Spectroscopy in high-temperature industrial processes on Earth

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Spectroscopy of Exoplanets
July 24th – 26th 2015

Spectroscopy in high-temperature industrial processes on Earth

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DTU Chemical Engineering
Department of Chemical and Biochemical Engineering
Spectroscopy in industrial processes | Outline

• Background

• Large scale measurements

• Example/Case 1: NH3

• Example/Case 2: SO2/SO3

• Example/Case 3/UV: C6H6O and C10H8

• 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)

DTU Chemical Engineering
Department of Chemical and Biochemical Engineering
Complexity:  
- get results first  
- trustful system  
- 1500C is not uncommon  

Expensive:  
- access possibilities  
- man power  
- time  

Campaign at Blok 7 Fynsværket (Denmark)
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 | **NH₃: experiment (500C, 0.09cm⁻¹) 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 NH₃ at high temperatures: 500 - 2100 cm⁻¹”
(submitted to JQSRT)

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Department of Chemical and Biochemical Engineering
Application case 1 | In Situ measurements on **Pyroneer (6MW) gasifier**

**NH3**: Q: Why to do measurements? A: NH3 contributes to NOx formation

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**Gas extraction (150°C):**

- **20-06-2014 (17:00-19:30)**: \( \text{NH}_3 = (0.4 \pm 0.02)\% \), \( \text{H}_2\text{O} = (35 \pm 0.6)\% \), \( \text{CO}_2 = (14 \pm 0.45)\% \), \( \text{CO} = (10 \pm 0.21)\% \)
- **24-06-2014 (15:00-17:00)**: \( \text{NH}_3 = (0.42 \pm 0.02)\% \), \( \text{H}_2\text{O} = (36 \pm 0.6)\% \), \( \text{CO}_2 = (13.5 \pm 0.45)\% \), \( \text{CO} = (10.3 \pm 0.21)\% \)

**In situ (547°C):**

- **24-06-2014 (20:00-21:00)**: \( \text{NH}_3 = (0.55 \pm 0.05)\% \), \( \text{H}_2\text{O} = (36 \pm 1)\% \)
Application case 2 | SO2/SO3/NH3 in a hot flue gas

SO2/SO3/NH3:  Q: Why to do measurements?
A: NOx reduction at SCR/NSCR units, NH3 slip/costs, corrosion/fouling
Example 2 | **SO3: measurements at 25C and 400C**

- Simple to generate, but difficult to measure/quantify
- No databases (SO2/SO3) are available at T>100C

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

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**SO3 at 25C: 0.5cm⁻¹ vs PNNL (0.12cm⁻¹)**

- **PNNL:** 1.2832E-17
- **DTU:** 1.2812E-17

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**T=400C SO3: effect of resolution 0.5cm⁻¹ vs 0.09 cm⁻¹**

- **28-10-2013 log10 b2 SO3=2500ppm 400C 0.09cm⁻¹ MCT**
- **28-10-2013 log10 a2 SO3=2500ppm 400C 0.5cm⁻¹ MCT**
Example 2 | **SO2/SO3 cross sections (0.5cm⁻¹)**

PhD (Dan Underwood) with UCL:
- **SO₂ and SO₃ line lists**
- ready by the end 2015
- **2nd Power plant measurement campaign, fall 2015**
Example 3/UV | Phenol/Naphthalene UV absorption cross-sections temperature effects

- Not too many reference data available even at low T (about 23°C)
- 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 23°C to 500°C
Phenol abs cross-sections: from 23°C to 500°C
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: SO2 UV absorption as an example
Application case 3/UV | In Situ measurements on LT-CFB (100kW) gasifier

Comparison of the measurements

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
<th>Temperature</th>
<th>Phenol</th>
<th>Naphthalene</th>
</tr>
</thead>
<tbody>
<tr>
<td>GC-MS</td>
<td>30 min</td>
<td>15°C</td>
<td>215 ppm</td>
<td>16 ppm</td>
</tr>
<tr>
<td>Extraction</td>
<td>3 min</td>
<td>150°C</td>
<td>360 ppm</td>
<td>31 ppm</td>
</tr>
<tr>
<td>In-situ</td>
<td>3 min</td>
<td>306°C</td>
<td>7700 ppm</td>
<td>1000 ppm</td>
</tr>
</tbody>
</table>
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 NH3/SO2/SO3
- 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$_3$Cl, KCl etc. (together with UCL)
- Combine several methods to obtain multi-parameters
- ... ?

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• 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