Process and environmental systems analysis of the BioBuF concept
Outline

• Conventional adipic acid production

• Process and environmental systems analysis in BioBuF

• Some environmental systems analysis results

• Assessment of processes in early development stages
Conventional adipic acid production

• Production from fossil resources $\rightarrow$ KA oil

\[ \text{Cyclohexanone} + 1\frac{1}{2} \text{HNO}_3 \xrightarrow{\text{Cu}^{2+}, \text{V}^{5+}} \text{Adipic acid} + \frac{3}{4} \text{N}_2\text{O} + \frac{3}{4} \text{H}_2\text{O} \]

\[ \text{Cyclohexanol} + 2 \text{HNO}_3 \xrightarrow{\text{Cu}^{2+}, \text{V}^{5+}} \text{Adipic acid} + \text{N}_2\text{O} + 2 \text{H}_2\text{O} \]

Process flow diagram of the BioBuF concept

Lutein
- Heat
- CO₂
- Nutrients
- Water

Adipic acid
- O₂
- CO₂

- GROT Processing
- Sugars
- Lysine
- Aromatic chemicals

- Microalgal Cultivation
- Biomass Fractionation
- Separation

- Microbial Cell Factory for Adipic Acid Prod.
- Adipic Acid Separation

- Carotenoids
- Lipids/fatty acids

- Adipic acid
- By products + residuals
- Nutrients (liquid fraction/bio-solids)

Lignin derivative

- Bioconversion of Lignin-Derived Chemicals

Utilities
- Anaerobic Digestion
- Heat & Power Production

- Residues + organic matter
- Raw biogas
- Water
- Electricity
- CO₂
- Heat + steam

Bioelectro-chemical Systems

- Nutrients

- Utilities
1. Modelling based on experimental, lab-scale data
2. Process integration
3. Economic and environmental analysis
4. Feedback to development
Information flow in the project – 2

• Development of systemic communication protocols → Maximize output from research of biorefineries

1. Lab scale → Experimental and in-silico data for enzyme selection, metabolic engineering and bio-reaction networks, biomass fermentation, anaerobic digestion, fractionation and lignin characterization, and bio-electrochemical systems

2. Process scale → Conceptual to rigorous process modelling and design of upstream and downstream separation technologies

3. Plant level → Process integration for material and energy recovery using scenario based and superstructure approaches

4. Economic and environmental assessment level → Operating and capital cost estimations, and environmental assessment using LCA
Life cycle assessment (LCA) framework

- **Goal and scope definition**
- **Inventory analysis**
- **Impact assessment**
  - Classification
  - Characterization
  - Normalization
  - Weighting
- **Interpretation**

Environmental loads e.g.
- MJ fossil energy
- g SO₂
- g NOₓ
- kg waste

Environmental potential effects, e.g.
- resource depletion
- global warming potential
- acidification potential

Final assessment e.g.
- one-dimensional index
Previous LCAs of adipic acid production

- ecoinvent process for adipic acid production\(^2,^3\)
  - Global warming \(\approx 25 \text{ kg CO}_2\text{-eq/kg adipic acid produced}\)
  - Elimination of \(\text{N}_2\text{O}\) emissions \(\rightarrow 75\%\) reduction of global warming
  - Switch to renewable resource \(\rightarrow 10\%\) reduction of global warming

- Production from cyclohexene using \(\text{H}_2\text{O}_2\)\(^4\)
  - Fossil-based feedstock but no use of \(\text{HNO}_3\)
  - Global warming \(\approx 6 \text{ kg CO}_2\text{-eq/kg adipic acid produced}\)

- Production from aromatic compounds via fermentation\(^5\)
  - Both fossil-based and bio-based feedstock, no \(\text{N}_2\text{O}\) emissions
  - Global warming reduction \(\rightarrow 9\) to \(17 \text{ kg CO}_2\text{-eq/kg adipic acid produced}\)

System description - 1

- Goal → Guide technology development\(^6\)
- Functional unit → 1 kg of adipic acid produced

System description - 2

- Pretreatment
  - Acid-catalyzed → SO₂
  - Alkaline → NaBH₄

- Additional fuel use → Fossil, biomass

- Fermentation yield
  - Concentration of product
  - Lignin use → As fuel, as product
Acid-catalyzed pretreatment

- Bio-based pathway → Significant environmental benefits
- Hotspots → Downstream, GROT pretreatment, enzyme production
Alkaline pretreatment

- Higher impacts when compared to the acid pretreatment
- Hotspots → NaBH₄, downstream processing, GROT neutralization
NaBH$_4$ production and use

- Switch to biomass use for energy purposes in NaBH$_4$ production

<table>
<thead>
<tr>
<th>Scenario</th>
<th>GWP change [%]</th>
</tr>
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<tr>
<td>Base case</td>
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<tr>
<td>1</td>
<td>-32</td>
</tr>
<tr>
<td>2</td>
<td>-19</td>
</tr>
<tr>
<td>3</td>
<td>-32</td>
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</tbody>
</table>

- Change in dosage of NaBH$_4$ in pretreatment step

![Graph showing change in GWP with NaBH$_4$ concentration]
What have we learned?

- **Technology**
  - Moving from fossil-based to bio-based adipic acid production creates environmental benefits
  - Moving from fossil-based to bio-based adipic acid production may also lead to environmental burden shifting
  - Acid-catalyzed pretreatment performs better than alkaline pretreatment

- **Methodology**
  - Using data from large LCA databases can result in misleading results
  - Assessment of the complete biorefinery concept
  - Quantifying the benefits of integration of processes into an overall biorefinery concept
Prospective LCA

• Definition → “Studies of emerging technologies in early development stages, when there are still opportunities to use environmental guidance for major alterations”

• Appropriate methodological choices need to be made
  • Technology alternatives
  • Foreground system
  • Background system

• Incorporating scale-up in LCA for technology under development

• Simulation and LCA

Thanks for your attention

Project partners:

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