Infrared Spectroscopy for High Temperature Estimation in Gases

Yudaya Sivathanu
En’Urga Inc.
1291 Cumberland Av., West Lafayette, IN 47906

Nancy Ulerich
Siemens Westinghouse Power Corp.
1310 Beulah Rd., Pittsburgh, PA 15235

Acknowledgement: This work was completed with support provided by NASA, NIST, and the Department of Energy.
Outline

• Background

• Laminar Flow Results

• Turbulent Flow Issues

• Applications to Turbulent Flow
<table>
<thead>
<tr>
<th>Contact</th>
<th>Non-contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermocouples (thin film, bead)</td>
<td>Absorption Spectroscopy</td>
</tr>
<tr>
<td>Resistance Temperature Devices</td>
<td>Raleigh Scattering</td>
</tr>
<tr>
<td>Optical Fiber</td>
<td>Spontaneous Raman Scattering</td>
</tr>
<tr>
<td>Semiconductor sensors</td>
<td>Coherent Anti-Stokes Raman</td>
</tr>
<tr>
<td>Thin Filament Pyrometers</td>
<td>Laser Induced Fluorescence</td>
</tr>
<tr>
<td>Phosphor Thermometry</td>
<td>Ultrasonic thermometry</td>
</tr>
<tr>
<td>Noise thermometry</td>
<td>Emission spectroscopy (UV, NIR, IR)</td>
</tr>
<tr>
<td>Spectroscopy using probes</td>
<td>Tomography</td>
</tr>
</tbody>
</table>
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; Gritzo 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

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

$C_1$ 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: \( \text{CO}_2 \), \( \text{H}_2\text{O} \), \( \text{CO} \) and \( \text{CH}_4 \)
- 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)**

<table>
<thead>
<tr>
<th>Species</th>
<th>Band</th>
<th>Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>2.0 μm</td>
<td>modeled</td>
</tr>
<tr>
<td></td>
<td>2.7 μm</td>
<td>modeled</td>
</tr>
<tr>
<td></td>
<td>4.3 μm</td>
<td>modeled</td>
</tr>
<tr>
<td></td>
<td>10.0 μm</td>
<td>modeled</td>
</tr>
<tr>
<td></td>
<td>15.0 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td>H₂O</td>
<td>1.38 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td></td>
<td>1.88 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td></td>
<td>2.70 μm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>6.30 μm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>20 to 200 μm</td>
<td></td>
</tr>
<tr>
<td>CO</td>
<td>4.6 μm</td>
<td>modeled</td>
</tr>
<tr>
<td>CH₄</td>
<td>2.4 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td></td>
<td>3.3 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td></td>
<td>7.7 μm</td>
<td>tabulated</td>
</tr>
<tr>
<td>soot</td>
<td>0.4 to 2000 μm</td>
<td>modeled</td>
</tr>
</tbody>
</table>

Siemens
Westinghouse
Flow Chart for Iterative Program

1. Guess temperature of segment
2. Guess gas concentrations
3. Calculate intensity
4. Compare with measured intensity
5. Update concentrations using MLE method
6. Update temperature using Fibonacci method

- Error1 converged: Y → EXIT
- Error2 converged: Y → EXIT
- N → N

Siemens Westinghouse
Evaluation in Laminar Flame

![Graph showing intensity vs. wavelength with data points and an iterative solution line.]

- Intensity (W/m²·μm-str.)
- Wavelength (μm)
- Data
- Iterative solution
## Deconvolution Results

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Emission spectroscopy</th>
<th>Thermocouple/GC</th>
<th>Theoretical (Adiabatic)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO$_2$ ($\Phi = 0.81$)</td>
<td>0.070</td>
<td>0.078</td>
<td>------</td>
</tr>
<tr>
<td>H$_2$O ($\Phi = 0.81$)</td>
<td>0.158</td>
<td>------</td>
<td>0.157</td>
</tr>
<tr>
<td>T(K) ($\Phi = 0.81$)</td>
<td>1940</td>
<td>1840</td>
<td>2034</td>
</tr>
<tr>
<td>CO$_2$ ($\Phi = 0.86$)</td>
<td>0.074</td>
<td>0.083</td>
<td>------</td>
</tr>
<tr>
<td>H$_2$O ($\Phi = 0.86$)</td>
<td>0.168</td>
<td>------</td>
<td>0.166</td>
</tr>
<tr>
<td>T(K) ($\Phi = 0.86$)</td>
<td>2011</td>
<td>1840</td>
<td>2112</td>
</tr>
</tbody>
</table>
Intensity Data from Microgravity Experiment

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

Siemens
Westinghouse

En’Urga Inc.
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

Siemens
Westinghouse
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
Equation of Radiative Transfer (Non-homogeneous Paths)

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

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

\[
\kappa_\lambda (l) = \int_0^l \alpha_\lambda (l^*) dl^*
\]
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
• 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

![Graph showing correlation between Planck weighted temperature and estimated temperature.](image)
Correlation of different variables with the instantaneous heat release

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

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

\[ T* = \frac{C_1}{\lambda \left( \ln(C_2 / I_\lambda \lambda^5) + 1 \right)} \]

En’Urga Inc.

Siemens

Westinghouse
# Industrial Ranking of Methods

<table>
<thead>
<tr>
<th>Category</th>
<th>Thermocouples</th>
<th>Absorption Spectroscopy</th>
<th>UV Emission</th>
<th>IR Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td>Detector</td>
<td>1</td>
<td>4</td>
<td>4</td>
<td>10</td>
</tr>
<tr>
<td>Sources</td>
<td>0</td>
<td>8</td>
<td>8</td>
<td>0</td>
</tr>
<tr>
<td>Development cost</td>
<td>2</td>
<td>10</td>
<td>5</td>
<td>20</td>
</tr>
<tr>
<td>Manufacturing cost</td>
<td>2</td>
<td>10</td>
<td>10</td>
<td>8</td>
</tr>
<tr>
<td>Utility</td>
<td>10</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>Intrusive</td>
<td>15</td>
<td>4</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>Operational ease</td>
<td>1</td>
<td>3</td>
<td>3</td>
<td>1</td>
</tr>
<tr>
<td>Longevity</td>
<td>10</td>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>Maintenance</td>
<td>5</td>
<td>8</td>
<td>8</td>
<td>2</td>
</tr>
</tbody>
</table>
High Speed Spectrometer

Model ES100

Entrance slit

Fold mirror 1

Fold mirror 2

Detector

Janos A8037-146 (off-axis parabola)

Janos A8037-164 (off-axis parabola)

two 1° equilateral CaF₂ prisms

4.7 μm

1.3 μm

aperture stop

Janos A8037-246 (off-axis parabola)
Validation of ES100 Measurements

![Graph showing mean intensity vs. wavelength with data points for ES100 Monochromator.

Mean intensity (W/m²-μm-str.)

- ES100 Monochromator

Wavelength (μm)

- φ = 0.54
- φ = 0.60

Siemens
Westinghouse
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\(_X\)
- Temperature from thermocouple is not correlated with NO\(_X\)

Siemens
Westinghouse
Westinghouse Turbine at NRC

- Results similar for data obtained with water addition
- Temperature from ES100 correlated with NOX
- Temperature from thermocouple is not correlated with NOX
Kerosene Spray Flame Data

- 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

General Electric Corporation (CRD)
Kerosene Spray Flame

<table>
<thead>
<tr>
<th>Equivalence Ratio ($\phi$)</th>
<th>IR sensor</th>
<th>Inverse</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.551</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.593</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.518</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Equivalence Ratio ($\phi$)

- 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

![Graph showing spectral intensity and mean intensity over wavelength. Peaks indicate CO₂ and H₂O gas bands.](image-url)
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

Siemens
Westinghouse
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
Non-Homogeneous Fields

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