Spectroscopy in high-temperature industrial processes on Earth

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Spectroscopy of Exoplanets
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Spectroscopy in high-temperature industrial processes on Earth

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Department of Chemical and Biochemical Engineering
• **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)**

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Department of Chemical and Biochemical Engineering
Complexity: Large Scale Measurements

**Complexity:**
- get results first
- trustful system
- 1500C is not uncommon

**Expensive:**
- access possibilities
- man power
- time

Campaign at Blok 7 Fynsværket (Denmark)
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 | **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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**Application case 1 | In Situ measurements on Pyroneer (6MW) gasifier**

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

**Gas extraction (150C):**

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 (547C):**

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**

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

**Simple to generate, but difficult to measure/quantify**

**No databases (SO2/SO3) are available at T>100C**
**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>

![Graph of Differential Optical Absorption Spectrum](image1)

Extraction

![Graph of Differential Optical Absorption Spectrum](image2)

In-situ
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: CH3Cl, KCl etc. (together with UCL)
- Combine several methods to obtain multi-parameters
- ... ?
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Thank you for your attention