Spectroscopy in high-temperature industrial processes on Earth

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Publication date: 2015

Document Version
Peer reviewed version

Citation (APA):

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Spectroscopy of Exoplanets

July 24th – 26th 2015

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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)
Complexity

**Complexity:**
- get results first
- trustful system
- 1500°C 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
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)
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): NH3=(0.4 ± 0.02)%, H2O=(35 ± 0.6)%, CO2=(14 ± 0.45)%, CO=(10 ± 0.21)%
24-06-2014 (15:00-17:00): NH3=(0.42 ± 0.02)%, H2O=(36 ± 0.6)%, CO2=(13.5 ± 0.45)%, CO=(10.3 ± 0.21)%

In situ (547C):

24-06-2014 (20:00-21:00): NH3=(0.55 ± 0.05)% , H2O=(36 ± 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

**Good news:**
- Excellent agreement with PNNL data at 25C
- No need to use high-resolution at high T
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 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: 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: CH3Cl, 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