Integrated Analysis in Support of the Separations Consortium

Bioenergy Technologies Office Peer Review

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Denver, Colorado

Consortium Analysis Team:

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Goal Statement

**Goal:** Provide an analysis-based foundation to support and guide the research strategies being pursued under the Separations Consortium

**Outcome:**
- A baseline comparison of the strategies being pursued by Separation Consortium compared to commercially relevant off the shelf technologies
- A series of TEAs and LCAs to identify technical targets to improve both economics and sustainability of the proposed projects and guide R&D
- Publications that utilize analysis results to motivate the various strategies developed under the Separations Consortium

**Relevance:** *Ensure that the proposed processes being developed under the Separations Consortium are economically viable, improve sustainability, and are scalable.*
**Quad Chart Overview**

**Timeline**

- **Start Date:** 10/1/2016
- **End Date:** 9/30/2019
- **Completion:** 75%

<table>
<thead>
<tr>
<th></th>
<th>Total Costs Pre FY17</th>
<th>FY 17 Costs</th>
<th>FY 18 Costs</th>
<th>Total Planned Funding (FY 19-Project End Date)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DOE Funded</strong></td>
<td>$500,000</td>
<td>$400,000</td>
<td>$175,000</td>
<td>$115,000</td>
</tr>
<tr>
<td><strong>Partners</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ANL</td>
<td>13%</td>
<td>20%</td>
<td>13%</td>
<td></td>
</tr>
<tr>
<td>LBL</td>
<td>15%</td>
<td></td>
<td>39%</td>
<td></td>
</tr>
<tr>
<td>NREL</td>
<td>38%</td>
<td>57%</td>
<td>39%</td>
<td></td>
</tr>
<tr>
<td>PNNL</td>
<td>38%</td>
<td>23%</td>
<td>48%</td>
<td></td>
</tr>
</tbody>
</table>

**Barriers Addressed**

**Ot-B:** Cost of Production. Advanced and robust separations and molecular efficiency are required to reduce the up to 50% share of separations costs in bioprocesses.

**Objective**

Develop cost-effective, high-performing separations technologies through coordinated separations research that targets challenges relevant to industry and BETO.

**End of Project Goal**

Demonstrate the consortium’s value to BETO and the biofuel and bioproduct communities through documentation of technical advances, influence on process economics, and potential industrial applications of consortium technologies.
Project Overview

History:

– At the consortium’s beginning, the analysis team reviewed current separations strategies utilized in design cases of BETO.
– Utilized this information to identify key cost and sustainability drivers in current design cases as areas to target R&D.

Motivation:

– Many separation options are available; which solutions best address the problem economically and sustainably?
– Provide feedback and guidance to help to bound problems and verify a path towards economic viability and sustainability
– Consider risk and help to define the research space to establish and implement a consortium research portfolio that is relevant at a commercial biorefinery scale
Assess technical, economic, & environmental feasibility of bioproduct/biofuel conversion processes:

- Detailed process analysis with rigorous mass and energy balances
- Identified data needs and further R&D need to improve overall cost and efficiency
- Assess environmental impacts (greenhouse gas emissions, fossil fuel and water consumption)
- Approach is consistent with other DOE BETO sponsored analyses

**Techno-economic Analysis (NREL and PNNL)**

**Life-cycle Analysis (ANL)**

**GREET™: Greenhouse gases, Regulated Emissions and Energy use in Transportation**
Assess technical, economic, & environmental feasibility of bioproduct/biofuel conversion processes:

- *Detailed process analysis with rigorous mass and energy balances*
- *Identified data needs and further R&D need to improve overall cost and efficiency*
- *Assess environmental impacts (greenhouse gas emissions, fossil fuel and water consumption)*
- *Approach is consistent with other DOE BETO sponsored analyses*

### Challenges:

- Data availability and quality
- Uncertainty of capital cost for new and novel technologies
- Ensuring rigor of separations process modeling – particularly when considering scale-up

### Critical Success Factors:

- Techno-economic and life-cycle analyses that have been vetted by stakeholders and that supports all of the Separations Consortium
- Identification of R&D needs to enable improved performance of separation strategies
Integrated Analysis Management Approach

Example data input for TEA:
Raw Material Flowrates
Recovery Efficiency
Regeneration Requirements

Example data feedback from TEA/LCA:
Cost and Sustainability Drivers
Key Data Gaps For Further R&D Needs
Technical Targets/Approach To Reduce Costs and Improve Sustainability

- Participate in monthly calls with entire consortia and BETO
- Participate in IAB meetings (every 6 months) including presenting latest results
- Analysis task QPMs are aligned with specific research areas
- Go/No-Go support for specific research and analysis contributes to decision metrics
- Analysis team has supported a yearly milestone in FY17 and FY18
Sample of input sheets provided to R&D team to Obtain key data for TEAs and LCAs

- Work closely with R&D team to obtain data needed to effectively model proposed separations technology
- Work with industrial advisory board to review TEA and LCA approach and outcome
- Adopt guidance from industrial advisory board to refine analyses
- Analysts participate in the regular calls with BC and TC experimentalists
- Meetings between analysts and experimentalists for data exchange to discuss enabled by open lines of communication among consortium PIs
Where we started
Review of 8 different biomass design cases to:

- Document the basis and cost/sustainability associated with current separations in designs
- Evaluate the impact of any assumptions on costs for separations technologies
- Highlight potential improvement and associated costs that separations could contribute to the design
- Presented and provided to R&D team -- help the development of R&D strategies

- Fast Pyrolysis
- Ex Situ Catalytic Pyrolysis
- Indirect Liquefaction
- Algae Dewatering
- Algae CAP process
- Algae - Hydrothermal liquefaction
- Biochemical biological conversion
- Catalytic Conversion of Sugars
**Accomplishments:**

*Review of separations included in recent design cases*

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**Sample of data collected for ex situ CFP (more details provided in back-up slides):**

<table>
<thead>
<tr>
<th>What are the main components?</th>
</tr>
</thead>
<tbody>
<tr>
<td>What is the basis for the values?</td>
</tr>
<tr>
<td>What is the current status (known)?</td>
</tr>
</tbody>
</table>

**Additional separations processes that could be included in the design base:**

<table>
<thead>
<tr>
<th>Additional separation strategies to be considered.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Advanced membrane technologies, such as Performance Architecture Surface Selective Membranes, could be utilized for the vapor quench step to improve efficiency of carbon recovery.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative strategies that might be required to mitigate risk</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot gas filtration (as discussed in the design base) is needed for the Ex Situ case if additional separation is required on the product stream. This hot gas filter will be placed after the catalytic upgrading reactor, which is a fixed bed.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Alternative strategies that might help improve conversion costs -- Use of waste streams/lost carbon for additional production.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reducing carbon losses to the aqueous phase helps improve the economics of the process. Liquid-phase CO2, if available, can be used to recover carbon lost to the aqueous phase.</td>
</tr>
</tbody>
</table>

**Process integration/intensification by condenser absorbers and decanters are inexpensive, and simple to operate and can be used to add an alternative separation process will most likely be justified if it reduces carbon losses to the aqueous phase and downstream cleanup equipment.**
**Biochemical Example:** Anaerobic production of biofuels are routes towards low cost hydrocarbons however separations is a key driver for both cost and sustainability. 

Focus of this analysis is on recovery strategy for acid intermediates
Accomplishments:
Developing Analyses for Separations Consortium Strategies

Simulated Moving Bed — Off the Shelf Technology

Electrodeionization — Separations Consortium Technology

Pertractive — Separations Consortium Technology

Simplified block flow diagrams of technologies considered

- **Simulated Moving Bed** considered as baseline to compare Separations Consortium Technologies
- **Electrodeionization** is linked with pH 7 fermentation in this study and future work will consider low pH case
- **Pertractive** separation is integrated with low pH fermentation
- Designs based on variation of Q3 BC design case (burned lignin and modified enzyme production)
Accomplishments:

Preliminary TEA Results – Biochemical Pathway

**Compared to baseline technology** -- Strategies being developed under separations consortium have the potential to lower separations costs as illustrated in the above graph (in orange)

**NOTE:** Designs have higher MFSP since lignin upgrading, not considered
Accomplishments:

Greenhouse gas emissions estimated with LCA

- Compared to the off-the-shelf SMB technology, EDI and pertractive separations exhibit lower life-cycle GHG emissions of the renewable diesel produced in the process.
- One key driver of the fuel stage, which includes the conversion step, is NaOH consumption.

Low Sulfur Diesel baseline: 94 g CO$_2$e/MJ
Accomplishments:

*Preliminary LCA results – Biochemical Pathway*

**Water consumption lower through pertractive approach**

Petroleum baseline is 0.06 L/MJ. If use solar energy, EDI becomes ~1 L/MJ.

Note: water consumption not optimized in process modeling.
Accomplishments:

**Summary of Results and Impacts – Biochemical Pathway**

- **Understanding key drivers:**
  - Pertractive technologies show the lowest overall MFSP and improved sustainability parameters, due to higher targeted yields (at 100%) and low raw material make-up (low pH fermentation and limited electricity demand).
  - The Electrodeionization approach has a higher MFSP than pertractive approach primarily due to lower targeted yields (at 95%) and raw material imports (which account for ~$0.03/GGE). Since EDI does not require low pH fermentation, this is a mitigation strategy for the anaerobic acids pathway.

- **Results reviewed by industrial advisory board and compared to expectations on costs**
- **Both technologies are highlighted in the recent update to the Biochemical design report (recently published)**
- **Initial analyses began in FY17 and supported a Q4 milestone for this project.**
- **These results supported an FY18 Q4 milestone for the projects as well as an inter-project Go/No-Go in FY18Q2.**
Thermochemical Example: *Sludge Hydrothermal Liquefaction to Renewable Diesel*

**BASELINE:**
- for WWT plants with nitrogen restrictions, ammonia is stripped out of the water stream (plus a small amount of non-condensable organics), neutralized, and thermally oxidized
- carboxylic acids are unrecovered

**SEPARATIONS CONSORTIUM:**
- ammonia recovered as an aqueous product
- low molecular carboxylic acids recovered (treated as acetic acid in LCA)
Accomplishments:

**Preliminary TEA Results – Thermochemical Pathway**

- Case shown uses the conservative Resin-Wafer (RW) EDI capex.
- At 90% ammonia recovery, selling the aqueous ammonia reduces the MSFP below the design case target.
- For the optimistic RW-EDI capex case ($2000/sq. meter, not shown), ammonia recovery reduces the MFSP even at zero sales value for aqueous ammonia.

**Graph:**

- LCA performed for 90% NH3 recovery case.
- RW Capex = $4000/sq. meter.
- No Co-Product Credit (Ammonia) and (Acid).
- Co-Product Credit (Ammonia) and (Acid).
- Design Case MFSP.

% Ammonia or Acid Recovery vs. $/gge Fuel.
EDI pathway offers lower GHG emissions and fossil fuel consumption than conventional NH$_3$ removal

NH$_3$ and acids are co-products. In case of acids, this is a best case estimate of displacement credit because acids are in aqueous stream and need additional separation. Fossil consumption also calculated (not shown, but has similar trend)
Accomplishments:

Summary of Results and Impacts

- Separations consortium technologies offer improvements in cost, fossil energy consumption, GHG emissions, and water consumption over baseline cases per analysis to-date.
- Once analysis finalized, a journal article will be prepared to highlight role of TEA and LCA in the consortium.
- Initial analyses began in FY17 – with a Q4 milestone for this project.
- These results supported an FY18 Q4 milestone for the projects as well as an inter-project Go/No-Go in FY18Q2.
Relevance

• **Goal:** Provide an analysis-based foundation to support and guide the research strategies being pursued under the Separations Consortium

• **Outcome:**
  – Develop baseline costs for comparison with research improvements
  – Complete TEA and LCA to guide R&D towards cost-effective solutions
  – Publish results for use by stakeholders
  – Identify data gaps for future research

• **Relevance to MYPP Platform Goals:**

  **Advanced Separations are a Key Focus:** Conversion R&D is working to “enable high-performance separations technologies to increase product yields and decrease cost.” (MYPP)

  **Integrated Analysis is working “to provide context and justification for decisions at all levels by establishing the basis of quantitative metrics, tracking progress toward goals, and informing portfolio planning and management”** (MYPP)
Relevance to Bioenergy Industry

Industry Review Undertaken

Example at right: BC separations

- Results presented to IAB board to ensure meaningful analysis
- Cost comparison results reviewed by IAB and compared to expectations for costs

IAB recommendations incorporated into practice (see Future Plans)
Enable focused research on key separations issues: TC Example for NH₃ recovery from HTL aqueous:

- Identified significant sustainability drivers for recovery of NH₃ from HTL aqueous stream
- Identified operating envelope for further research that will result in reduce cost of fuel production

Quick lime (CaO) consumption in conventional removal case prompts large water consumption
Future Work:

Near Term

• Continue to support TEA/LCA needs of consortium
  – Expand beyond design case separation issues by further integration to assist R&D and other consortiums, including
    • Agile Biofoundry
    • Co-Optima
    • ChemCatBio
    • Performance Advantaged Bioproducts

• Support overall consortium goal and provide data needed for public report (Q4 milestone)
  – Document technical advances from each consortium team and their influence on process economics.
  – Review industry-relevant applications of the technologies under investigation
  – Summarize feedback received from the advisory board on the consortium’s progress and impact.
Provide an analysis-based foundation to support and guide the research strategies being pursued under the Separations Consortium.

**Approach**
- Detailed process analysis with rigorous mass and energy balances
- Identified data needs and further R&D need to improve overall cost and efficiency
- Assess environmental impacts (greenhouse emissions, fossil fuel consumption and water consumption)
- Approach is consistent with other DOE BETO sponsored analyses

**Technical Progress**
- Review of design cases – Document current separation technologies utilized in design reports and additional separation needs to improve process performance
- TEA of BC and TC pathways- Developed initial TEAs and LCAs for BC and TC pathways. Compared designs to current off-the-shelf technologies. Identified key R&D drivers to improve cost and sustainability.

Ensure that the proposed processes being developed under the Separations Consortium are economically viable, improve sustainability, and are scalable.

**Future Work**
- Continue to support TEA/LCA of Separation Consortium strategies
- Document technical advances from each consortium team and their influence on process economics.
Responses to Previous Reviewers’ Comments

• This project was not reviewed in FY17
• None
Sample of data collected for ex situ CFP (more details provided in back-up slides):

The outlined process converts lignocellulosic biomass to pyrolysis vapors, which are then upgraded via ex situ catalytic conversion. After condensation and water removal, the upgraded pyrolysis liquid is further deoxygenated in a hydrotreater and fractionated in two distillation columns to produce a blend of diesel and gasoline-range hydrocarbons; heavier products are sent to a hydrocracker before being recycled to the distillation columns. The primary separations required for the process include:

1. Two condenser/absorbers in series, followed by a decanter; they separate the pyrolysis vapor into three streams: non-condensable gases, liquid pyrolysis oil, and wastewater.
2. Product recovery utilizes standard commercially-relevant processes such as distillation columns and flash drums. There is limited potential for improvement in these processes and thus are not reviewed in this effort.
Pyrolysis vapor quench design summary

- The first stage is a high-temperature absorber/condenser that condenses heavy organics using light organics from the low-temperature absorber/condenser as the condensing agent. Using condenser/absorbers, rather than indirect heat exchange, to condense heavy organics helps mitigate fouling concerns.
- Non-condensable gas stream is split to the pyrolysis reactor and to \( \text{H}_2 \) production/recovery.
- The aqueous fraction, which contains water-soluble organics, is sent to the wastewater management area, where most is boiled to produce process steam, while the remaining concentrated stream with carbon is combusted in a regenerative thermal oxidizer.
### Describe the separations designs in the baseline design cases.

<table>
<thead>
<tr>
<th>Question</th>
<th>Vapor Quench</th>
<th>Fuel recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td>What is the basis for these designs?</td>
<td>Two-stage condenser/absorber system that utilizes varying temperatures (low/high). Separates organic fraction from non-condensable gases and an aqueous phase.</td>
<td>Distillation columns</td>
</tr>
<tr>
<td>Where are the costs derived from?</td>
<td>Estimated from Aspen Icarus – standard equipment, off the shelf equipment</td>
<td>Aspen Icarus estimates</td>
</tr>
<tr>
<td>Where did key assumptions/targets come from?</td>
<td>Based on Aspen projections</td>
<td>Aspen simulation projections and literature</td>
</tr>
<tr>
<td>What cost impacts does the separations have on the MFSP?</td>
<td>Will show cost breakout in later slides</td>
<td></td>
</tr>
<tr>
<td>Are there sustainability implications around this proposed design (high electricity use or large amounts of chemicals required)?</td>
<td>Yes – Some electricity demand for chiller that could impact LCA. Higher carbon losses to wastewater will result in lower fuel yields impacting both TEA and LCA.</td>
<td>No</td>
</tr>
</tbody>
</table>
## What are the R&D targets?

<table>
<thead>
<tr>
<th>What is the basis of these values?</th>
<th>Vapor Quench</th>
<th>Fuel Recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Aspen model predictions</td>
<td>No targets Identified</td>
</tr>
<tr>
<td></td>
<td>Targeting 1.3wt% carbon loss to aqueous</td>
<td></td>
</tr>
<tr>
<td>What is the current SOT (if known)?</td>
<td>Current SOT is 2.9wt% based on experimental data (2015)</td>
<td></td>
</tr>
<tr>
<td>What are assumptions/risks associated with meeting these targets (cost impacts?)?</td>
<td>Higher losses of carbon could increase MFSP and impact LCA due to lower fuel yields.</td>
<td></td>
</tr>
</tbody>
</table>
## What are the process design assumptions?

<table>
<thead>
<tr>
<th></th>
<th>Vapor Quench</th>
<th>Fuel Recovery</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>What is the basis of these values?</strong></td>
<td>Design is standard equipment – cost based on Aspen Icarus estimates</td>
<td>Aspen modeling results</td>
</tr>
<tr>
<td></td>
<td>Heat and electricity requirements based on Aspen estimates</td>
<td>Design is standard equipment – cost based on Aspen Icarus estimates</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Heat and electricity requirements based on Aspen estimates</td>
</tr>
<tr>
<td><strong>What is the current SOT (if known)?</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>What are assumptions/risks associated with meeting these targets (cost impacts)?</strong></td>
<td>Lower yields because of lower carbon recovery.</td>
<td>Lower fuel recovery could result in higher costs.</td>
</tr>
</tbody>
</table>