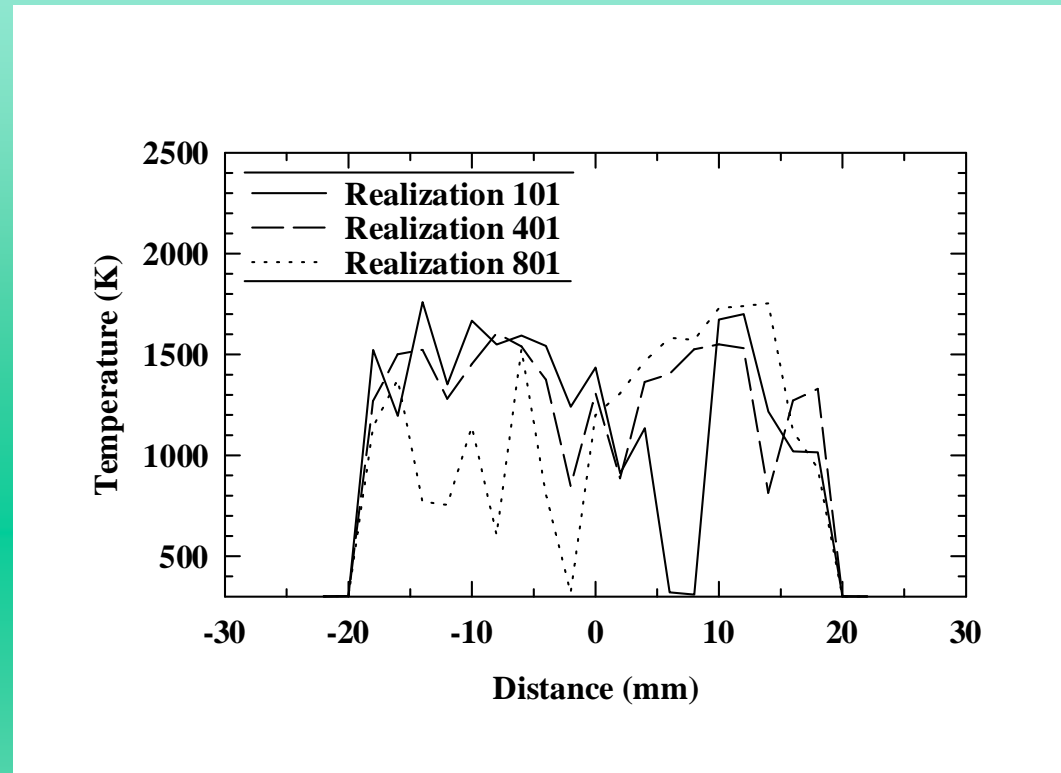
- **Discretized equation of Radiative Transfer**
- **Calculation started from cold or hot boundary**
- **For laminar flames, relative straightforward**
- **For turbulent flames, turbulence/radiation interactions are important**
- **Spatial and temporal correlations modeled using Monte Carlo or Time Series Methods**

# Statistical simulation of Combustor Volume



- **Statistically simulate the instantaneous temperature and gas concentrations in a small control volume**
- **Obtain total heat release rate and pollutants produced in the control volume**
- **Simultaneously obtain signatures of possible measurement variables within the control volume**

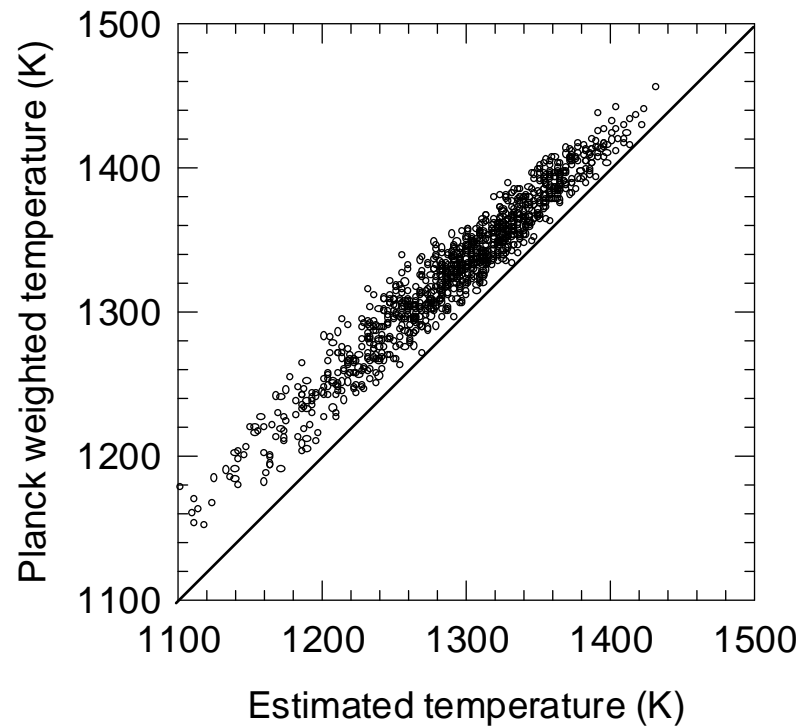
## Sample temperature realizations in the control volume



- Temperature and gas concentrations fluctuate
- Experimental data used to create 1000 sample realizations
- Simple reaction models for heat release rate and pollutant formation



# Correlation between Planck Function Temperature and Temperatures Estimated using Emission Spectroscopy



## Correlation of different variables with the instantaneous heat release

Quantity	Mean	RMS	Correlation
T* (0.30 μm)	1611 K	36 K	0.6011
T* (2.52 μm)	1327 K	54 K	0.995
T* (4.26 μm)	1255 K	60 K	0.984
T <sub>max</sub>	1529 K	295 K	0.293
T <sub>max/2</sub>	1294 K	325 K	0.289
T <sub>C/L</sub>	1118 K	301 K	0.176
T <sub>avg</sub>	1118 K	71 K	0.925
T (ES100)	1285 K	59 K	0.965
a <sub>λ</sub> (2.64 μm)	0.991	0.00055	-0.224
a <sub>λ</sub> (4.26 μm)	0.493	0.0237	-0.315

**T\* is the Planck-Function weighted average temperature of the control volume (function of wavelength)**

$$T^* = \frac{C_1}{\lambda(\ln(C_2 / I_\lambda \lambda^5) + 1)}$$



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# Industrial Ranking of Methods

Category	Thermo-couples	Absorption Spectroscopy	UV Emission	IR Emission
Detector	1	4	4	10
Sources	0	8	8	0
Development cost	2	10	5	20
Manufacturing cost	2	10	10	8
Utility	10	4	4	2
Intrusive	15	4	4	1
Operational ease	1	3	3	1
Longevity	10	2	2	2
Maintenance	5	8	8	2

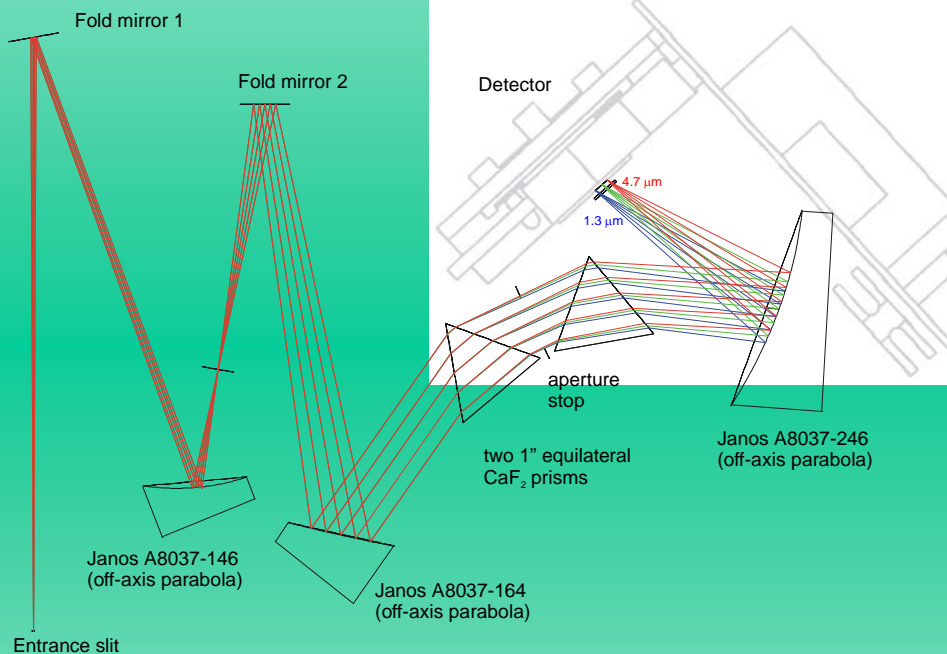


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# High Speed Spectrometer



Model ES100

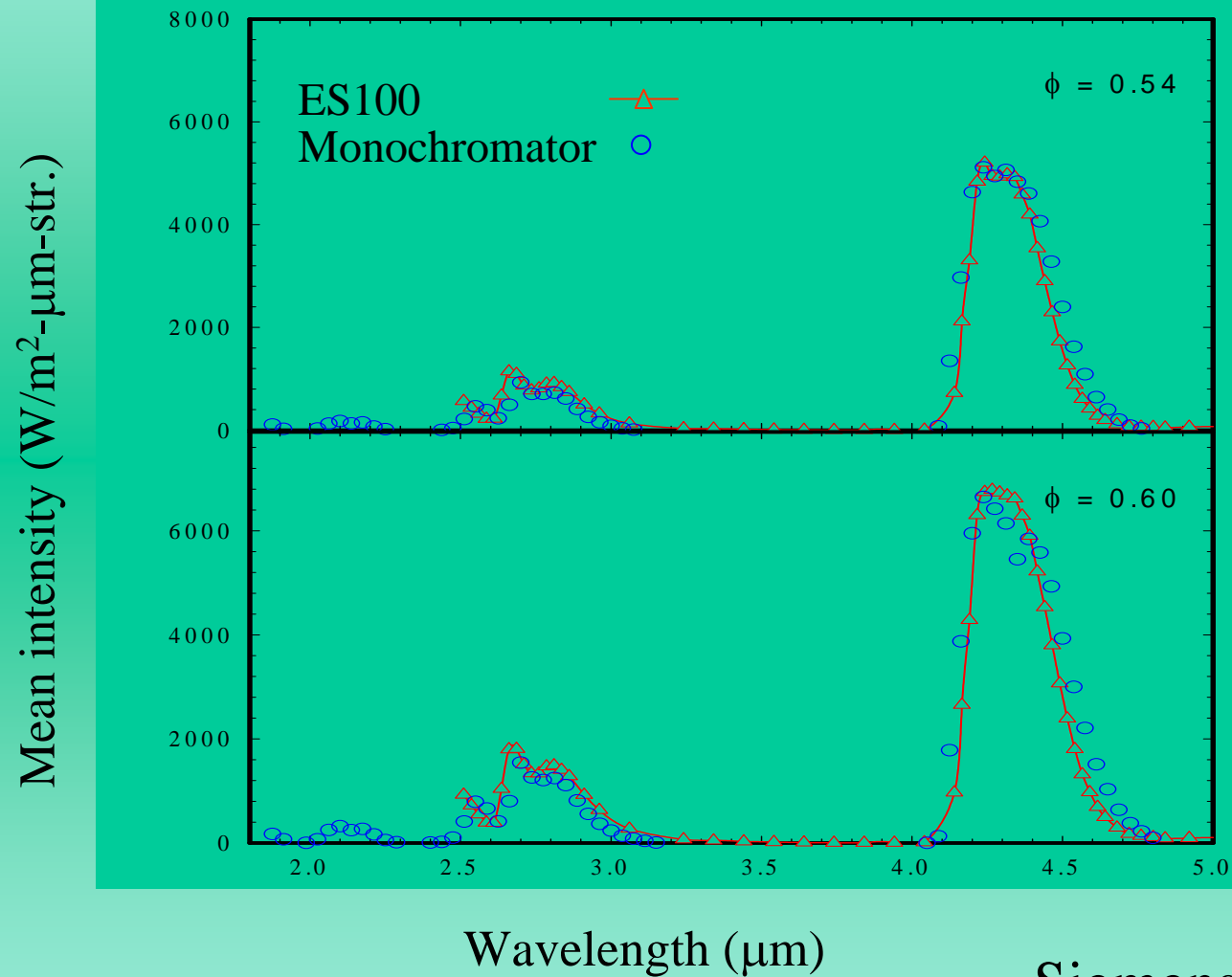


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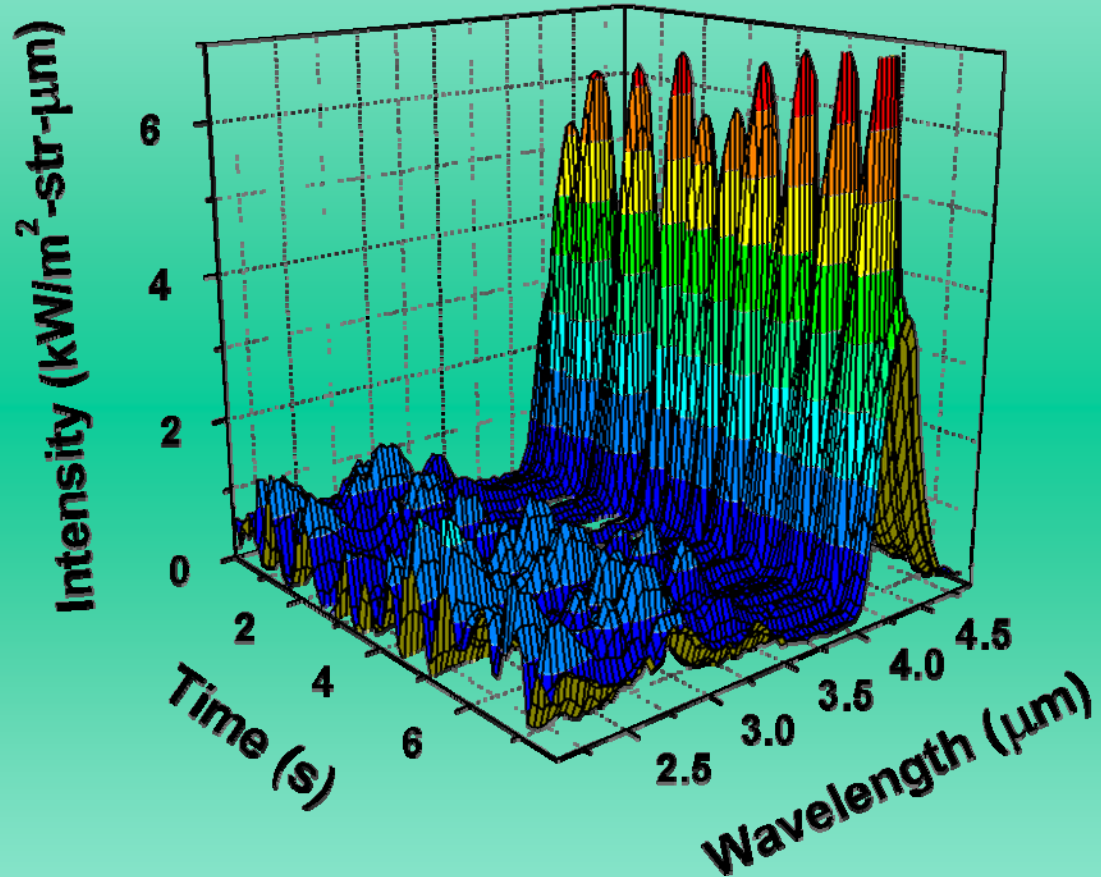
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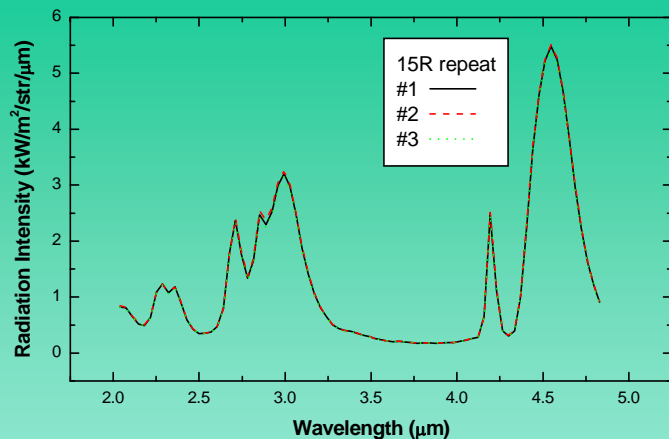
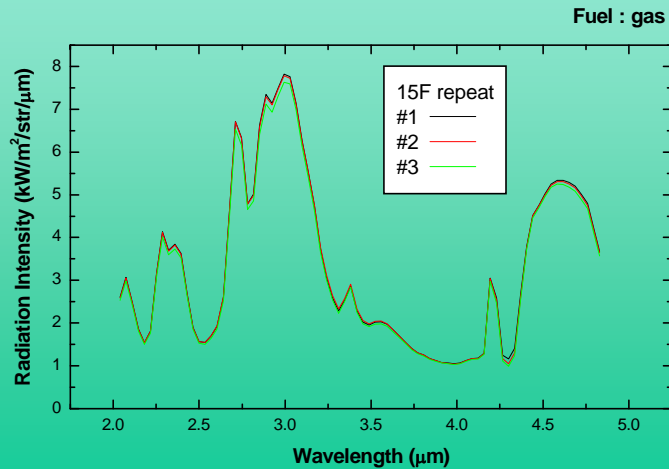
# Validation of ES100 Measurements



## Typical Spectra from a Turbulent Flame

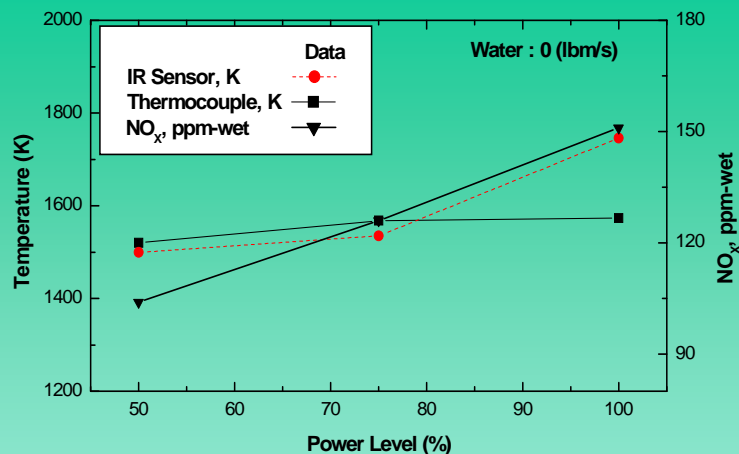
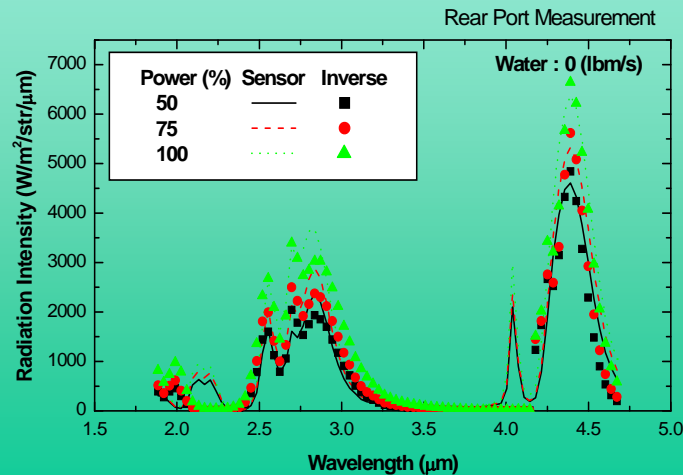


# Measurements from a Turbine Inlet



- Spectral intensity data collected at 1320 Hz
- Very high repeatability for mean intensities
- Temperature and gas concentrations obtained assuming homogeneous paths

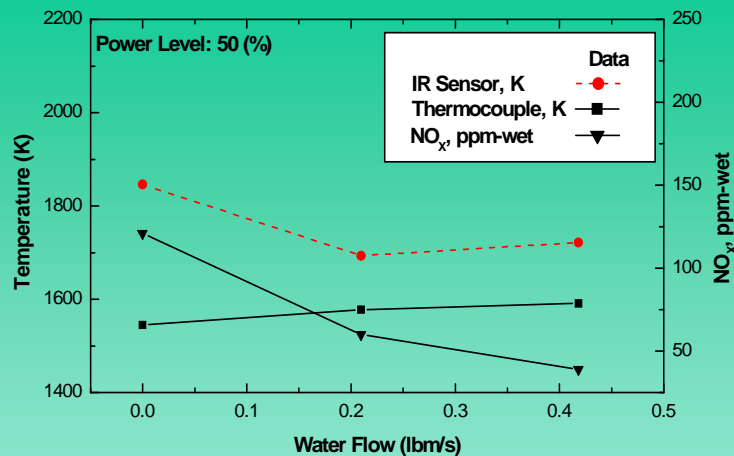
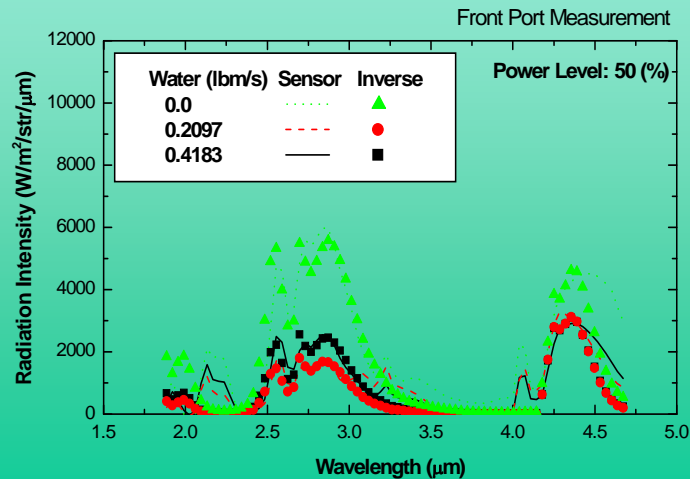
# Westinghouse Turbine at NRC



- Temperature and gas concentrations obtained using iterative algorithm
- Calculations assumed lack of methane and CO in the primary zone
- Temperature from ES100 correlated with NO<sub>X</sub>
- Temperature from thermocouple is not correlated with NO<sub>X</sub>



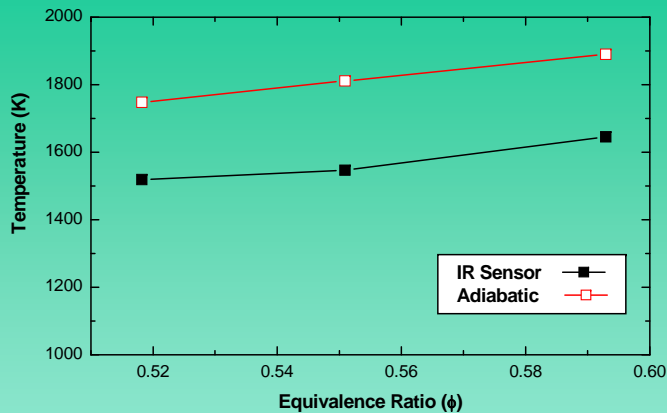
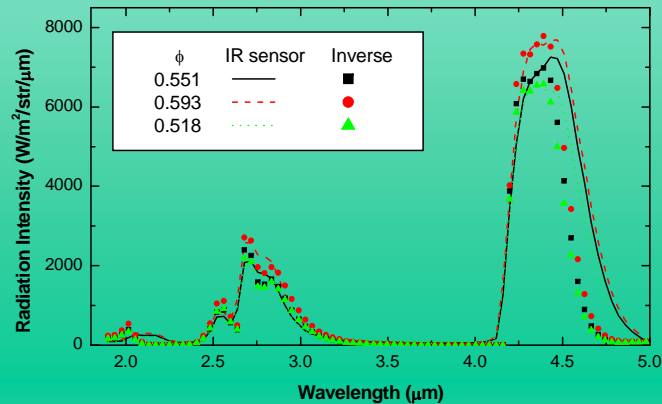
# Westinghouse Turbine at NRC



- Results similar for data obtained with water addition
- Temperature from ES100 correlated with NO<sub>X</sub>
- Temperature from thermocouple is not correlated with NO<sub>X</sub>

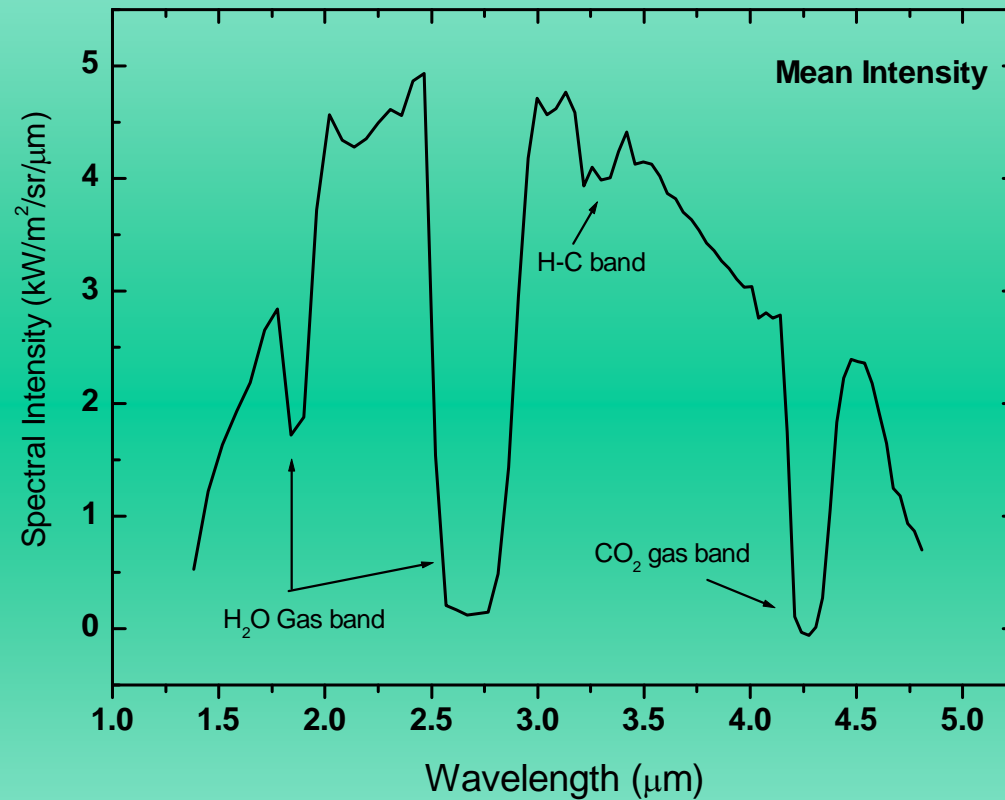
# Kerosene Spray Flame Data

General Electric Corporation (CRD)  
Kerosene Spray Flame

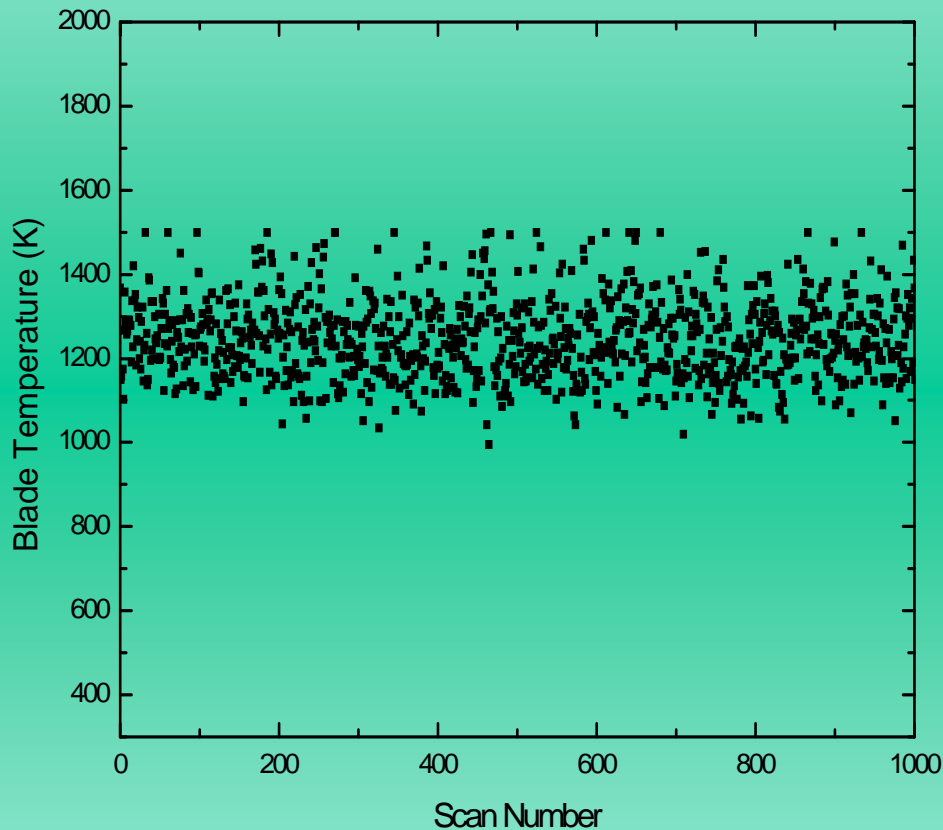


- Temperature from ES100 correlated with global equivalence ratio
- No thermocouple data available
- Global equivalence ratio is also a direct measure of power output or heat release rate

# High Pressure Data including Blade Radiation



# Blade Temperature Estimation



- Radiation from blades synchronized to data collection
- Intensity measurement spread over three blades
- Four gas band free wavelengths used to estimate temperature
- Mean Temperature is 1273 K and mean emissivity is 0.85

# Current Uses of Infrared Emission Spectrometer

## *Fundamental studies of turbulent flame structure*

- Sandia National Laboratories, NIST, NASA, DoD, varied universities

## *Radiation from turbines and internal engines*

- Westinghouse, KIMM

## *Steel, Aluminum, and Molten Glass Manufacturing*

- Pohang Steel Company, KAIST, Alcoa, etc.

## Future Directions in Infrared Emission Spectroscopy

- Hyper spectral scanning
- Multiple Element Sensors
- Advanced deconvolution algorithm
- Hyper speed spectral scanning



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## Non-Homogeneous Fields

- Multiple view angles and slices
- Tomography for Local transmittances/emission intensities
- Absorption measurements are typically required

