Absolute gas thermometry using IR emission spectroscopy

Ared Cezairliyan Best Paper Award of the Int. Journal of Thermophysics

27 November 2020

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Radiative Transfer in 1D uniform T case:

\[ I_\eta(\nu) = L(\nu) \varepsilon(\nu) \text{ or } I_\eta(\nu) = L(\nu) (1 - \exp(-k(\nu)L)) \]

- \( L(\nu) \) is Planck’s function
- \( k(\nu) \) is an (molecular) absorption coefficient
- \( L \) dimension
- \( \varepsilon(\nu) \) emissivity, if \( \varepsilon(\nu) = 1 \) then BB

Two “magic” wavelengths: 4.3 \( \mu \text{m} \) (2326 cm\(^{-1}\)) and 3.9 \( \mu \text{m} \) (2564 cm\(^{-1}\))

If \( 1 \ll k(\nu)L \) then \( I_\eta(\nu) \approx L(\nu) \) and

- CO\(_2\) band at 4.3 \( \mu \text{m} \) can be used for \( T_{\text{gas}} \) measurements

No “if” then (inverse) RHT equation should be solved with use of spectra modeling tools (HITEMP/HITRAN databases)

3.9 \( \mu \text{m} \) can be used for particles and/or surface temperature measurements (assuming some known \( \varepsilon(\nu) \))

Requires a calibration with a reference (calibrated) BB source

Detectors:
- 1D: (handheld) pyrometer or FTIR Spectrometer
- 2D: Imaging Camera (array) or Hyperspectral Imaging System

\( L \): from few cm to few m

“Gas” ↔ “Detector” distance: close or far-away

*IR* source*)

\( * \)BB, hot wall

**What is IR emission spectroscopy?**
**Why IR emission spectroscopy:**
- non-intrusive
- fast
- can be used for *in situ* process control
- can be realized in a *mid-price* range

**Where:**

Globally (broad spectral range):
- Gas and particle temperatures

Locally (narrow spectral range):
- Band-shapes P/T dependent
- Gas temperature

(Very) high price-range

(Very) low price-range
BUT:

Various optical emission spectroscopy methods need a validation with a known temperature and composition source traceable to ITS-90

The aims:

- to develop a portable flame temperature standard, calibrated via the Rayleigh scattering thermometry technique, traceable to ITS-90, with an uncertainty of 0.5 % of temperature ($k = 1$).
- to use standard flame for validation of
  - hyperspectral imaging FTIR spectrometer (2D species and temperature maps)
  - high-precision single line-of-sight FTIR spectrometer
The NPL portable standard flame

“Region of hot gas of known temperature and species”

The NPL standard flame:

- Hencken Burner – diffusion flamelets
- Propane / air flame – $0.8 < \phi < 1.4$
- Low uncertainty flowmeters - $U_r(\text{flow}) < 0.5\%$
- Known post flame composition
- Traceable to ITS-90
- Portable!
- Reproducible temperature - $U_r(\phi) = 0.5\%$

$$\phi = \frac{(V_{\text{fuel}}/V_{\text{air}})}{(V_{\text{fuel}}/V_{\text{air}})_{\text{stoichiometric}}}$$

Stoichiometric $\rightarrow$ fuel/air ratio for a balanced reaction (i.e. no excess oxygen)
Burner performance

Temperature profile example, $\phi = 1.0$
(Rayleigh scattering: point measurements)

- Flame is flat over +/- 10 mm region
- Knowledge of the profile useful for line of sight techniques

Green – HAB = 10 mm
Blue – HAB = 20 mm
Red – HAB = 30 mm

HAB = Height Above Burner
Temperature uncertainty

Table A1 Uncertainty budget for the temperature 20 mm above the centre of the NPL STD flame.

<table>
<thead>
<tr>
<th>Source</th>
<th>Type</th>
<th>Distr.</th>
<th>Size / ± %</th>
<th>Multiplier</th>
<th>Sensitivity Coefficient</th>
<th>Size (1σ) / %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molar refractivity data</td>
<td>B</td>
<td>Rect</td>
<td>0.20</td>
<td>0.58</td>
<td>1.00</td>
<td>0.12</td>
</tr>
<tr>
<td>Flow-meter uncertainty</td>
<td>B</td>
<td>Rect</td>
<td>1.00</td>
<td>0.58</td>
<td>0.40</td>
<td>0.23</td>
</tr>
<tr>
<td>Chemical equilibrium assumption</td>
<td>B</td>
<td>Rect</td>
<td>0.30</td>
<td>0.58</td>
<td>1.00</td>
<td>0.17</td>
</tr>
<tr>
<td>Air calibration PRT</td>
<td>A</td>
<td>Norm</td>
<td>0.05</td>
<td>1.00</td>
<td>1.00</td>
<td>0.05</td>
</tr>
<tr>
<td>Background scattered signal</td>
<td>A</td>
<td>Norm</td>
<td>0.10</td>
<td>1.00</td>
<td>0.50</td>
<td>0.05</td>
</tr>
<tr>
<td>Laser stability</td>
<td>A</td>
<td>Norm</td>
<td>0.20</td>
<td>1.00</td>
<td>1.00</td>
<td>0.20</td>
</tr>
<tr>
<td>Inlet air temperature (15-25 °C)</td>
<td>B</td>
<td>Rect</td>
<td>3.00</td>
<td>0.58</td>
<td>0.10</td>
<td>0.17</td>
</tr>
<tr>
<td>Atmospheric pressure</td>
<td>B</td>
<td>Rect</td>
<td>5.00</td>
<td>0.58</td>
<td>0.05</td>
<td>0.15</td>
</tr>
<tr>
<td>Gas purity</td>
<td>B</td>
<td>Rect</td>
<td>2.50</td>
<td>0.58</td>
<td>0.05</td>
<td>0.07</td>
</tr>
<tr>
<td>Flame temperature reproducibility</td>
<td>A</td>
<td>Norm</td>
<td>0.20</td>
<td>1.00</td>
<td>1.00</td>
<td>0.20</td>
</tr>
</tbody>
</table>

Total uncertainty (combined in quadrature)

- Long term stability = 0.2 % of T
- Combined uncertainty (k=1) = 0.5 % of T
European project to enhance process efficiency through improved temperature measurement:

- STD flame calibrated at NPL
- Partner organisations – developing novel optical combustion thermometers

- STD flame – circulated to partners
- Comparison of techniques – publication
- NPL facility available for others

IR spectroscopy

Portable STD Flame Rayleigh scattering

IR hyperspectral imaging

DFWM / LIGS

EMRESS - Enhancing Process Efficiency through Improved Temperature Measurement:
http://journals.sagepub.com/doi/pdf/10.1177/0020294016656892
**Hyper-spectral IR imaging at UC3M**

FTIR Hyperspectral Imaging System

- Operates in the MIR (2 \(\mu m\) to 5.5 \(\mu m\))
- Michelson interferometer, coupled to an InSb focal plane array (320 x 256 pixels)
- Similar to FTIR spectrometer but provides 2D maps of species and temperature
- Measures the emitted power from the CO\(_2\), CO and H\(_2\)O bands (post flame region)
- Comparison with HITEMP-2010 synthesised spectra \(\rightarrow\) determine the flame temperature
Hyper-spectral IR imaging: data analysis and modelling
Example measurement and spectral fit

- Model accounts for absorption in the ambient air
- Temperature profile assumed to be ‘top-hat’ (out of the page)
- Good agreement between measured and synthesised spectra
Measurements on the NPL STD flame

- $\phi = 1.0$, propane/air flame
- Temperature, CO$_2$ and CO are measured

<table>
<thead>
<tr>
<th>Visible image</th>
<th>Temperature (K)</th>
<th>CO$_2$ (ppm.m)</th>
<th>CO (ppm.m)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>2500</td>
<td>4000</td>
<td>1200</td>
</tr>
<tr>
<td></td>
<td>2000</td>
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<td>1200</td>
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</tr>
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<td></td>
<td>1000</td>
<td>4000</td>
<td>1200</td>
</tr>
</tbody>
</table>

**UC3M vs NPL**

$\phi = 1.0$, HAB = **20 mm**
Precision IR emission spectroscopy

Measurement configuration

STD flame installed at DTU

NPL STD flame

N2 purged system

Al-coated 60deg off-axis mirror

Au-coated flat mirror

FTIR spectrometer
Measurement principle

• The flame spectral intensity at wavenumber $\eta$ measured at $L$ is given by:

$$I(\eta) = \int_0^L \kappa \eta I_{B\eta}(T) e^{-\int_s^L \kappa \eta ds'} ds$$

• Where:
  • $I_{B\eta}(T)$ is the Planck function
  • $\kappa \eta$ is the spectral absorption coefficient

Determining the temperature profile

• Measure the emission spectra
• Estimate temperature profile $T_{est}(s)$ and calculate $\kappa \eta$ from HITEMP2010
• Synthesise the emission spectra
• Minimise the differences between the two
• Determine the true temperature profile $T_{true}(s)$

Assumed to be a smooth symmetric or asymmetric function
Validation of HITEMP spectral database

Modelled spectra agree very well with measured

Differences between measured/modelled:

- $\text{H}_2\text{O}/\text{CO (1500-2000cm}\text{-}^1) = 0.63\%$
- $\text{CO}_2/\text{CO (2160-2400cm}\text{-}^1) = -0.17\%$
- CO$_2$ band is most sensitive to $T(x)$ profile
- H$_2$O band is less sensitive

An overall excellent agreement

No CO$_2$ self-absorption (ambient air)
Verification of NPL temperature profiles

- NPL temperature profile is input parameter for modelled HITEMP2010 spectra
- NPL profile has been improved
- Example 2: $\phi = 0.8$, HAB = 20 mm

**Spectra ($\phi = 0.8$)**

**Temperature profile ($\phi = 0.8$)**
Inspired by industry: NOx reduction in SNCR systems

NOx Selective Non-Catalytic Reduction (SNCR) on power plants and waste incinerators:

- Narrow temperature range (nature of the process): \( \text{NH}_3 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O} \)
- Ammonia/urea consumption optimization (costs)
- NOx high-efficiency removal (environment, pollution)
- Accurate \textit{in situ} \( T_{\text{gas}} \) measurements is a must
- 2D temperature profiles with a sweeping technique (several line-of-sights measurements combined in 2D plot)
- Fast T-profiles retrievals
- Possibility for a “moderate” system cost
- Only 1x access point

From Bernd von der Heide (2008), Mehldau & Steinfath Umwelttechnik GmbH
Multi-Layer Perceptron

\[ I(\eta) = I_0 \eta e^{-\int_0^L \kappa_d ds} + \int_0^L \kappa_\eta I_0 \eta e^{-\int_0^L \kappa_d ds} \, ds \]


**Contents lists available at ScienceDirect**

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Machine learning applied to retrieval of temperature and concentration distributions from infrared emission measurements

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Predicted mean temperatures within 10 mm from the center of the burner differ by

- $\phi = 1$: 0.23%
- $\phi = 0.8$: -0.21%
- $\phi = 1.4$: 1.88%

from the measured temperatures.

Target: an overall temperature uncertainty below 0.5 %
In Situ measurements at a waste incinerator

Challenges:

- Keep optics clean (CO₂ self-absorption)
- HITEMP2010 “weak” line intensities become “strong” at long L (10 m)
- Reference CO₂/H₂O high-T spectra can be in house measured
- There are (natural) temporal T_gas-variations due to turbulence (from ± 20 °C to ± 60 °C)
  - 1% from 1000°C is 10°C (∆T = 50 °C window for SNCR)
Conclusions

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Acknowledgements:

These projects have received funding from the EMPIR programme co-financed by the Participating States and from the European Union’s Horizon 2020 research and innovation programme.