



## Spectroscopy in high- temperature industrial processes on Earth

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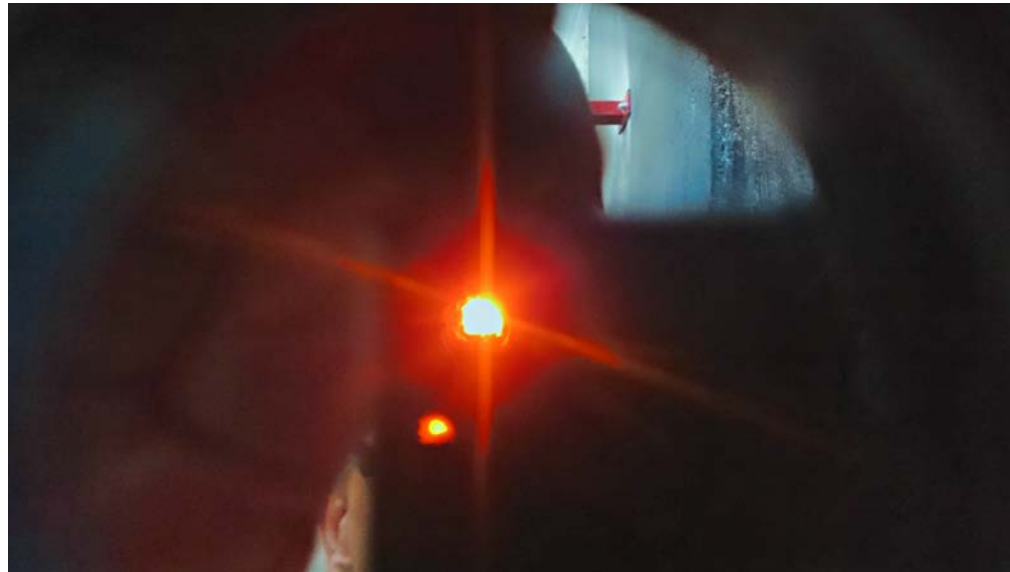
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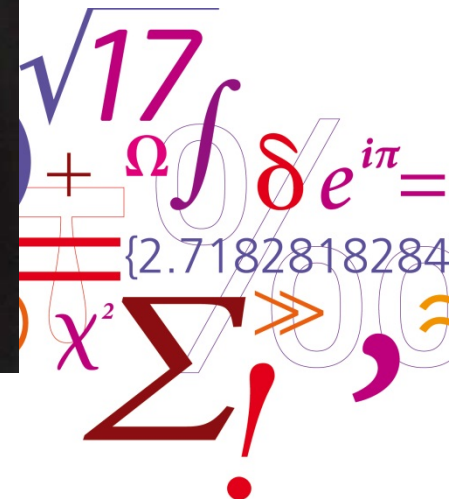
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Spectroscopy of Exoplanets | Spectroscopy in high- temperature  
July 24<sup>th</sup> – 26<sup>th</sup> 2015 industrial processes on Earth

Senior Scientists **Alexander Fateev**

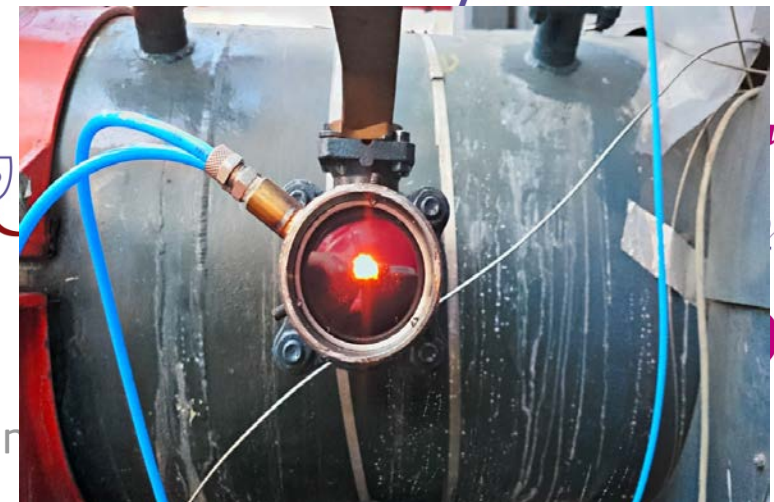
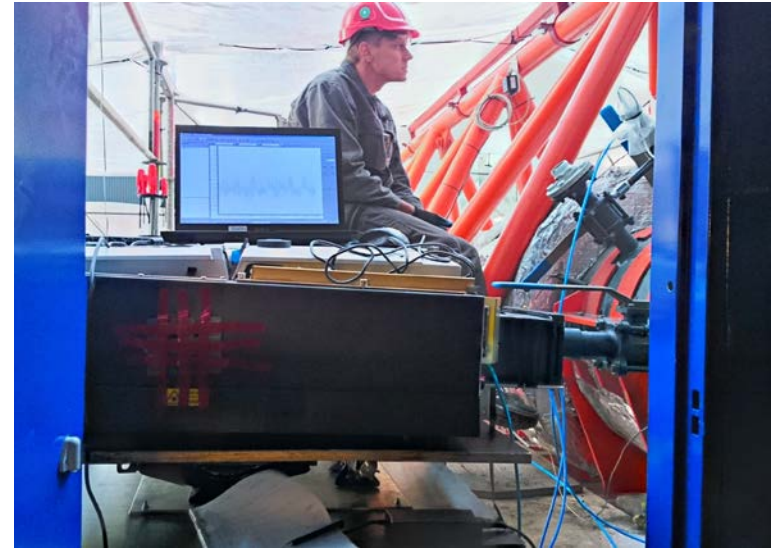


DTU Chemical Engineering  
Department of Chemical and Biochemical Engineering



# Spectroscopy in industrial processes | Outline

- **Background**
- **Large scale measurements**
- **Example/Case 1: NH<sub>3</sub>**
- **Example/Case 2: SO<sub>2</sub>/SO<sub>3</sub>**
- **Example/Case 3/UV: C<sub>6</sub>H<sub>6</sub>O and C<sub>10</sub>H<sub>8</sub>**
- **Conclusions**

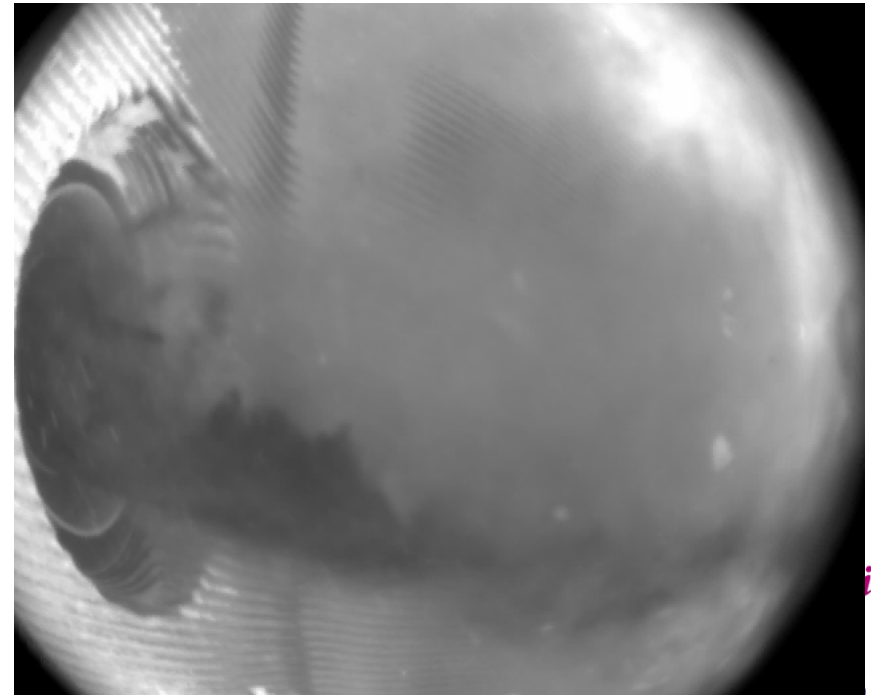


## Needs | Large Scale Measurements

- Boilers,
- Flames (oil, gas, bio-masses),
- Engines (ships, jets),
- Field campaigns (explosions)



VIS image grade flame (waste)



IR image wood dust flame (video fuel mixing)



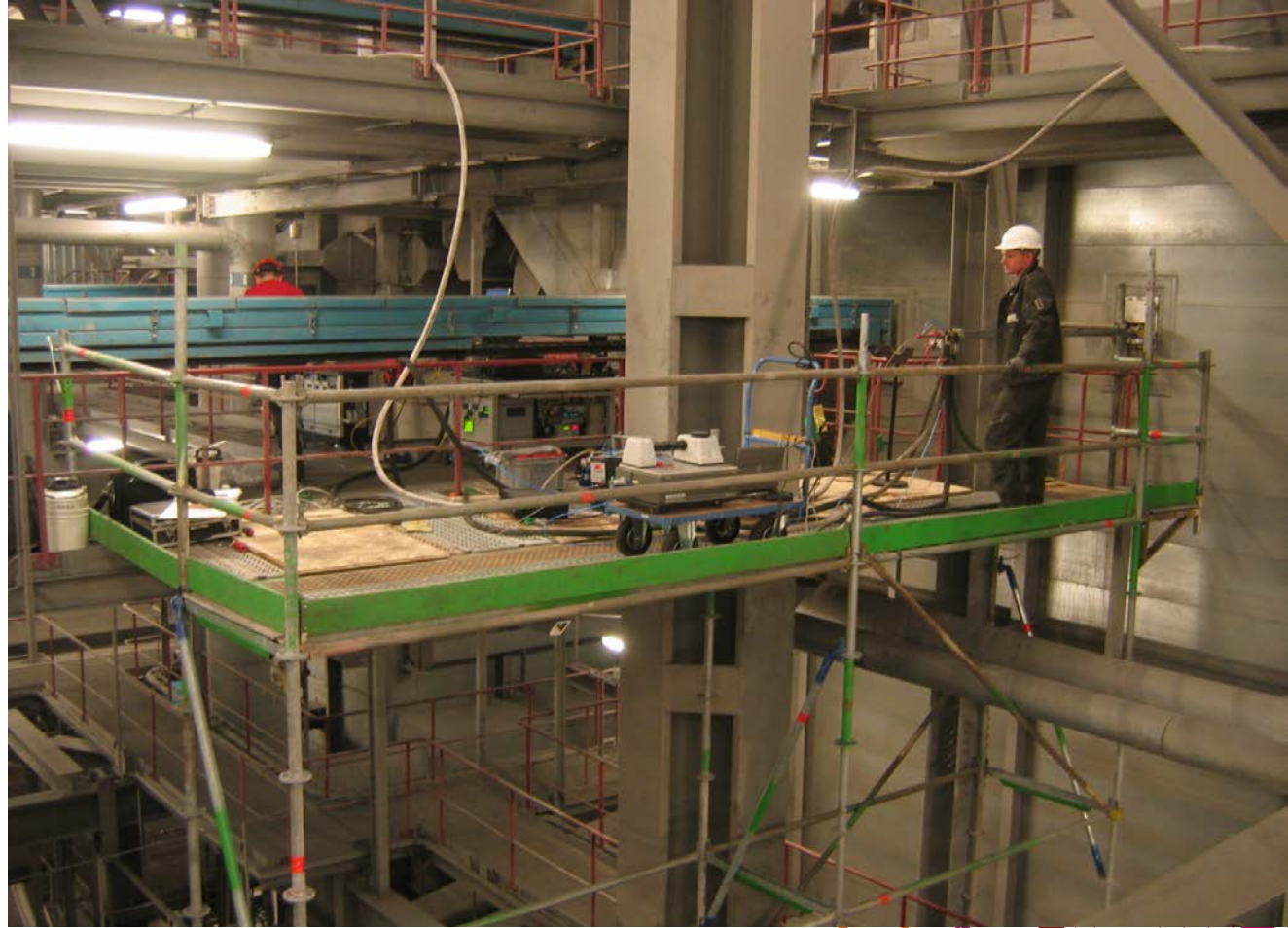
# Complexity | Large Scale Measurements

## Complexity:

- get results first
- trustful system
- 1500C is not uncommon

## Expensive:

- access possibilities
- man power
- time



# Data analysis | Large Scale Measurements

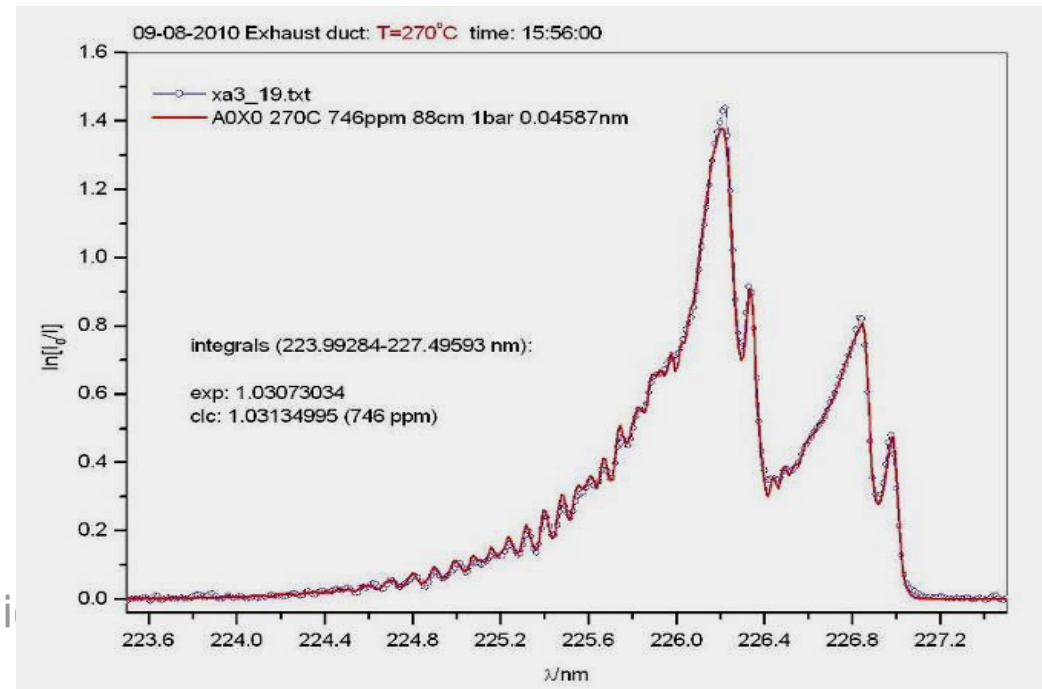
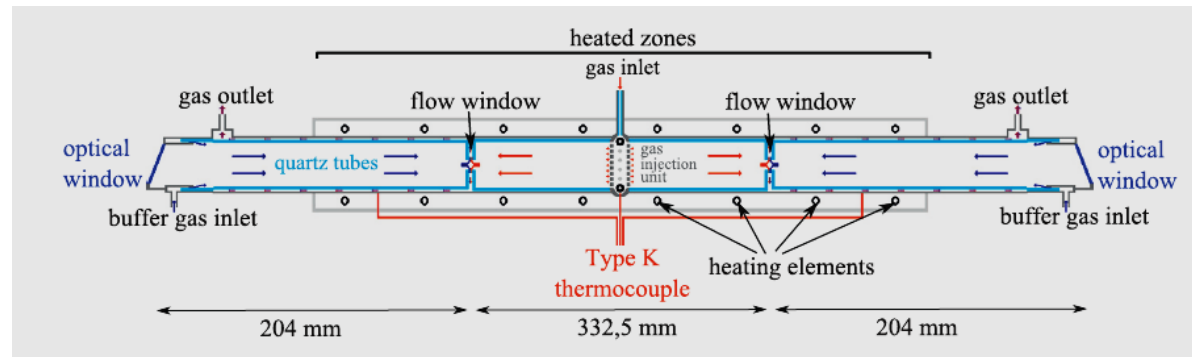
## Data analysis:

- on-line
- at home

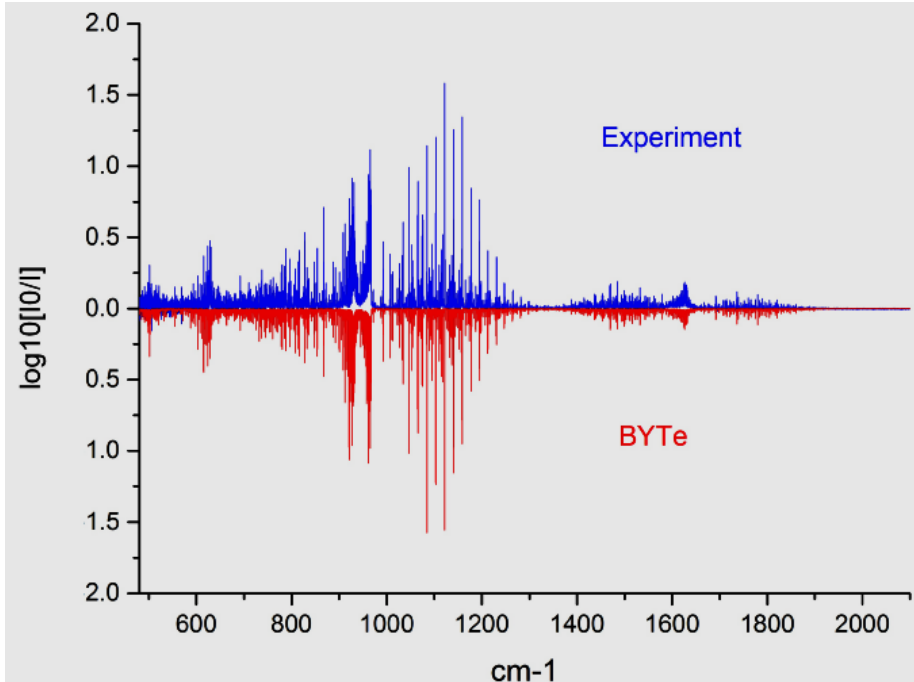
## Source of reference data:

- measurements in a cell with pre-mixed gases
- **databases (IR/UV)**

NO measurements in exhaust duct of a large ship engine



# Example 1 | NH<sub>3</sub>: experiment (500C, 0.09cm<sup>-1</sup>) vs calculations (BYTe)



Can we use BYTe at 500C for practical apps?

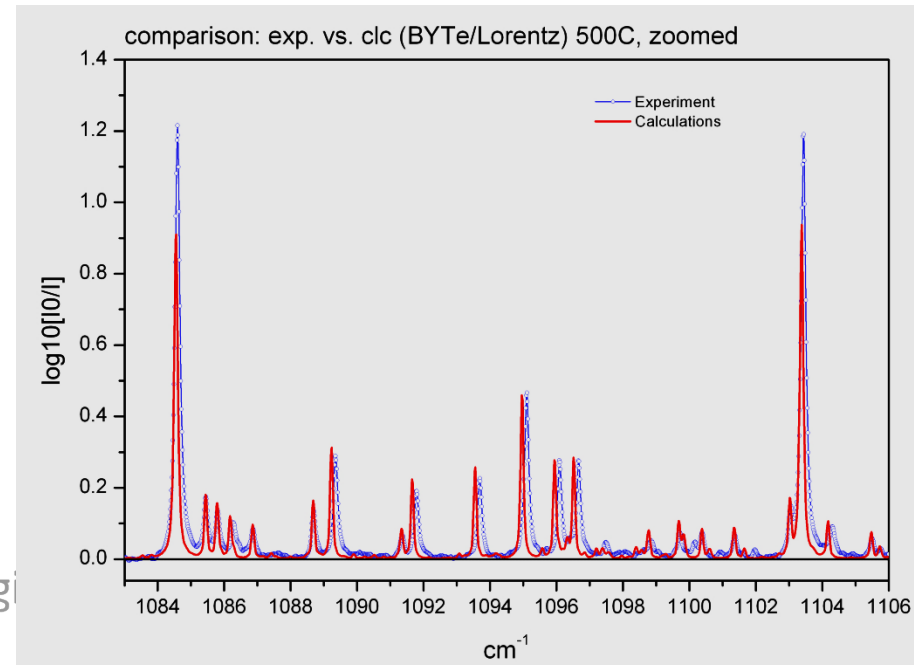
- in general a good agreement
- some difficulties with strong line intensities
- some frequency shifts in line positions

More work to do at even higher T (>500C)

## More details:

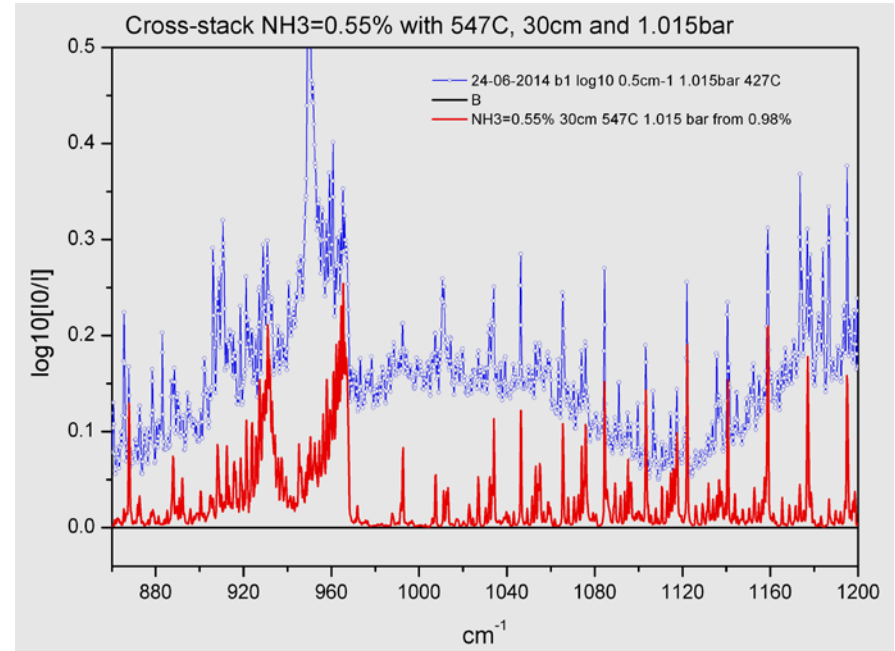
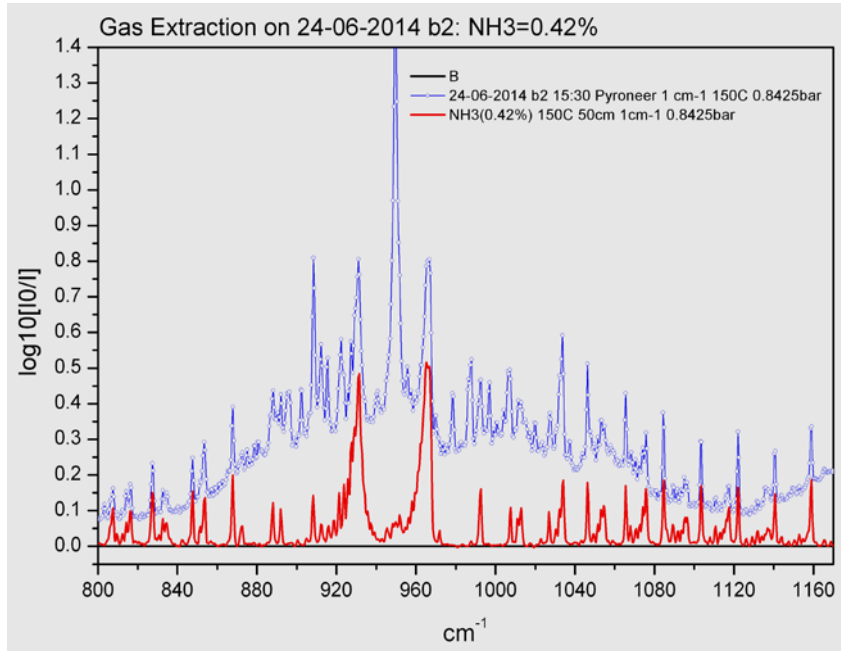
Emma J. Barton et al

“High-resolution absorption measurements of NH<sub>3</sub> at high temperatures: 500 - 2100 cm<sup>-1</sup>”  
(submitted to JQSRT)



# Application case 1 | In Situ measurements on **Pyroener (6MW) gasifier**

**NH<sub>3</sub>: Q: Why to do measurements? A: NH<sub>3</sub> contributes to NO<sub>x</sub> formation**



## Gas extraction (150C):

20-06-2014 (17:00-19:30) : **NH<sub>3</sub>=(0.4 ± 0.02)%**, H<sub>2</sub>O=(35 ± 0.6)%, CO<sub>2</sub>=(14 ± 0.45)%, CO=(10 ± 0.21)%

24-06-2014 (15:00-17:00): **NH<sub>3</sub>=(0.42 ± 0.02)%**, H<sub>2</sub>O=(36 ± 0.6)%, CO<sub>2</sub>=(13.5 ± 0.45)%, CO=(10.3 ± 0.21)%

## In situ (547C):

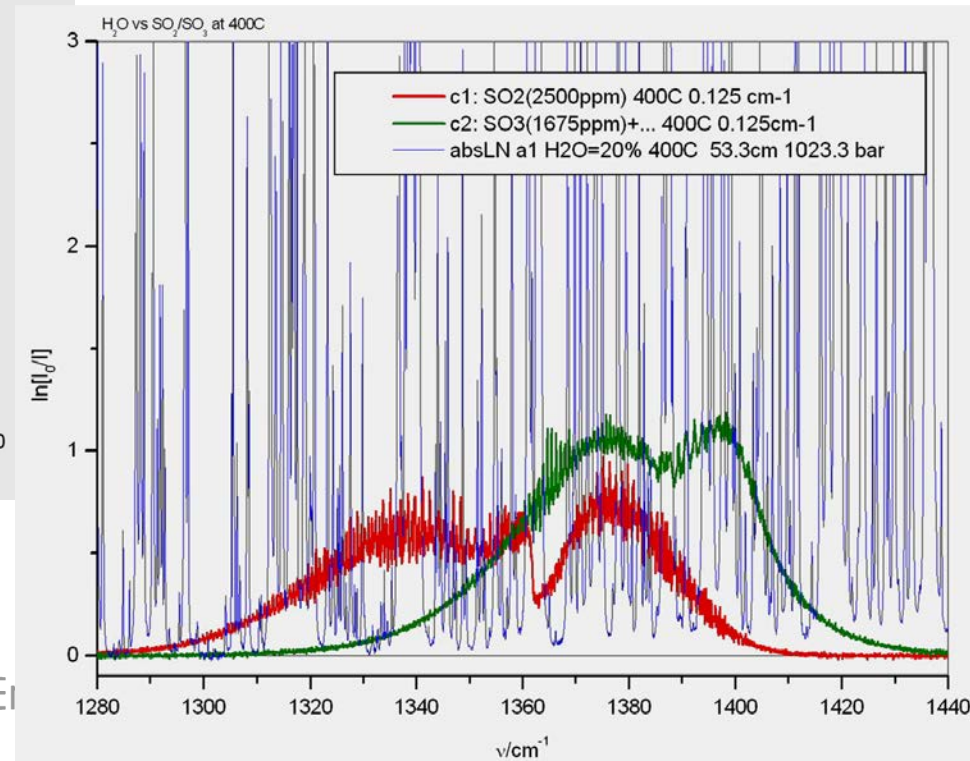
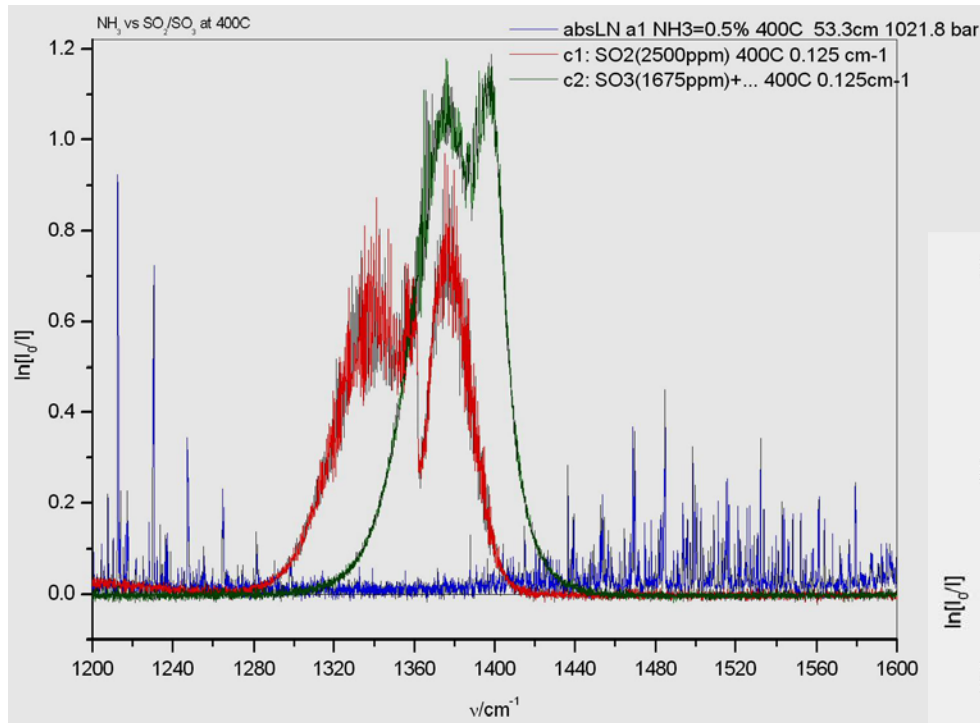
24-06-2014 (20:00-21:00): **NH<sub>3</sub>=(0.55 ± 0.05)%**, H<sub>2</sub>O=(36 ± 1)%



# Application case 2 | SO<sub>2</sub>/SO<sub>3</sub>/NH<sub>3</sub> in a hot flue gas

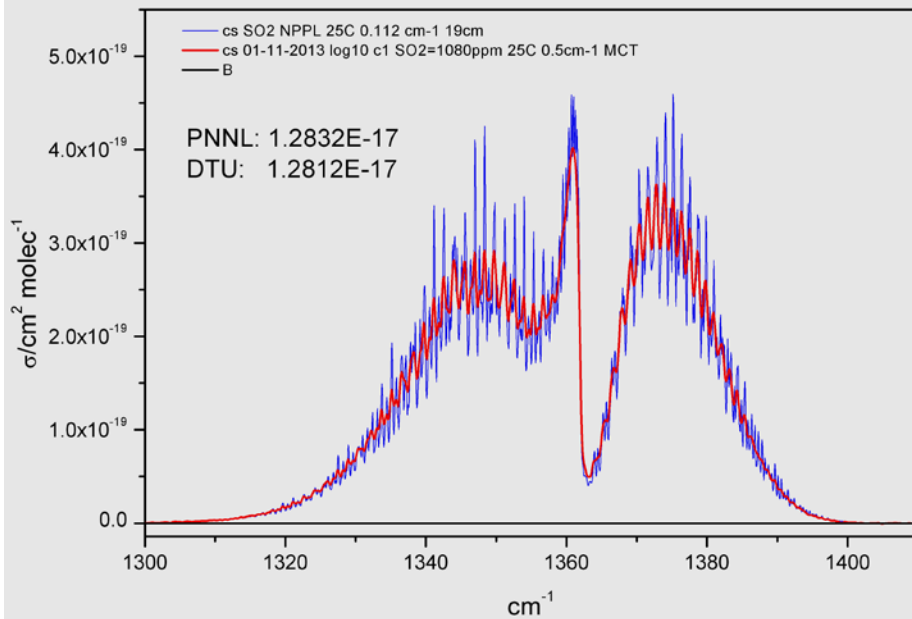
**SO<sub>2</sub>/SO<sub>3</sub>/NH<sub>3</sub>: Q: Why to do measurements?**

**A: NO<sub>x</sub> reduction at SCR/NSCR units, NH<sub>3</sub> slip/costs, corrosion/fouling**



## Example 2 | SO<sub>3</sub>: measurements at 25C and 400C

SO<sub>3</sub> at 25C: 0.5cm<sup>-1</sup> vs PNNL (0.12cm<sup>-1</sup>)

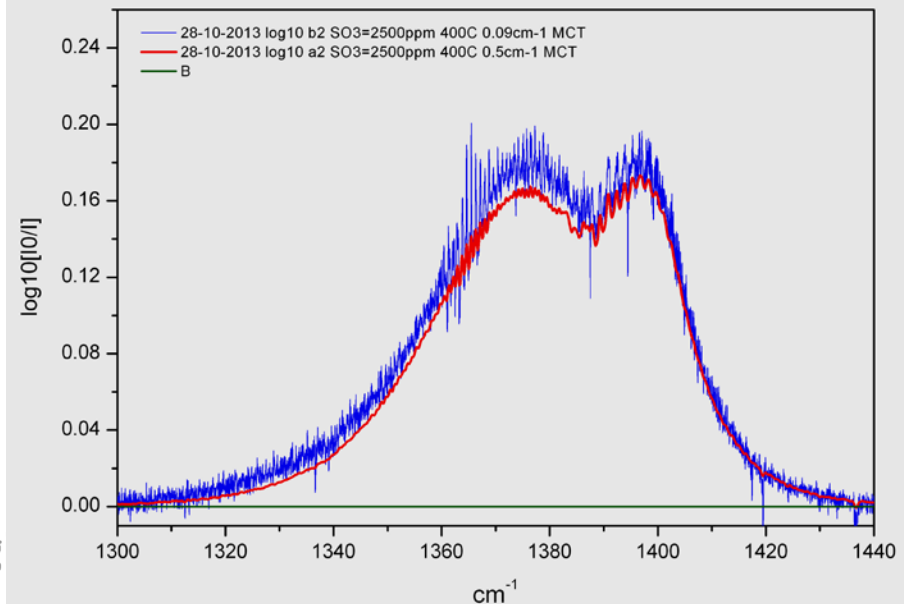


- Simple to generate, but difficult to measure/quantify
- No databases (SO<sub>2</sub>/SO<sub>3</sub>) are available at T>100C

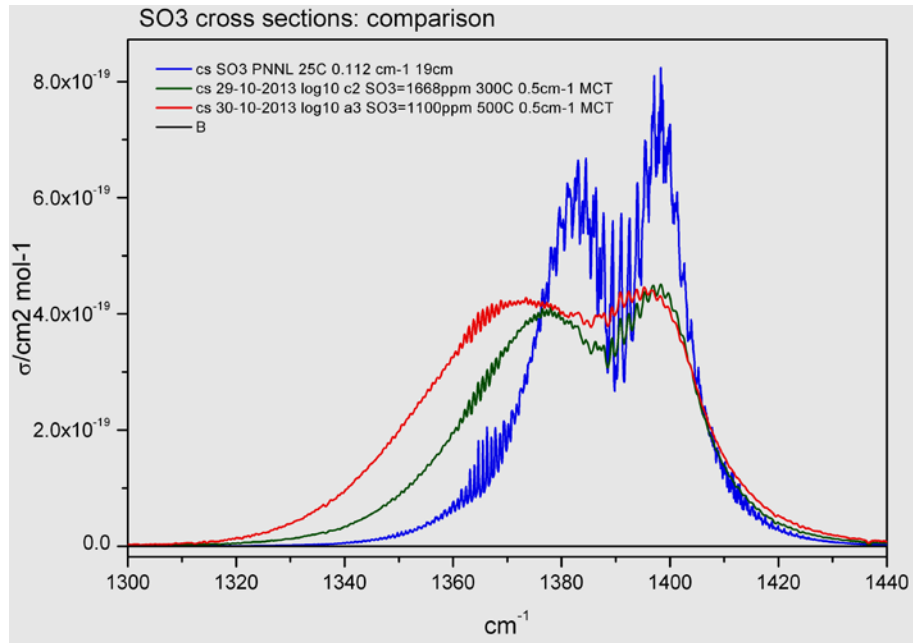
### Good news:

- Excellent agreement with PNNL data at 25C
- No need to use high-resolution at high T

T=400C SO<sub>3</sub>: effect of resolution 0.5cm<sup>-1</sup> vs 0.09 cm<sup>-1</sup>

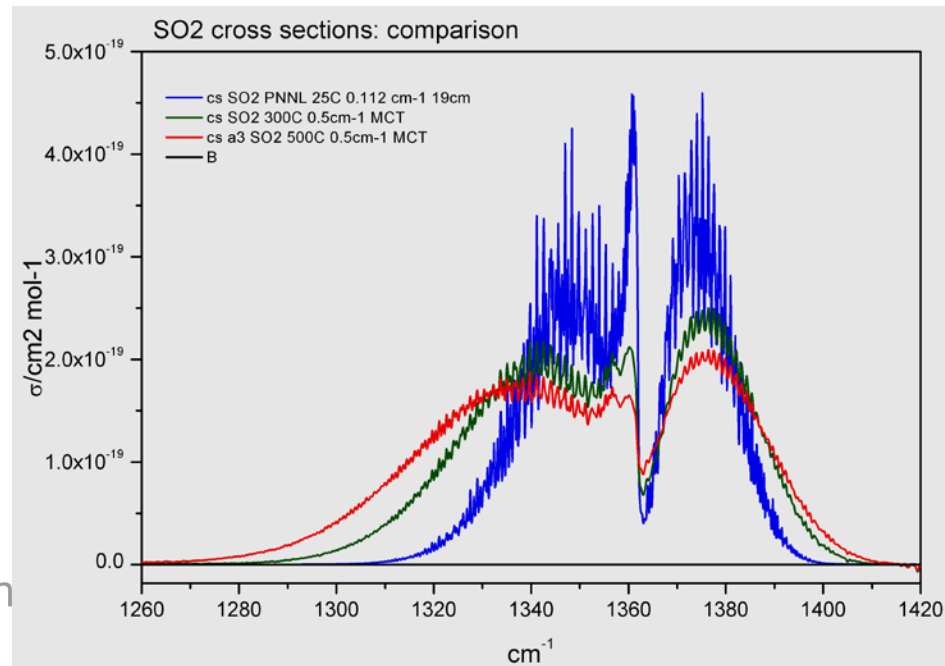


## Example 2 | SO<sub>2</sub>/SO<sub>3</sub> cross sections (0.5cm-1)



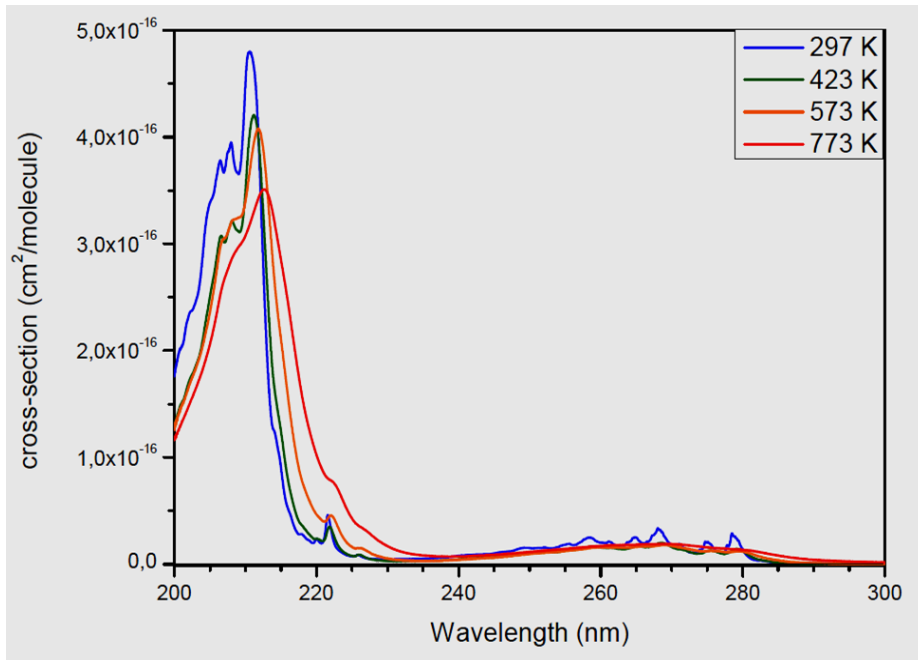
PhD (Dan Underwood) with UCL:

- SO<sub>2</sub> and SO<sub>3</sub> line lists
- ready by the end 2015
- **2<sup>nd</sup> Power plant measurement campaign, fall 2015**

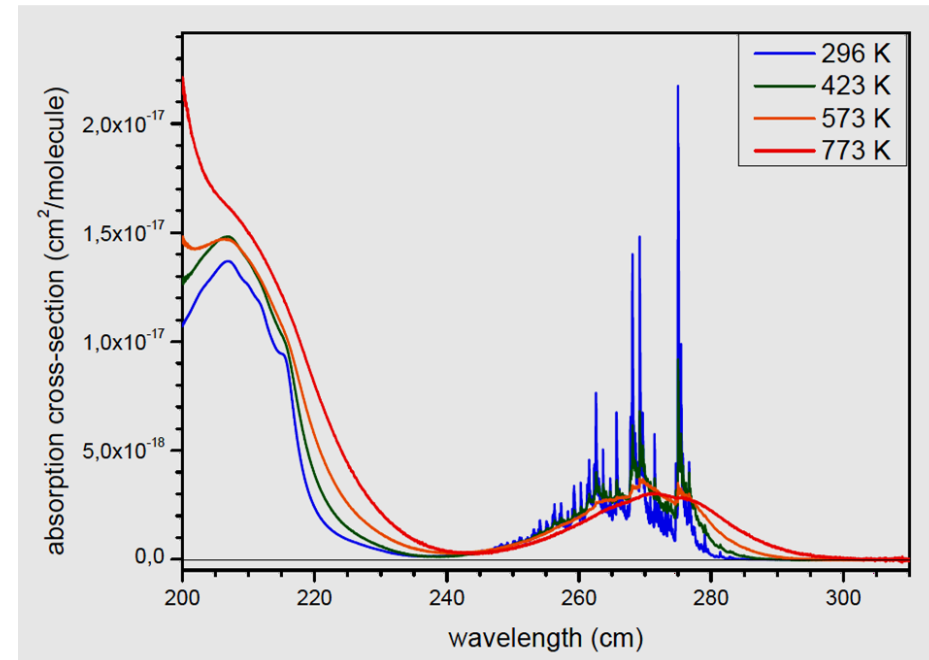


- Not too many reference data available even at low T (about 23C)
- An excellent agreement with published data at low T
- Significant changes in the fine structure of the cross-section spectra with T

Naphthalene abs cross-sections: from 23C to 500C



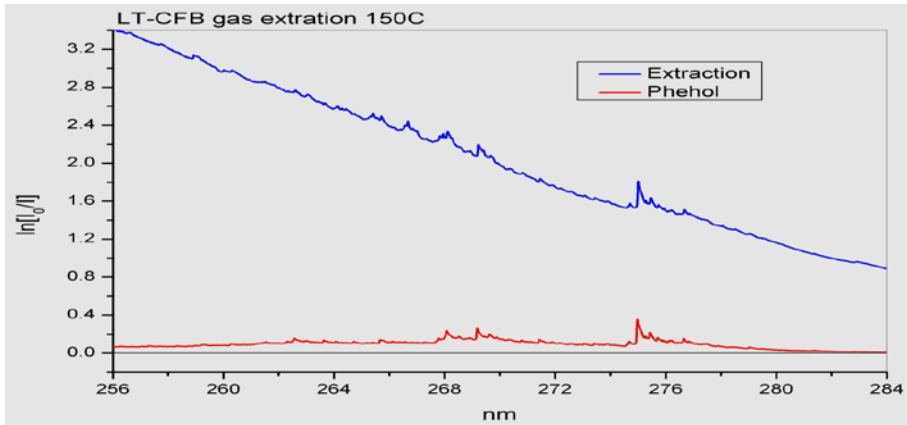
Phenol abs cross-sections: from 23C to 500C



# Application case 3/UV | In Situ measurements on LT-CFB (100kW) gasifier

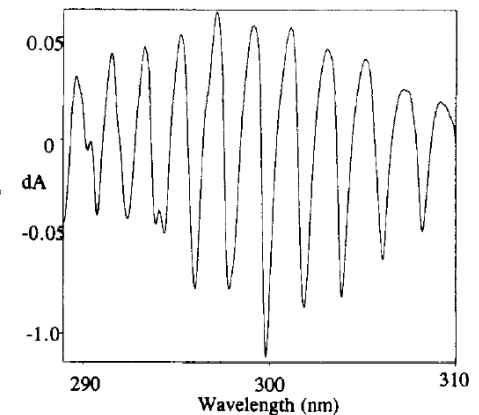
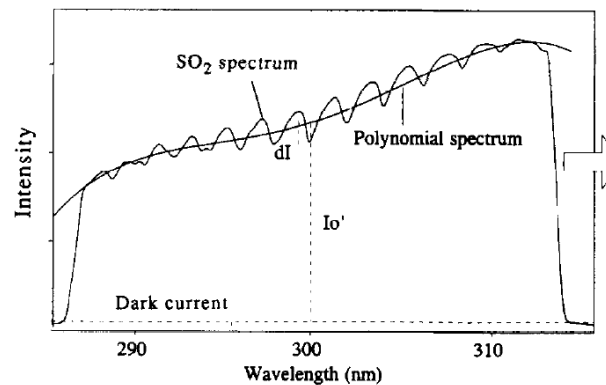
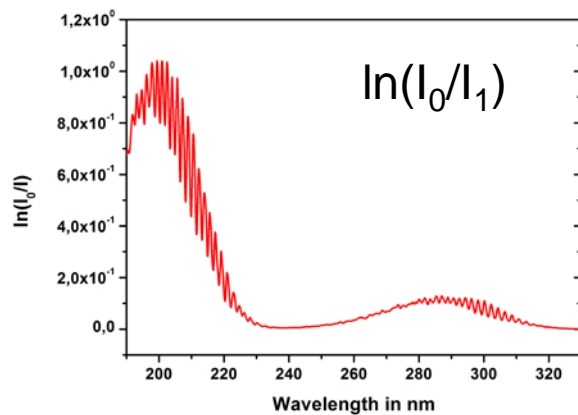
**Phenol/Naphthalene: Q: Why to do measurements?**

**A: Phenol/Naphthalene – major trace gases from PAH's in low temperature gasification**



- Few new challenges:
- Very strong UV light attenuation
  - Very broad continuum-like abs structures
  - Very small L for in situ measurements

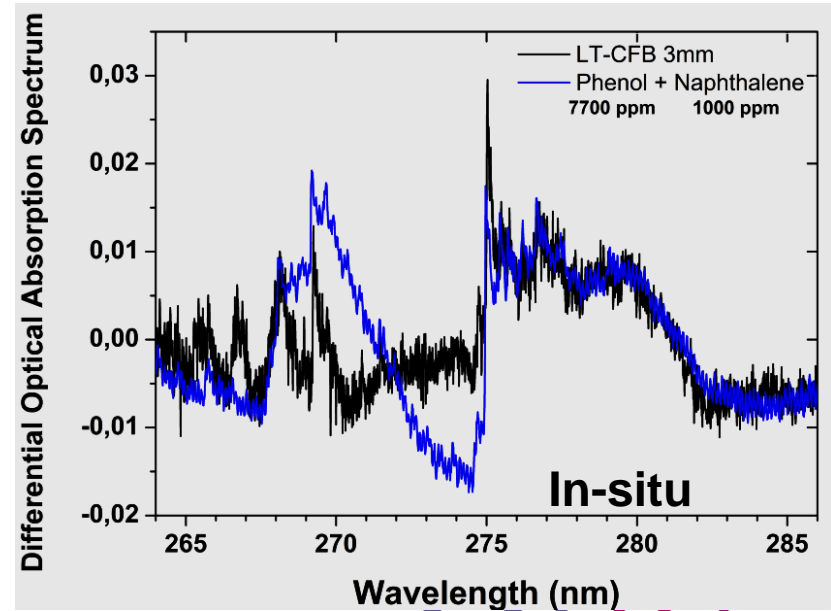
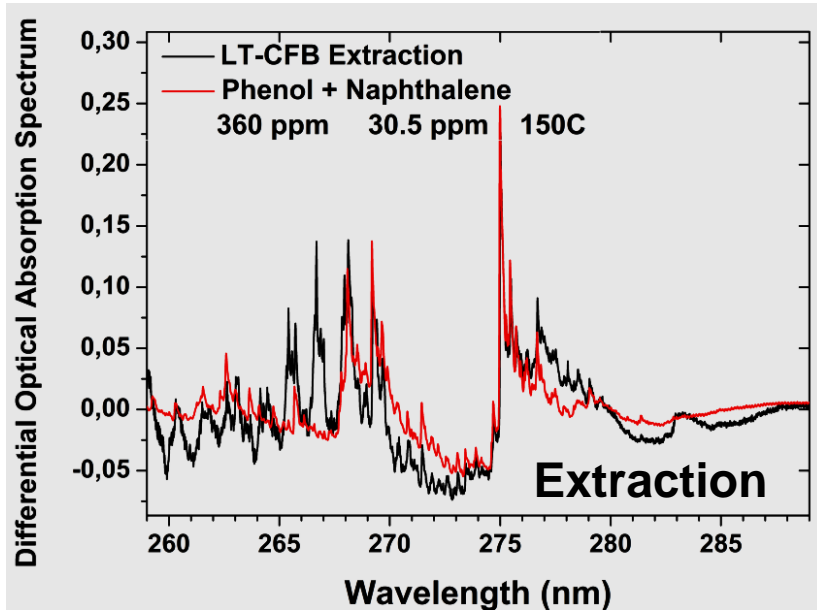
## DOAS approach: SO<sub>2</sub> UV absorption as an example



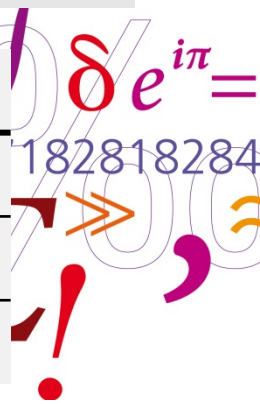


Application case 3/UV | **In Situ measurements on LT-CFB (100kW) gasifier**

**Comparison of the measurements**



Method	Time	Temperature	Phenol	Naphthalene
GC-MS	30 min	15°C	215 ppm	16 ppm
Extraction	3 min	150°C	360 ppm	31 ppm
In-situ	3 min	306°C	7700 ppm	1000 ppm



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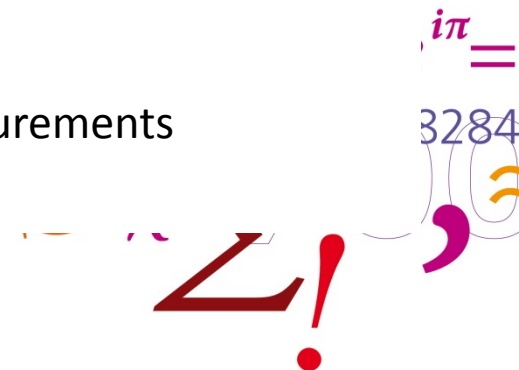
## Conclusions | **Now**

### **In general**

- You can find a lot inspirations for the work on the Earth
- Different research areas can have the same origin
- Scientists can make industry guys happy

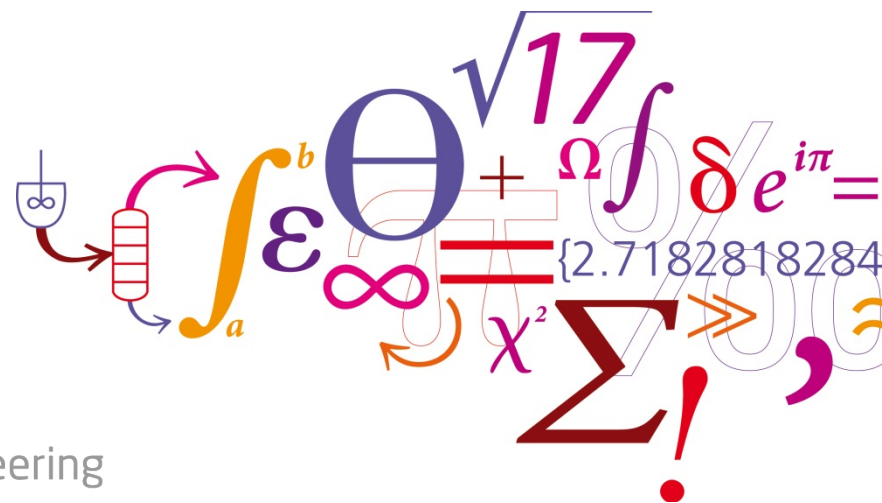
### **In particular:**

- Excellent experimental tools are available for (VUV) UV-FIR optical measurements
- Temperature range can be also negative (e.g. gases at low T)
- New data/lines for NH<sub>3</sub>/SO<sub>2</sub>/SO<sub>3</sub>
- New data for phenol/naphthalene
- Try always In Situ and avoid any Ex Situ (extraction) measurements

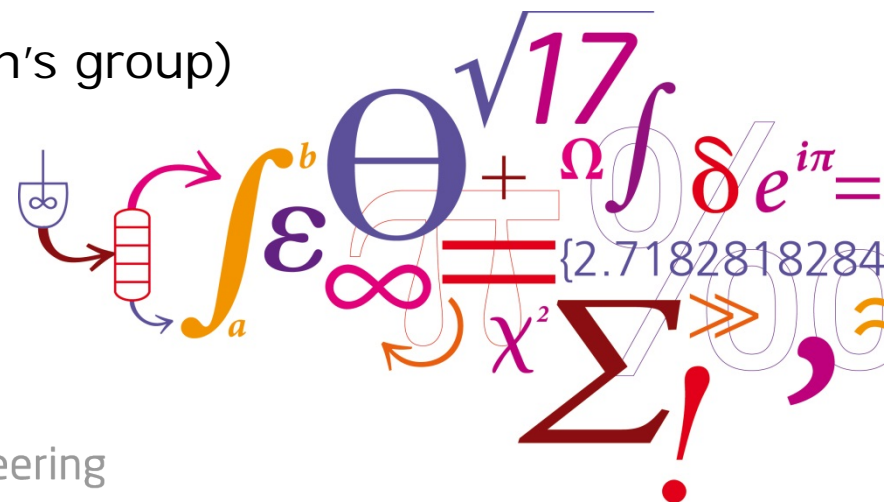


## Conclusions | Future

- Inspiration comes from industry (small, middle large, ...)
- Possible spin offs: innovation (patents)
- New **gas components: CH<sub>3</sub>Cl, KCl etc. (together with UCL)**
- Combine several methods to obtain **multi-parameters**
- ... ?
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+45 23652906



- To Energinet.dk: projects No. 2013-12027, 2011-1-10622, 2010-1-10422
- To MST.dk
- To DONG Energy and Vattenfall
- To UCL (Prof. Jonathan Tennyson's group)



# Thank you for your attention

