Biomass Based Chemicals for the Oil and Gas Industry

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Green Chemicals for the Oil Industry

Green Chemistry???
Relevance for the oil industry?

“Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances.... Reduces the negative impacts of chemical products and processes on human health and the environment. Lessens and sometimes eliminates hazard from existing products and processes”

98% of all products and materials needed for modern economies is still derived from petroleum and/or natural gas
Green chemistry's 12 principles

1. Prevent waste.

4. Design safer chemicals and products.

7. Use renewable feedstocks.

10. Design chemicals and products to degrade after use.
“Green Chemicals” within the Oil and Gas Industry

**Oilandgas360**: “Shifting focus toward the usage of green chemicals is likely to provide opportunities for the market growth in the future”

**McKinsey and Company**: “An oil and gas giant finds green growth opportunities in biobased chemicals”

The big companies...?
Our Expertise and Approach

• ~20 years experience in organic synthesis

• Specialized in carbohydrate chemistry, biomass conversion, molecular interactions

• Use abundant biomolecules as templates for new green chemicals.
  • Benefits: cheap, recyclable or disposable (bio-degradable), one chemical more functions, tailor made properties.

• Demonstrated POC in two RIS projects – **Green chemicals with multiple properties**
Renewable Oil/Gas Production Chemicals

• Iron control agents: isoascorbic acid as a reducing agent.

• Scale inhibitor: phytic acid (inositol hexaphosphate).

• Cationic flocculants: Starch derivatives, chitosan
The ideal biomass for production chemicals

Requirements

• Cheap and abundant
• Biodegradable
• Safe and easy to handle
• Renewable

Candidate: Carbohydrates

• Glucose the most abundant molecule in the biosphere.
• Commodity chemical
• Yearly production >185 mio tons
• Price ~ 0.4 $/kg
Current Focus

- $\text{H}_2\text{S}$ scavenging
- Avoid triazine or alike
- Scalability and price
- POF in realistic setting
- Kinetics
- Property prediction
- Degradability
Background

H$_2$S is produced down-well

\[
\text{SO}_4^{2-} \xrightarrow{\text{SRB}} \text{H}_2\text{S} \quad \text{hydrogen sulfide}
\]

Triazine H$_2$S scavenging

Produced water @NCS in 2016: 180000000 m$^3$
Synthesis of New Scavengers

- Few scalable steps from common sugars.
- Limit solvents and reagents.
- Catalysis in water preferred.
- No or simple purification, i.e. low waste production.
- Evaluation of scavengers...
Evaluation and Analysis of the Green Scavengers

• At UCPH – Qualitative
  • Laboratory test: \( \text{H}_2\text{S} \) generation, bubbling through solution of scavenger at 80°C.
  • Analysis of spend scavenger: incorporation of sulphur = success
    • NMR spectroscopy, HRMS, IR

• At AAU Esbjerg – Qualitative and quantitative
  • Raman spectroscopy under relevant conditions
  • Reaction kinetics
  • Comparison with commercial scavengers (triazines)
  • Mechanistic studies together with UCPH.
The AAU setup:
The AAU setup:

- **pH sensor**
- **Injection hose**
- **Vial**
- **Isolating layer**
- **Heating plate**
- **Temperature sensor**
- **Probe cooling tube**
- **Raman probe**
Green Scavengers vs MEA-Triazine
Preliminary Conclusion from AAU

- Green scavengers remove H$_2$S completely
  - Less pH dependent
- MEA-triazine removes H$_2$S faster initially, but is inhibited by change in pH.
  - Very pH dependent
- One green scavenger stands out and is the lead compounds for 2$^{nd}$ generation scavengers.
- More studies will clarify mechanistic aspects and scope of the new green scavengers.
Relative binding energies for divalent cations to the spent green scavenger

<table>
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<tr>
<th>Ion</th>
<th>Relative reaction energy (kJ/mol)</th>
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<tbody>
<tr>
<td>Ba$^{2+}$</td>
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</tr>
<tr>
<td>Ca$^{2+}$</td>
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<tr>
<td>Fe$^{2+}$</td>
<td>-38</td>
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<tr>
<td>Mg$^{2+}$</td>
<td>11</td>
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<tr>
<td>Sr$^{2+}$</td>
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Advantages of our approach

• Tailor made properties
  • pH dependence, oil-water partitioning, biocide, H$_2$S-scavenger, shale inhibitor, corrosion inhibitor etc. combined in one molecule.

• A molecular “swiss army knife”

• Biomass-based and cheap

• Bio-degradable

• The synthesis is simple, scalable and high yielding.

• H$_2$S scavenging has been confirmed by NMR, Raman and High-resolution mass spectrometry (HRMS).

• Molecular modelling shows promising properties of the novel chemicals as corrosion inhibitors and anti-scale compounds.
Participants

**UCPH – CHEM: Synthesis and Analysis**
- PI: Christian Marcus Pedersen
- PhD student Asger Koue (from 15/12-2020)

**AAU – Esbjerg: Raman spectroscopy - Kinetic studies**
- Assoc. Prof. Marco Maschietti (AAU Esbjerg)
- Assoc. Prof. Sergey Kucheryavskiy (AAU Esbjerg)
- PhD student Fernando Raul Montero Revelo (from 15/11-2020)

**DTU – KT: Computational modelling**
- Assoc. Prof. Martin Andersson (DTU)
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