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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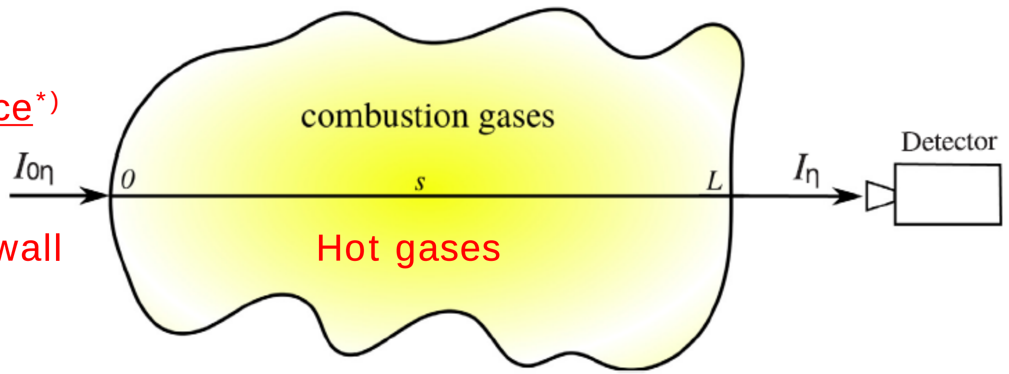
What is IR emission spectroscopy?

(IR) source*)

*)BB, hot wall



Detector:

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

Radiative Transfer in 1D uniform T case:

$$I_\eta(v) = L(v)\ \varepsilon(v)\ or$$

$$I_\eta(v) = L(v)\ (1 - \exp(-k(v)L)$$

- $L(v)$ is Planck's function
- $k(v)$ is an (molecular) absorption coefficient
- L dimention
- $\varepsilon(v)$ emissivity, if $\varepsilon(v)$ = 1 then BB

Two "magic" wavelengths: 4.3 μm (2326 cm^{-1}) and 3.9 μm (2564 cm^{-1})

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

- CO_2 band at 4.3 μm can be used for T_{gas} measurements

No "if" then (inverse) RHT equation should be solved with use spectra modeling tools (HITEM/HITRAN databases)

3.9 μm can be used for particles and/or surface temperature measurements (assuming some known $\varepsilon(v)$)

Requires a calibration with a reference (calibrated) BB source

Why IR emission spectroscopy:

- ✓ non-intrusive
- ✓ fast
- ✓ can be used for *in situ* process control
- ✓ can be realized in a *mid-price* range

Where:

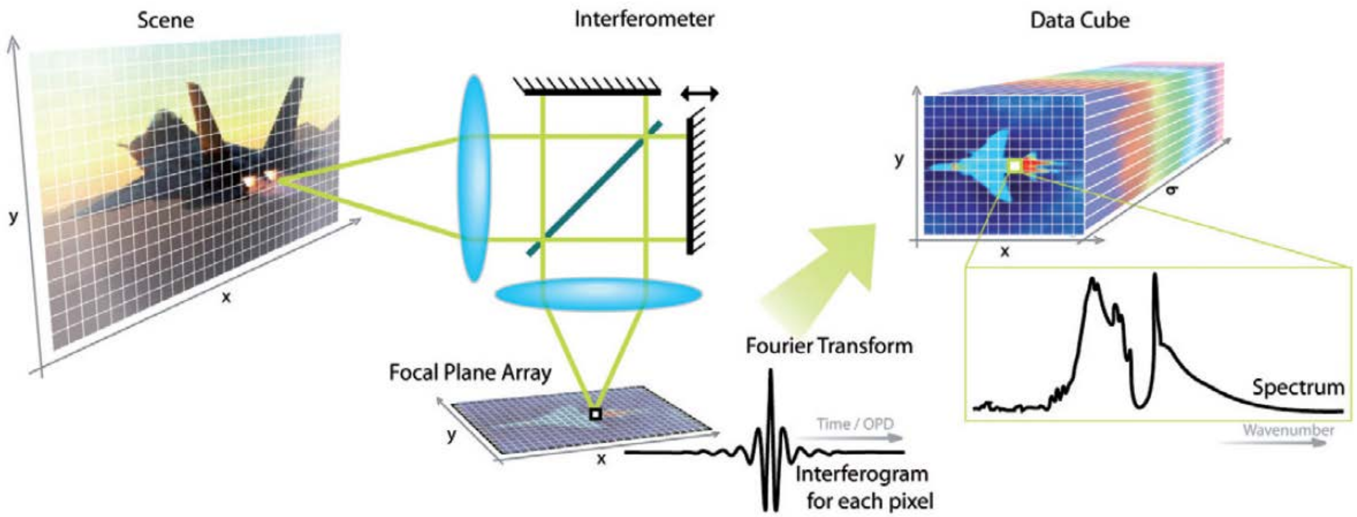
Globally (broad spectral range):

- ➢ Gas and particle temperatures

Locally (narrow spectral range):

- ❑ Band-shapes P/T dependent
- ➢ Gas temperature

(Very) high price-range



(Very) low price-range

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BUT:

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

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https://doi.org/10.1007/s10765-019-2557-6

Check for updates

Validation of Emission Spectroscopy Gas Temperature Measurements Using a Standard Flame Traceable to the International Temperature Scale of 1990 (ITS-90)

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Received: 30 November 2018 / Accepted: 9 October 2019

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

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The NPL portable standard flame

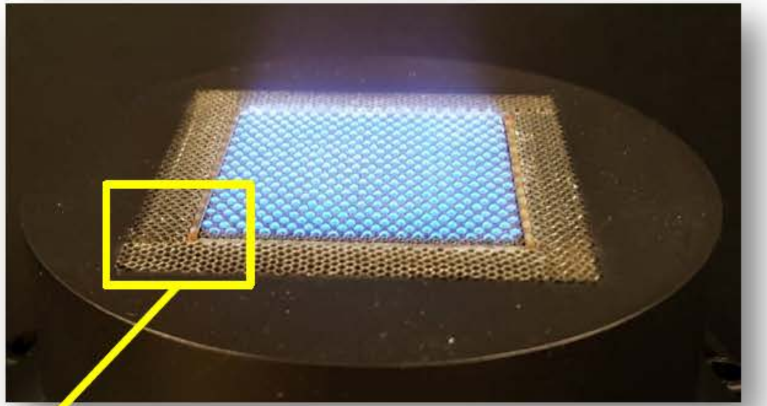
"Region of hot gas of known temperature and species"

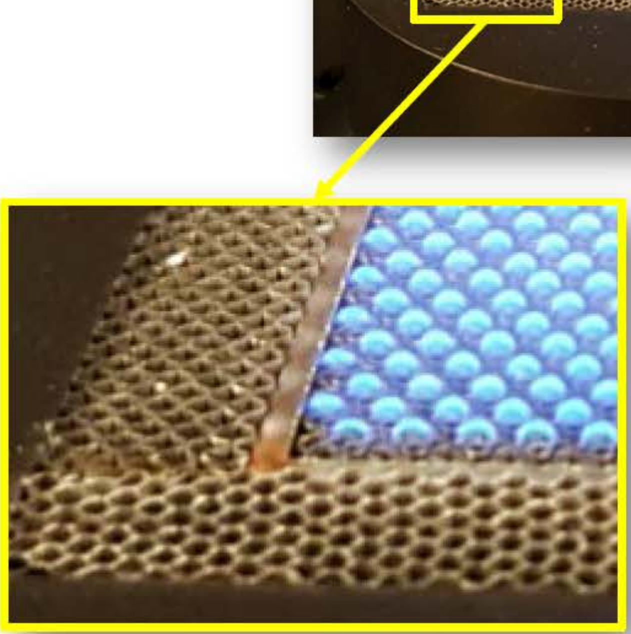
The NPL standard flame:

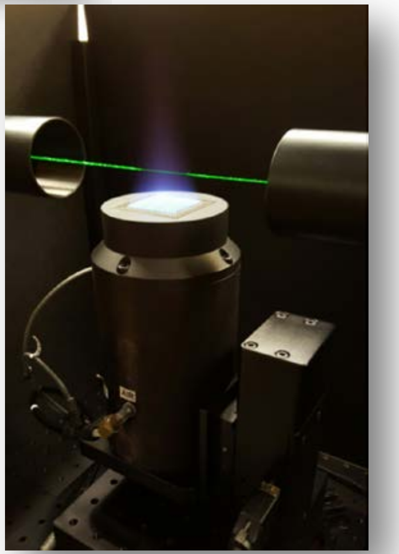
- Hencken Burner – diffusion flamelets
- Propane / air flame – $\{0.8 < \phi < 1.4\}$
- Low uncertainty flowmeters - $U_r(flow) < 0.5\%$
- Known post flame composition
- Traceable to ITS-90
- Portable!
- Reproducible temperature - $U_r(\phi) = 0.5\%$

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

Stoichiometric → fuel/air ratio for a balanced reaction (i.e. no excess oxygen)

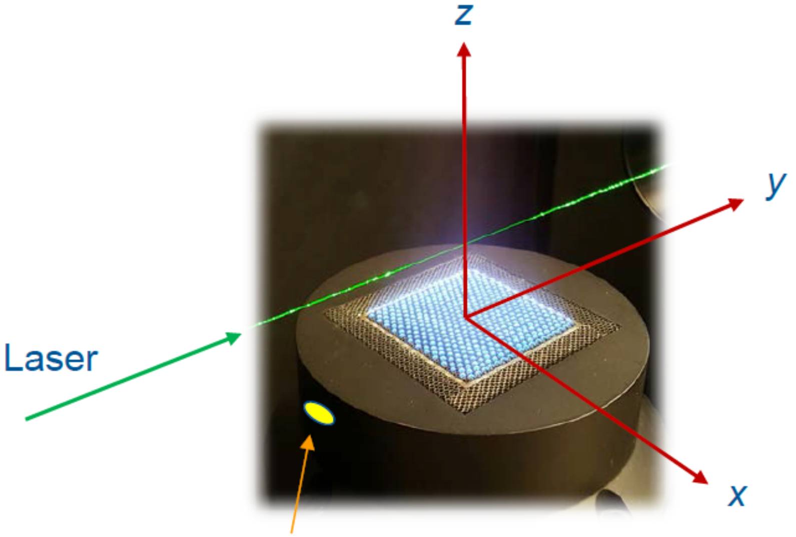






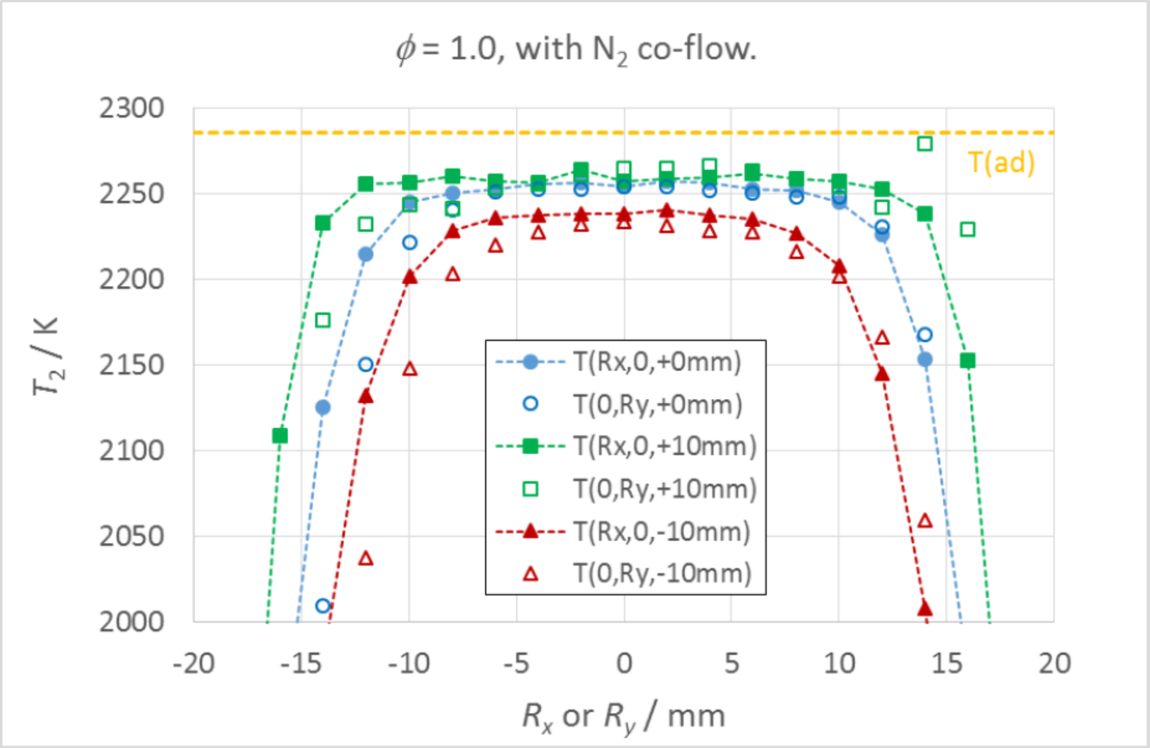
Burner performance

Temperature profile example, ϕ = 1.0
(Rayleigh scattering: point measurements)



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

Dotted Lines/symbols - x-profile
Symbols only - y-profile



HAB = Height Above Burner

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

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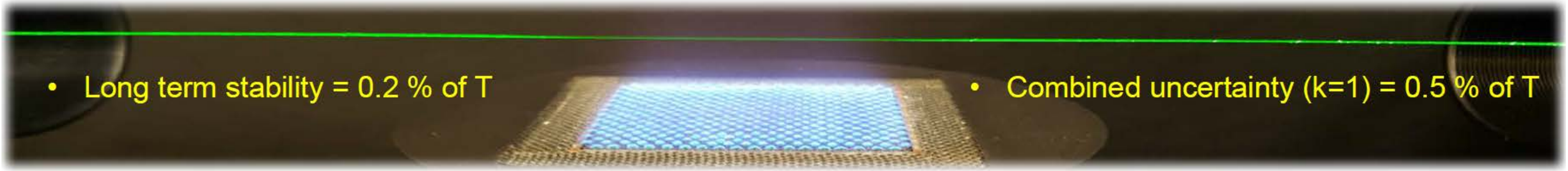
Temperature uncertainty

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

Source	Type	Distr.	Size / ± %	Multiplier	Sensitivity Coefficient	Size (1σ) / %
Molar refractivity data	B	Rect	0.20	0.58	1.00	0.12
Flow-meter uncertainty	B	Rect	1.00	0.58	0.40	0.23
Chemical equilibrium assumption	B	Rect	0.30	0.58	1.00	0.17
Air calibration PRT	A	Norm	0.05	1.00	1.00	0.05
Background scattered signal	A	Norm	0.10	1.00	0.50	0.05
Laser stability	A	Norm	0.20	1.00	1.00	0.20
Inlet air temperature (15-25 °C)	B	Rect	3.00	0.58	0.10	0.17
Atmospheric pressure	B	Rect	5.00	0.58	0.05	0.15
Gas purity	B	Rect	2.50	0.58	0.05	0.07
Flame temperature reproducibility	A	Norm	0.20	1.00	1.00	0.20
Total uncertainty (combined in quadrature)						**0.5 %**



NPL National Physical Laboratory

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

Portable STD Flame Rayleigh scattering (NPL)

- Technical University of Denmark (DTU): IR spectroscopy
- University of Oxford: DFWM / LIGS
- Universidad Carlos III de Madrid; Centro Español de Metrología (CEM): IR hyperspectral imaging

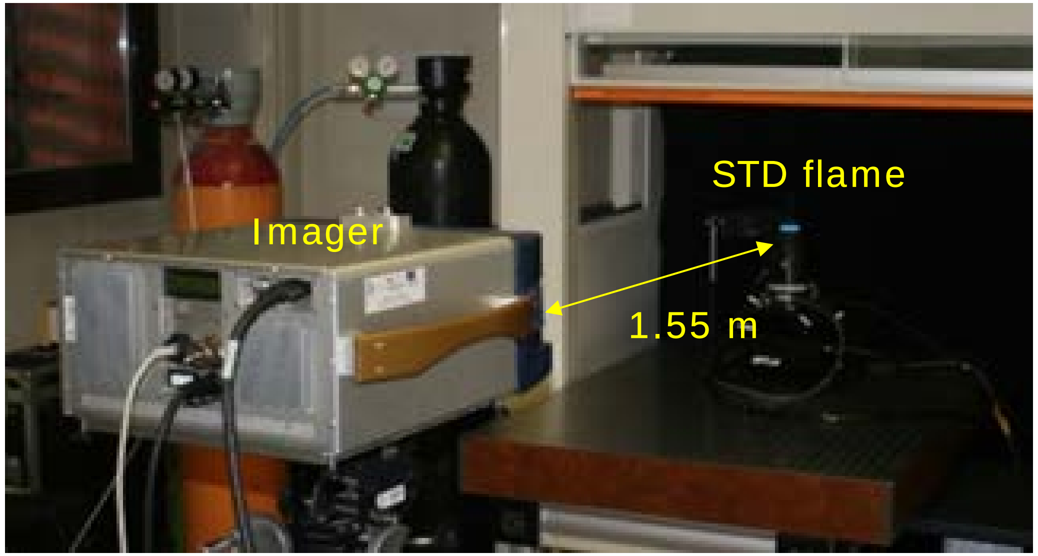
EMPRESS - Enhancing Process Efficiency through Improved Temperature Measurement: http://journals.sagepub.com/doi/pdf/10.1177/0020294016656892

Hyper-spectral IR imaging at UC3M

FTIR Hyperspectral Imaging System

- ✓ Operates in the MIR (2 μm to 5.5 μm)
- ✓ 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_2O bands (post flame region)
- ✓ Comparison with HITEMP-2010 synthesised spectra → determine the flame temperature

Hyper-spectral imager measuring the NPL STD flame



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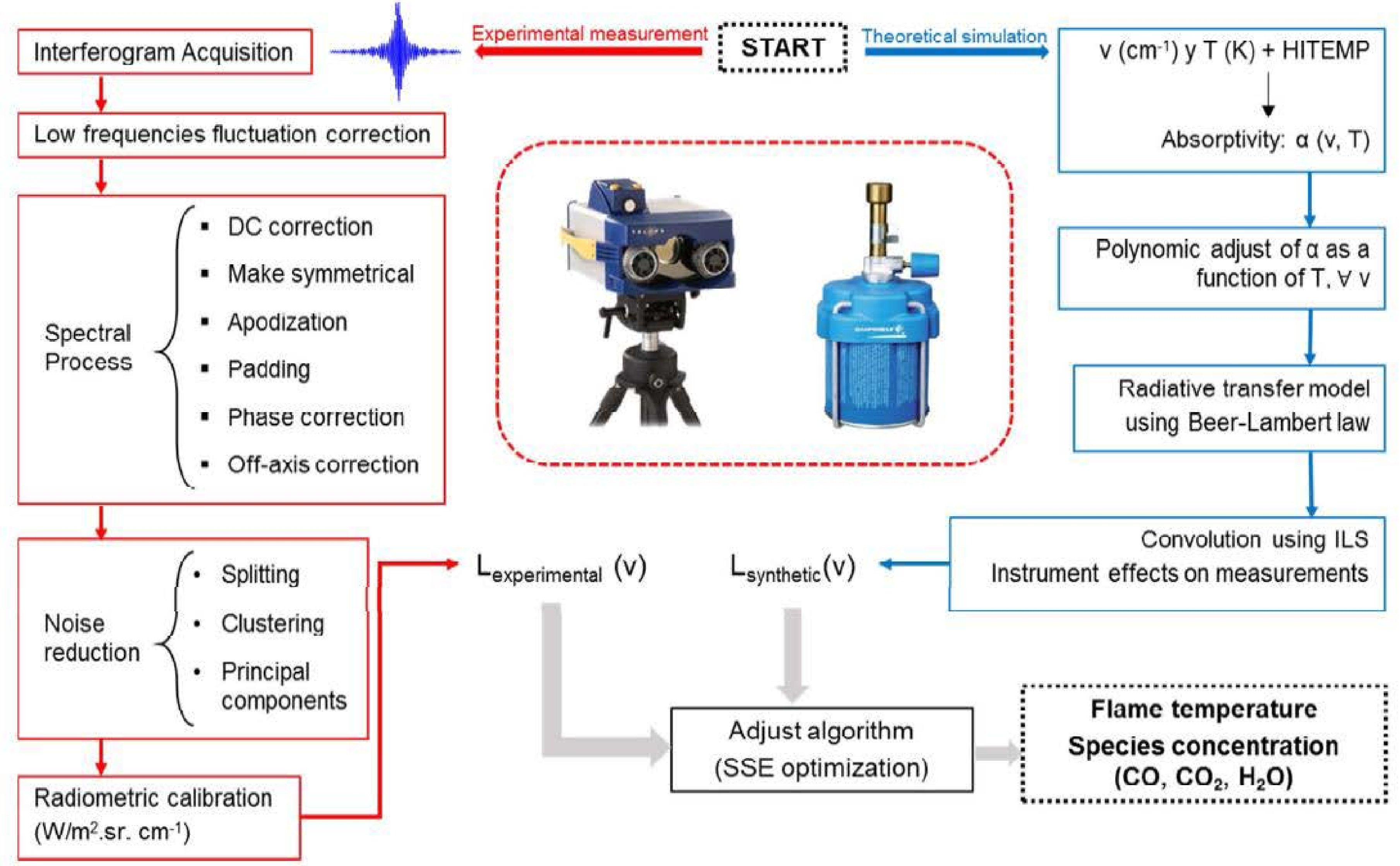
Hyper-spectral IR imaging: data analysis and modelling



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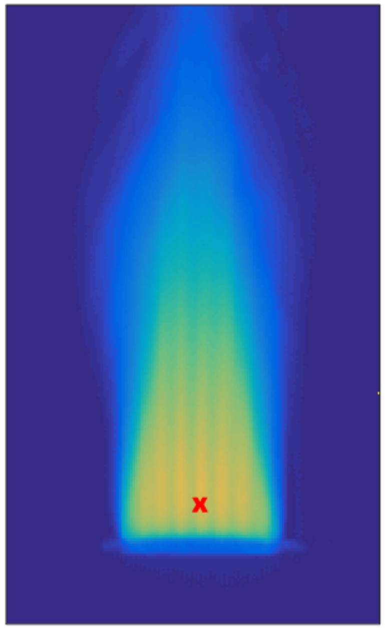
Example measurement and spectral fit

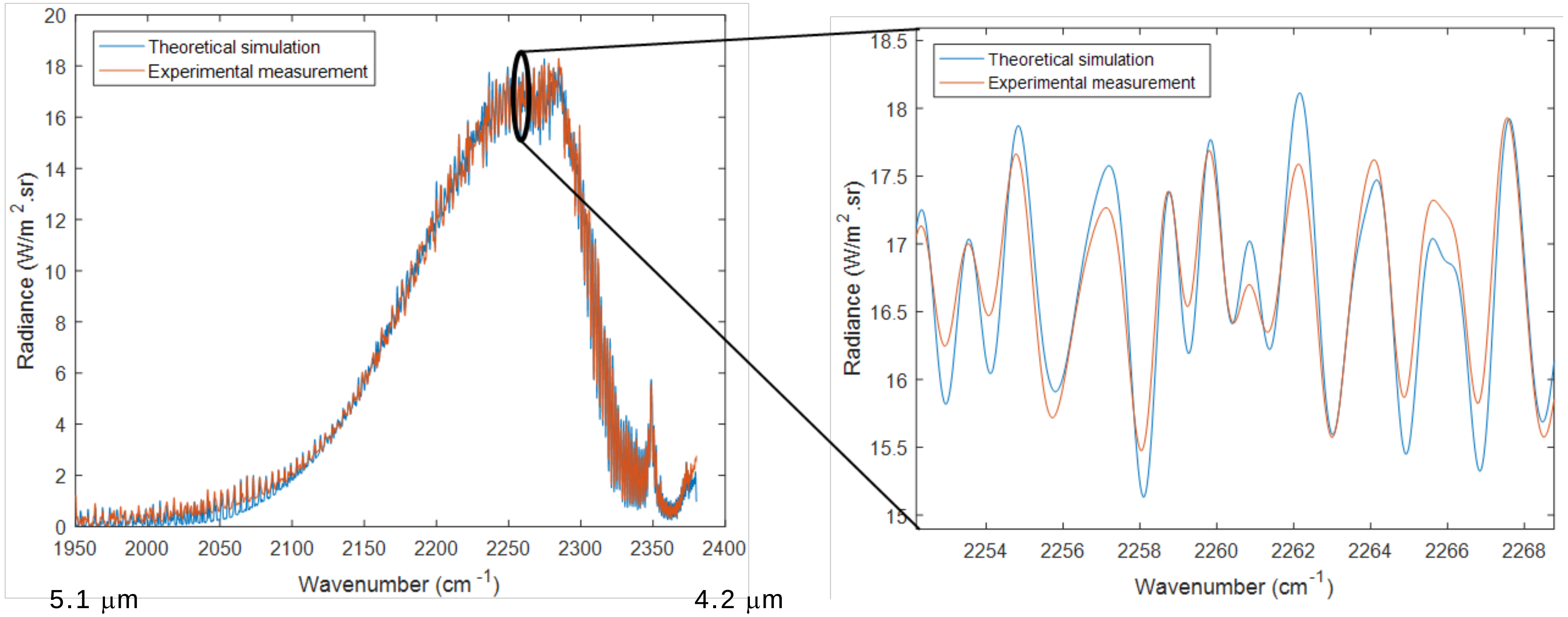
- Model accounts for absorption in the ambient air
- Temperature profile assumed to be ‘top-hat’ (out of the page)
- Good agreement between measured and synthesised spectra

Radiance image of STD flame



Measured and best fit simulated spectra at x

Close-up of spectral region around 2250 cm^{-1}



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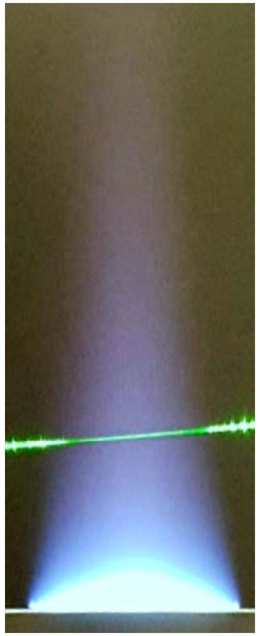
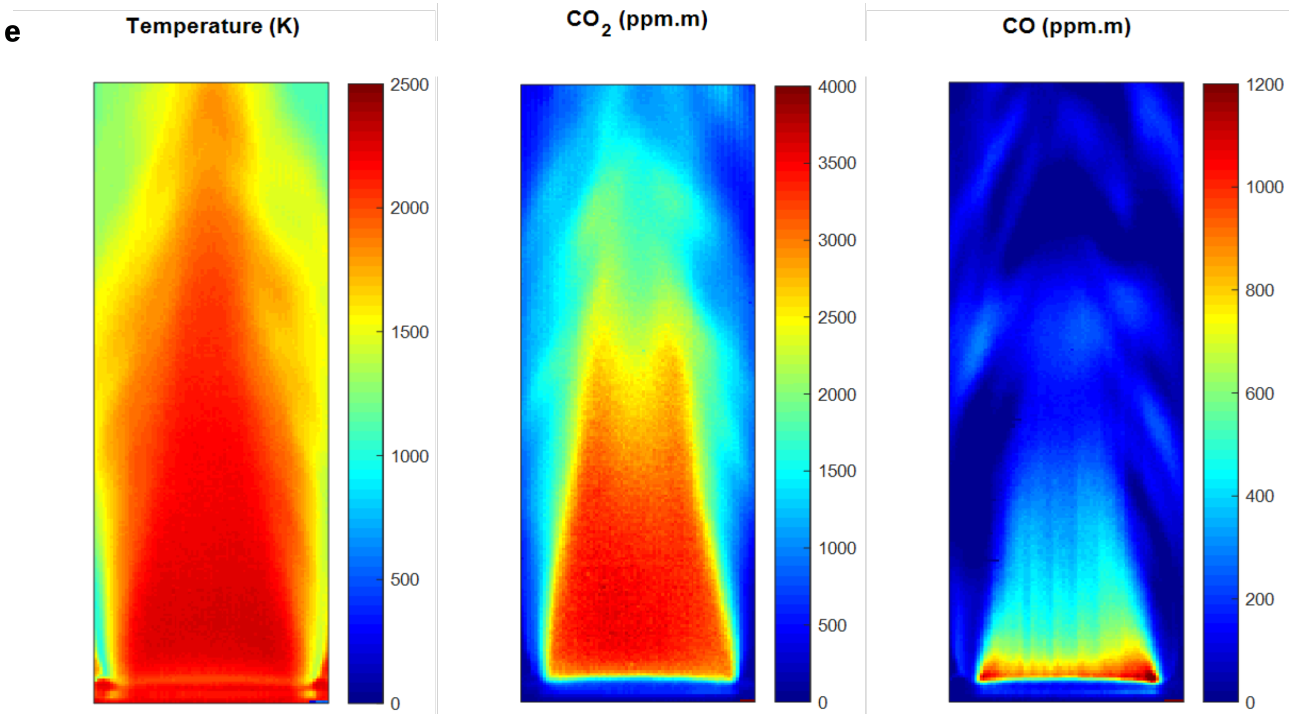
Measurements on the NPL STD flame

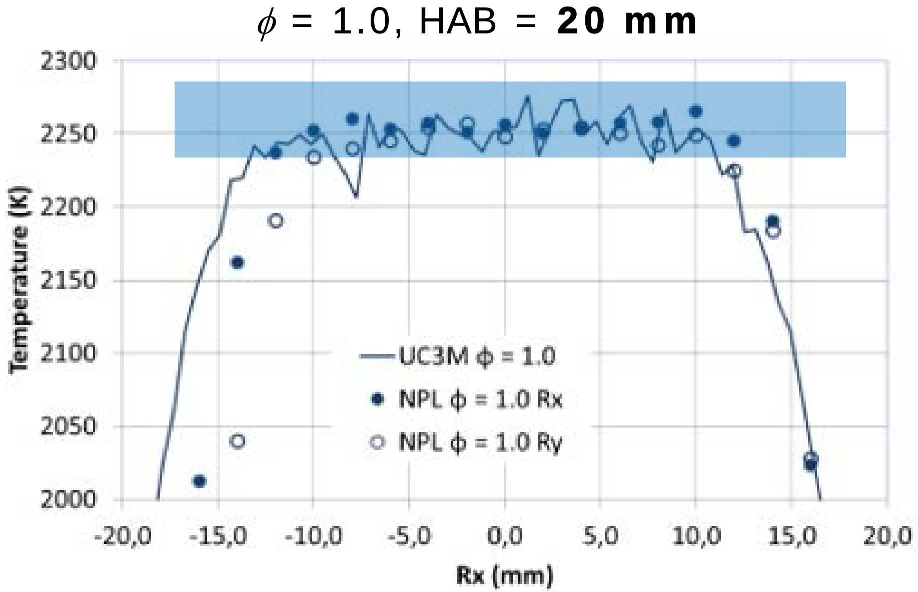
- ϕ = 1.0, propane/air flame
- Temperature, CO_2 and CO are measured

Visible image





UC3M vs NPL



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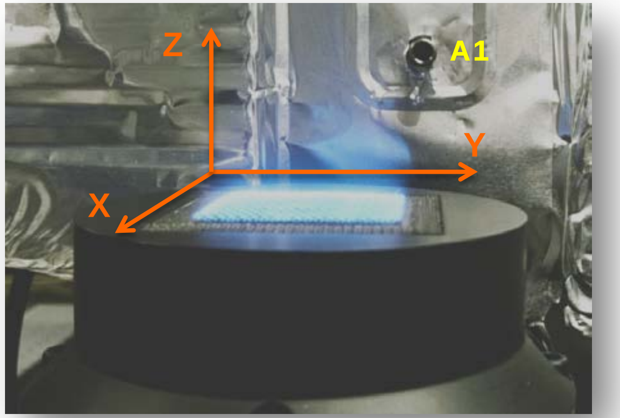
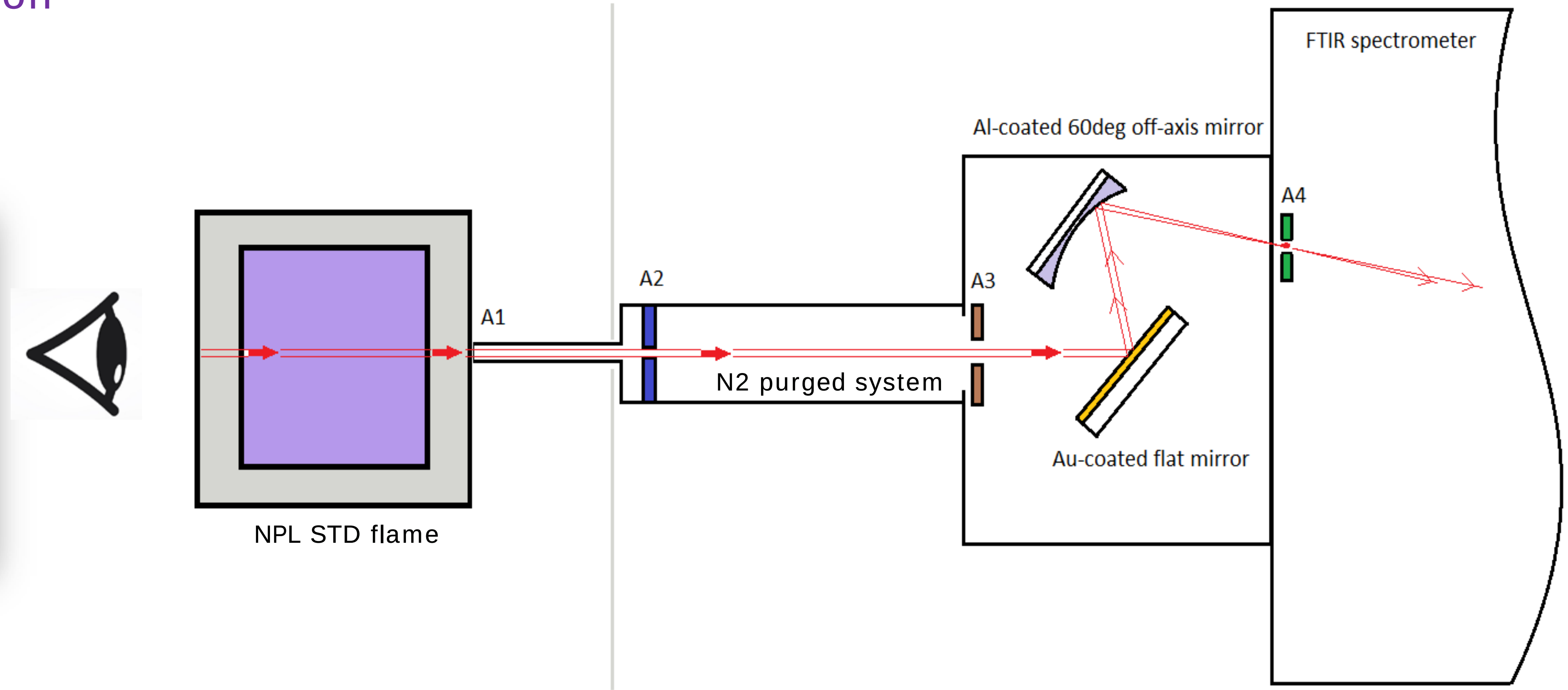
Precision IR emission spectroscopy

Measurement configuration

STD flame installed at DTU



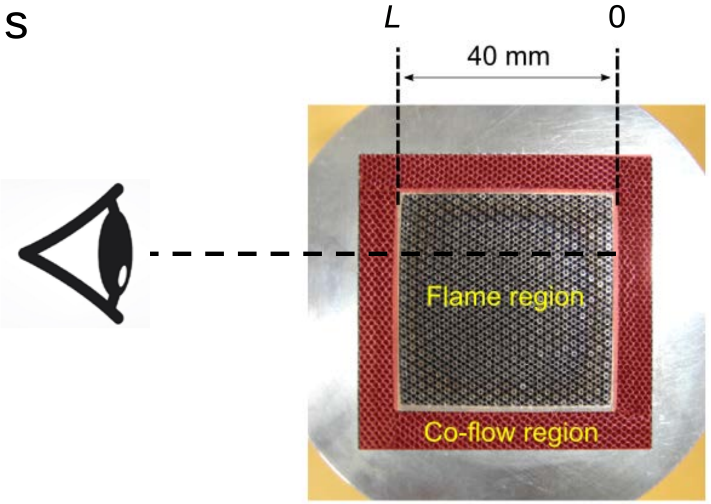


Measurement principle

- The flame spectral intensity at wavenumber η 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
  - κ_η is the spectral absorption coefficient



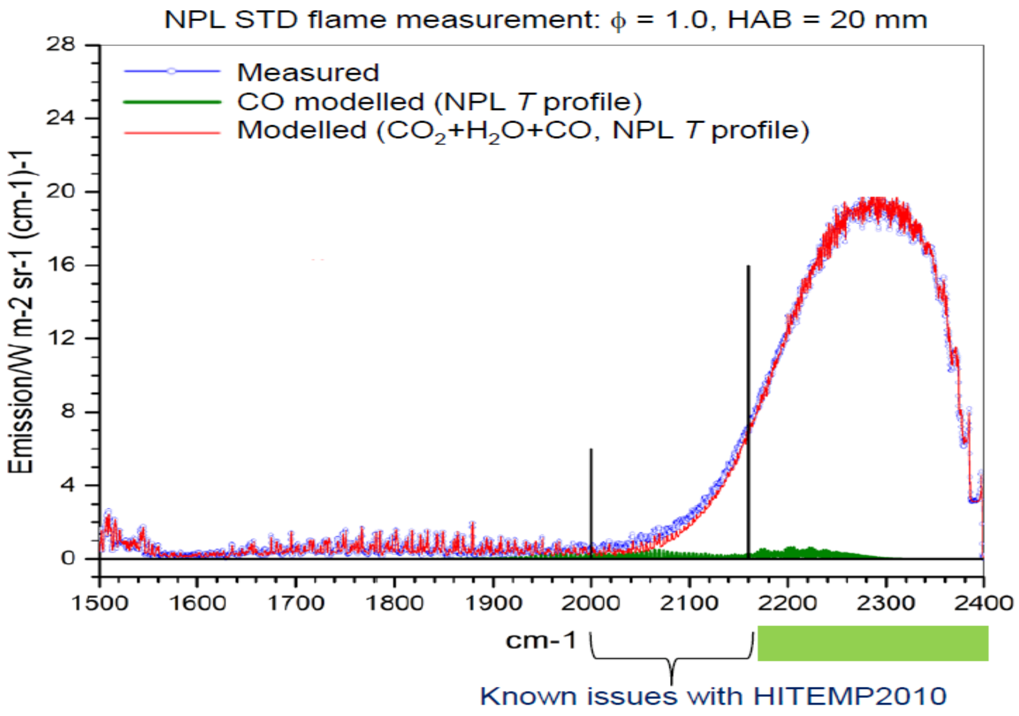
Determining the temperature profile

- Measure the emission spectra
- Estimate temperature profile $T_{est}(s)$ and calculate κ_η 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

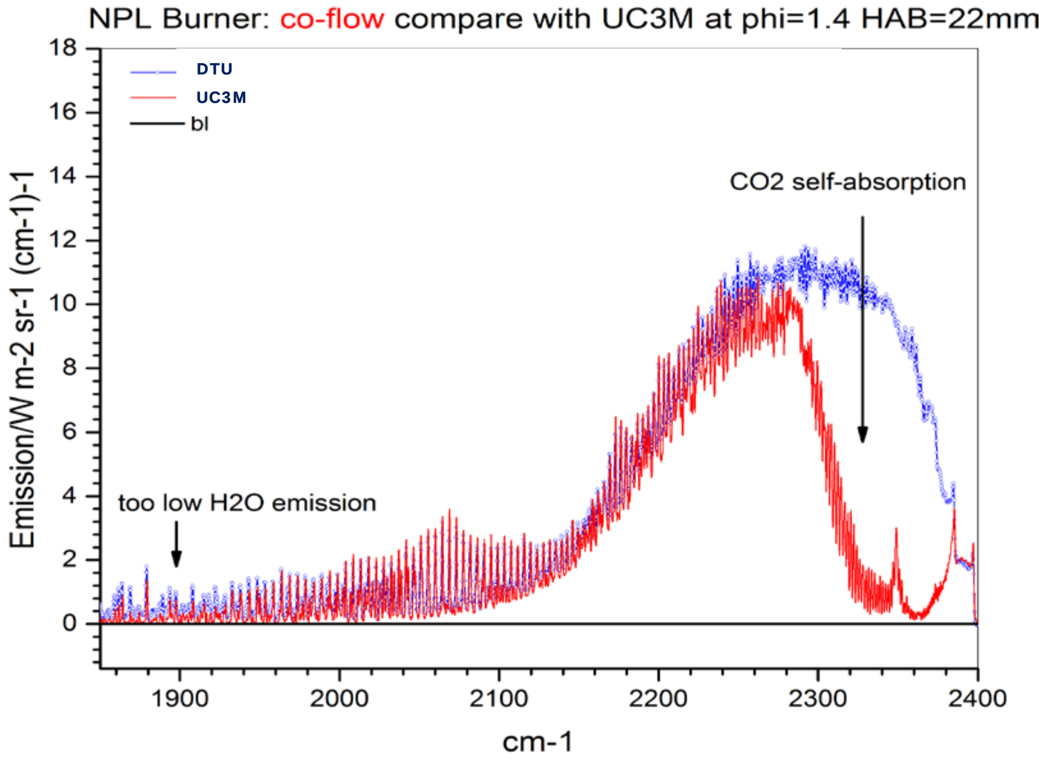


Modelled spectra agree very well with measured

Differences between measured/modelled:

- H_2O/CO (1500-2000cm^{-1}) = 0.63%
- CO_2/CO (2160-2400cm^{-1}) = -0.17%
- CO_2 band is most sensitive to $T(x)$ profile
- H_2O band is less sensitive

Comparison with Hyper-Spectral measurements

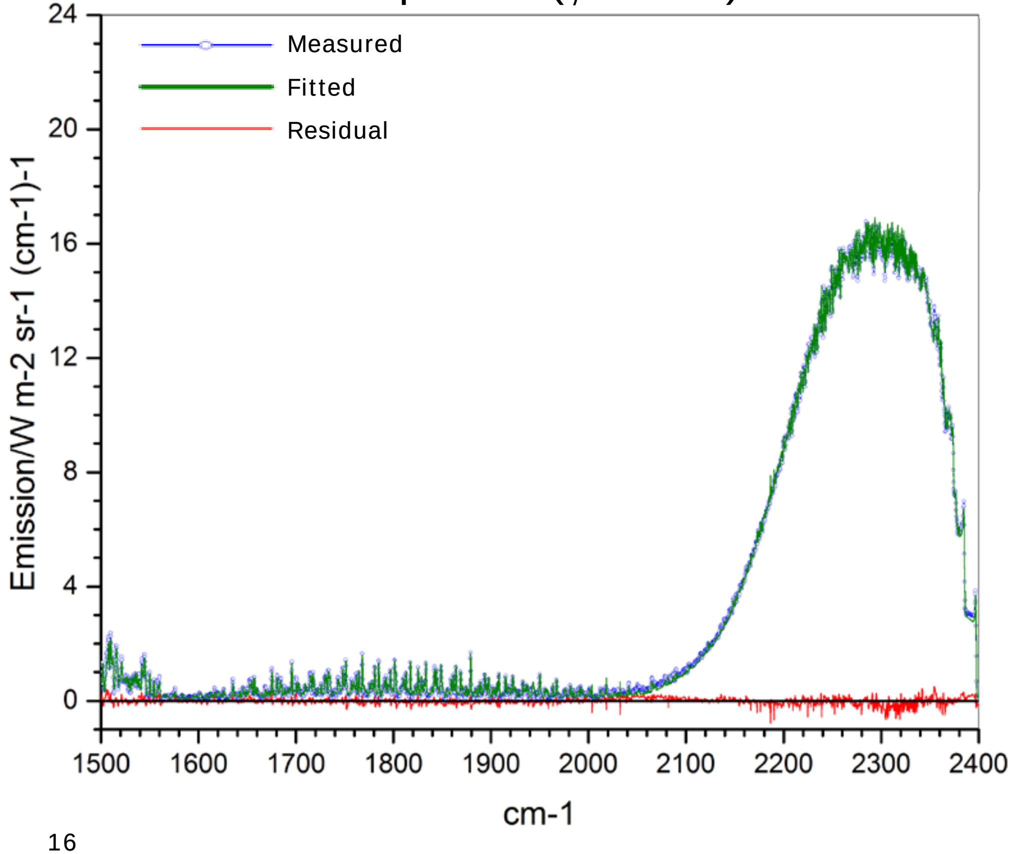


- An overall excellent agreement
- No CO_2 self-absorption (ambient air)

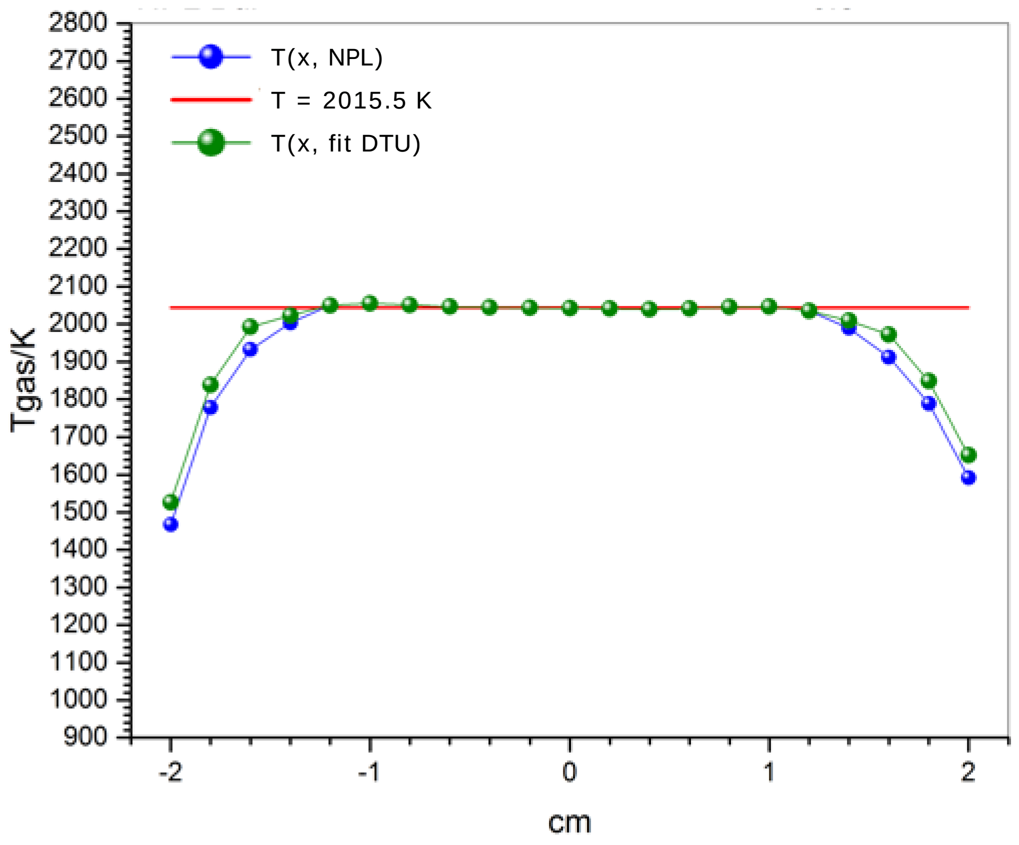
Verification of NPL temperature profiles

- NPL temperature profile is <u>input</u> parameter for modelled HITEMP2010 spectra
- NPL profile has been improved
- Example 2: ϕ = 0.8, HAB = 20 mm

Spectra (ϕ = 0.8)



Temperature profile (ϕ = 0.8)



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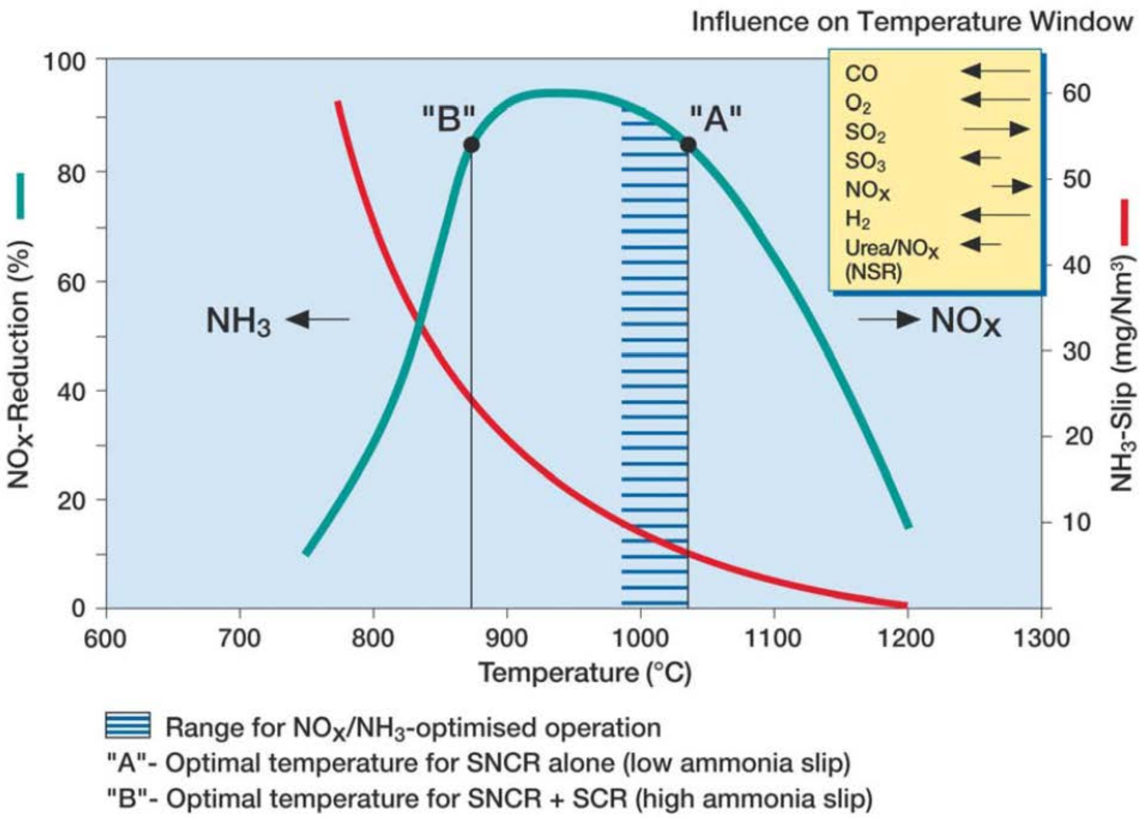
Inspired by industry: NOx reduction in SNCR systems



From Bernd von der Heide (2008), Mehldau & Steinfath Umwelttechnik GmbH

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

- Narrow temperature range (nature of the process): $NH_3 + NO \rightarrow N_2 + H_2O$
- Ammonia/urea consumption optimization (costs)
- NOx high-efficiency removal (environment, pollution)
- Accurate *in situ* T_{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

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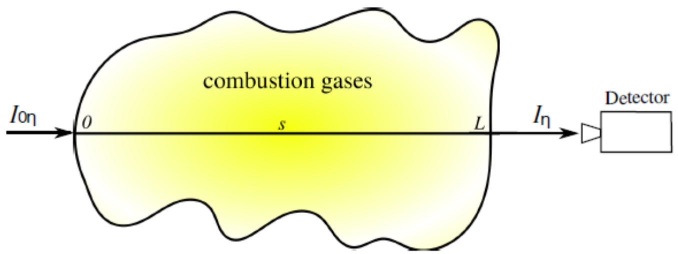
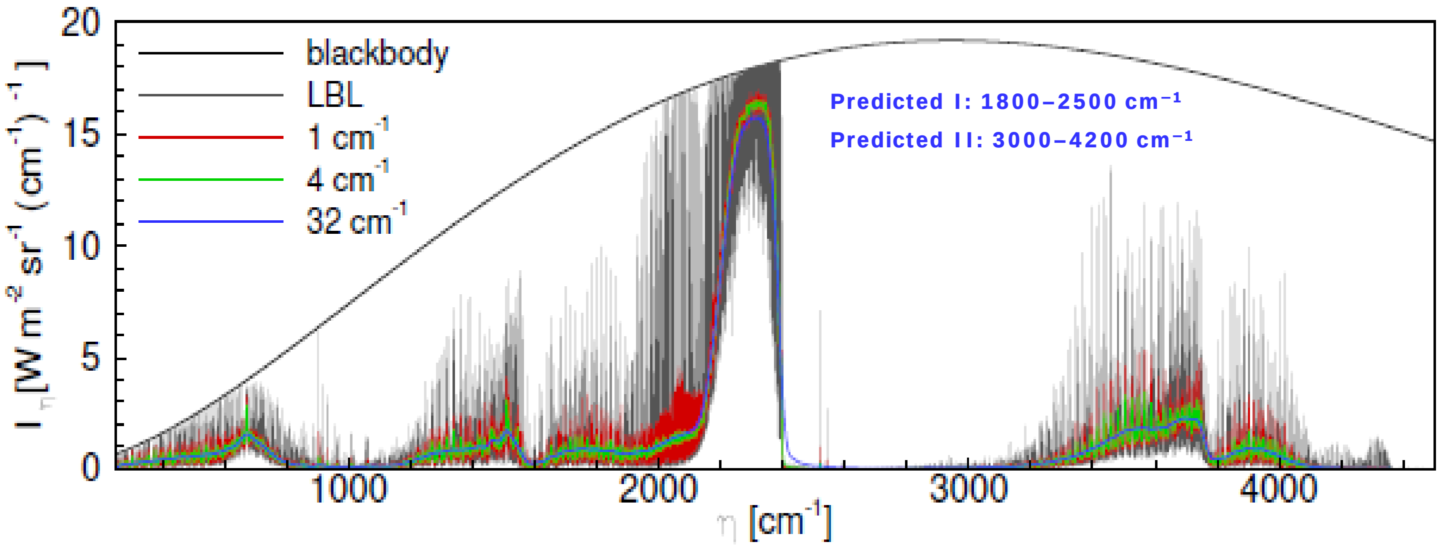
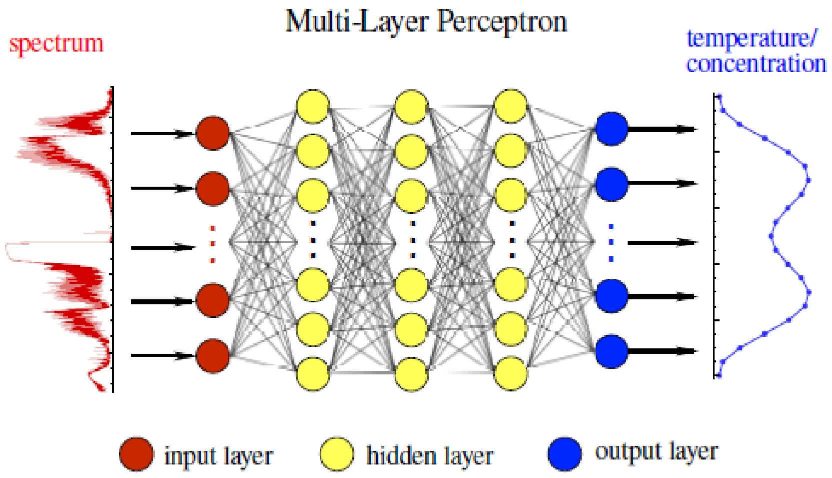
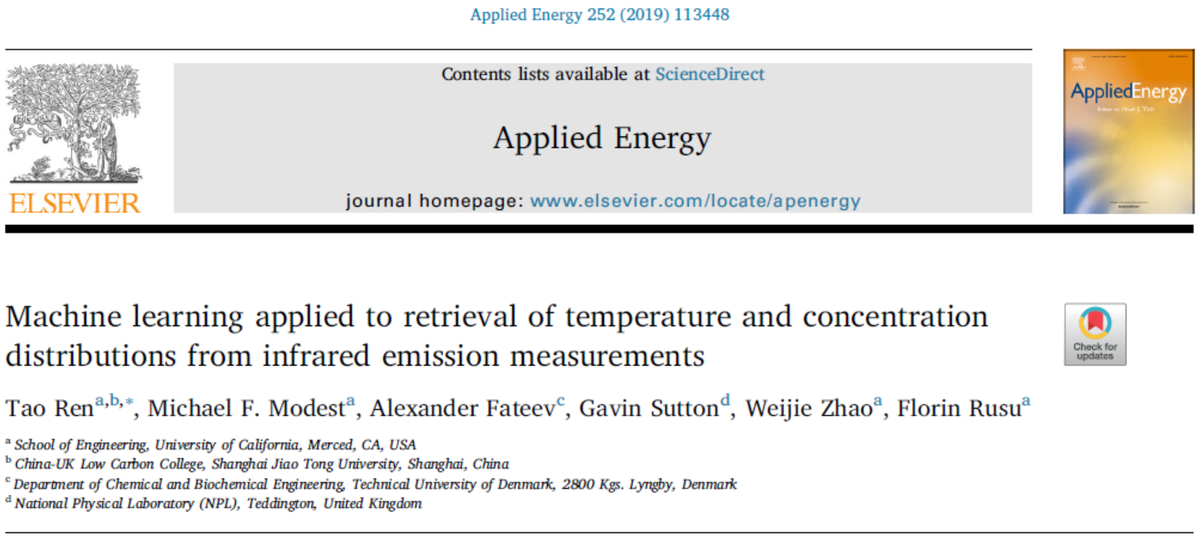


$$I(\eta) = I_{0\eta} e^{-\int_0^L \kappa_\eta ds} + \int_0^L \kappa_\eta I_{b\eta} e^{-\int_s^L \kappa_\eta ds'} ds$$



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

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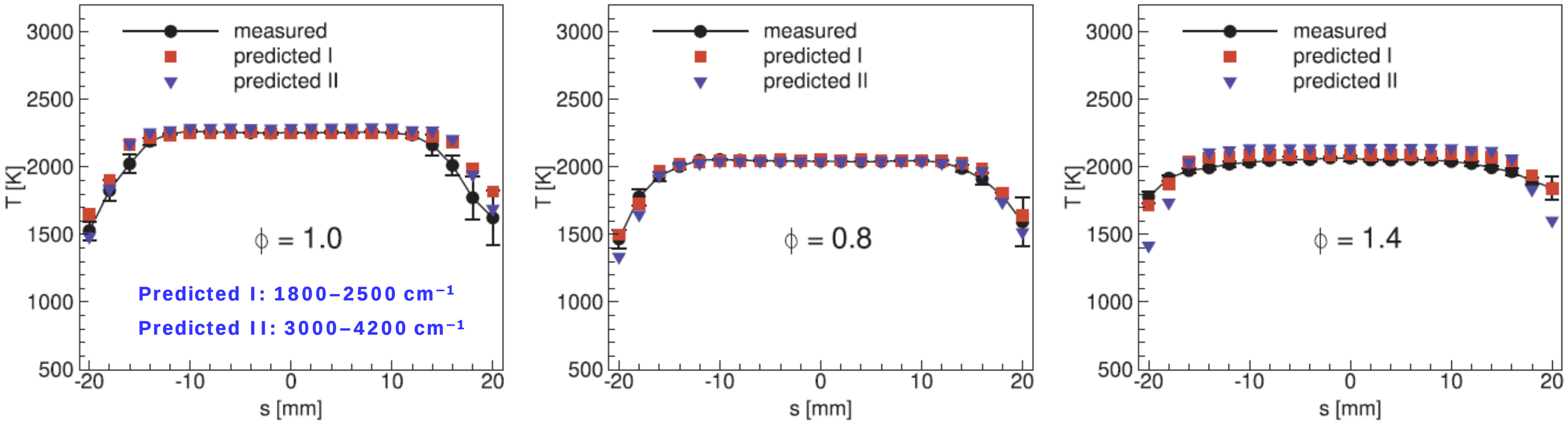
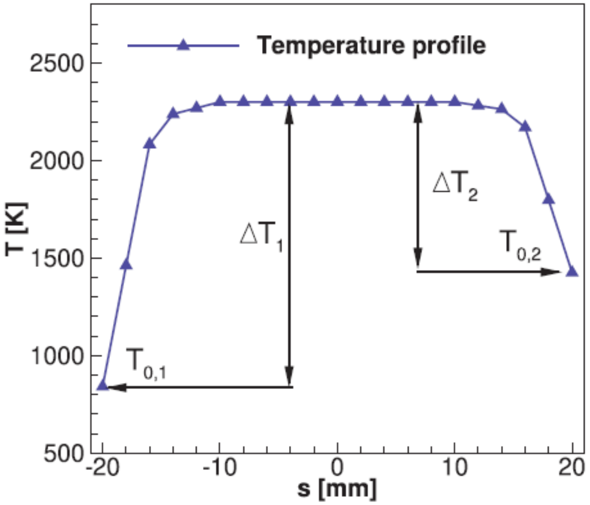
Machine learning approach for retrievals of temperature profiles





Example of temperature profile used for generating training data sets

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

- ϕ=1: 0.23%
- ϕ=0.8: −0.21%
- ϕ=1.4: 1.88%

from the measured temperatures.

Target: an overall temperature uncertainty below 0.5 %

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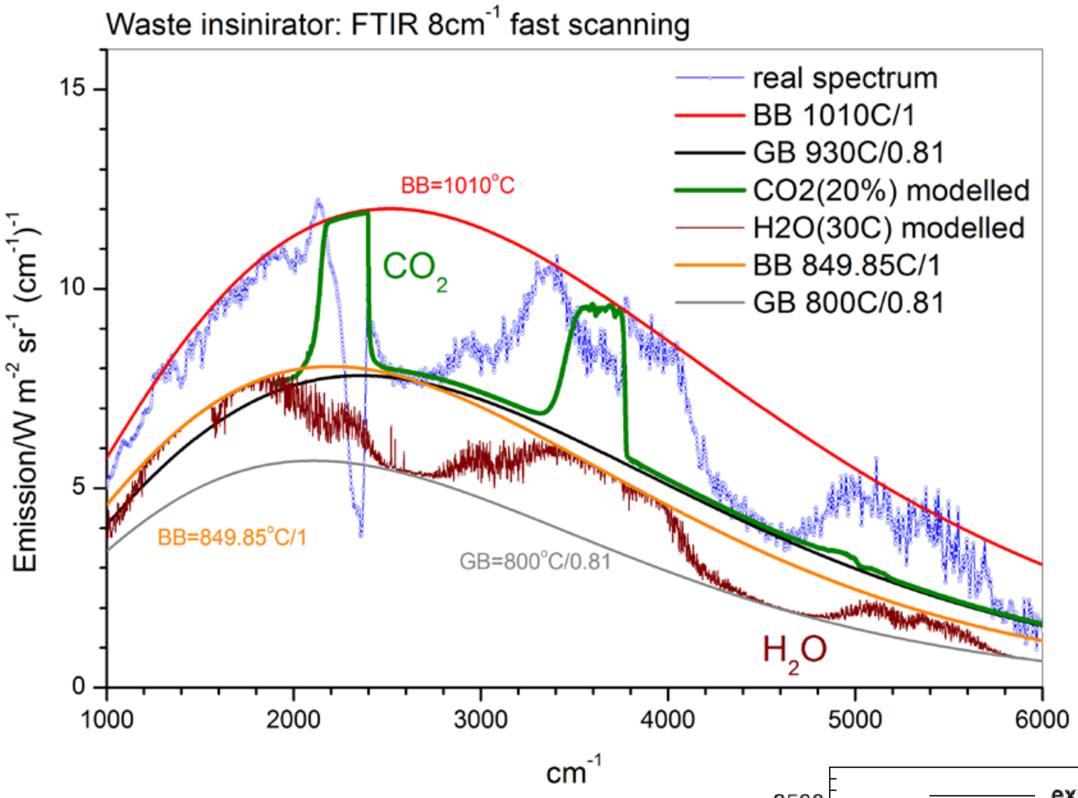
Waste insinirator: FTIR 8cm^{-1} fast scanning

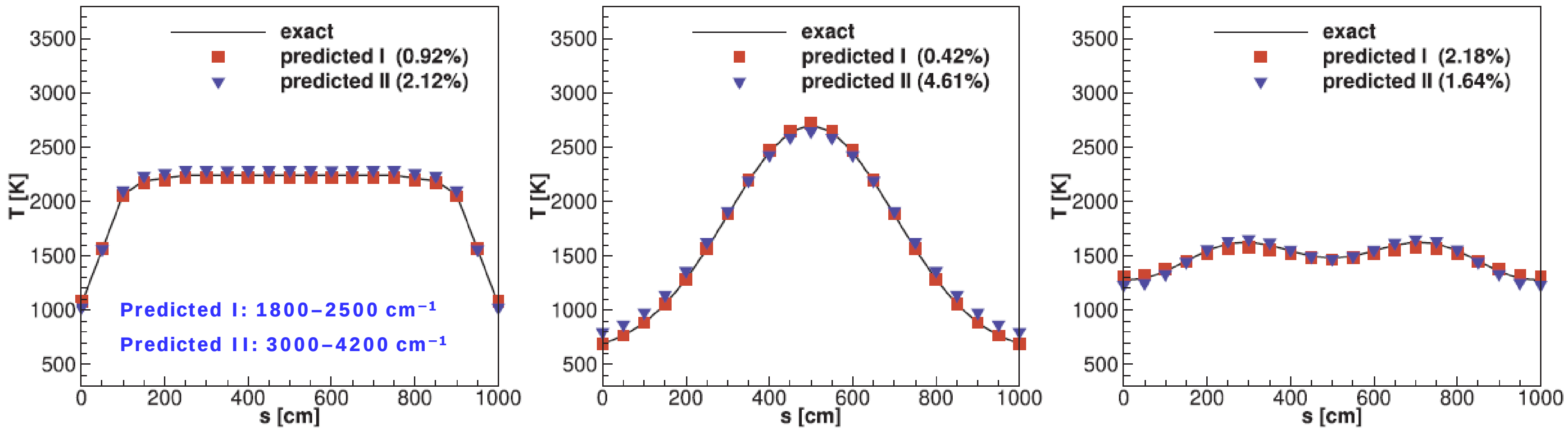


In Situ measurements at a waste incinerator

Challenges:

- ✓ Keep optics clean (CO_2 self-absorption)
- ✓ HITEMP2010 “weak” line intensities those become “strong” at long L (10 m)
- ✓ Reference CO_2/H_2O 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 (ΔT = 50 °C window for SNCR)



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Conclusions

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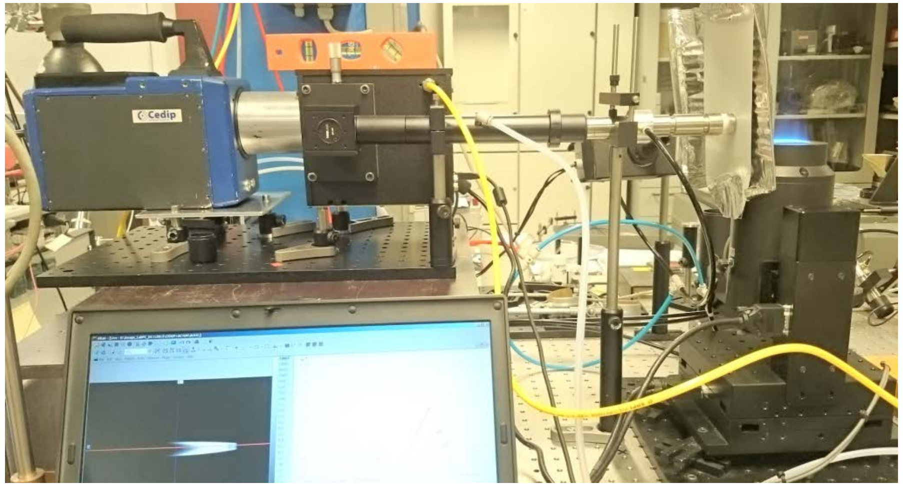

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