DOE Bioenergy Technologies Office (BETO) 2015 Project Peer Review

Biochemical Platform Analysis

Biochemical Platform Review
March 23, 2015
Alexandria, VA

Ryan Davis
National Renewable Energy Laboratory

This presentation does not contain any proprietary, confidential, or otherwise restricted information
Goal Statement

Biochemical Platform Analysis Objective:

- Provide **process design and economic analysis support** for the biochemical conversion platform, to **guide R&D priorities** for both NREL and BETO
  - Translate demonstrated or proposed research advances into economics quantified as $/gal ($/GGE) selling price

- Project develops benchmark process models in Aspen Plus and related economic analysis tools, used to:
  - Assess cost-competitiveness and **establish process/cost targets** for biofuel production pathways
  - **Track progress** towards goals through State of Technology (SOT) updates
  - Quantify **sustainability metrics** associated with modeled biorefinery conversion operations
  - **Disseminate** rigorous, objective modeling and analysis information in a transparent way (the “design report” process)

- This project **directly supports the BETO Program** by assisting in the development of cost benchmarks and future targets for use in MYPP planning
  - **Guide R&D towards economic viability, eventual adoption of hydrocarbon biofuels into U.S. market**
Quad Chart Overview

Timeline
• Started: 2010
• Finish: 2017
• 75% complete

Barriers
• Barriers addressed
  – BT-H: Cleanup/Separation
  – BT-J: Biochemical Conversion Process Integration
  – BT-K: Product Acceptability and Performance

Budget

<table>
<thead>
<tr>
<th></th>
<th>Total Costs FY 10 – FY 12</th>
<th>FY 13 Costs</th>
<th>FY 14 Costs</th>
<th>Total Planned Funding (FY 15-Project End Date)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Funded ($MM)</td>
<td>$1.8</td>
<td>$1.1</td>
<td>$0.9</td>
<td>$2.7</td>
</tr>
<tr>
<td>Project Cost Share (Comp.)*</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

Partners
• Partners
  • No partners with shared funding
• Other interactions/collaborations
  • INL – Feedstock interface activities, supply chain analysis
  • ANL – GREET modeling team, water quality assessment team
  • PNNL – Biochemical modeling/report reviews
  • Industrial partners
  • Engineering subcontractors
Project Overview

- NREL has a long history of establishing, maintaining, and exercising rigorous process models
  - Set objective, transparent benchmarks for a single plausible conversion pathway
  - Quantify economic impact of funded R&D improvements relative to benchmarks
  - Evaluate sensitivities to uncertainties, process alternatives
  - “Basic engineering” and process optimization
- Phased approach:
  1) Develop baseline models using best available data
  2) Validate and peer review modeling assumptions, publish “design reports”
  3) Assist in cost target development
  4) Iterate with researchers and external stakeholders as new data becomes available to refine models
- Types of analysis:
  - Techno-economic analysis (TEA)
  - Lifecycle analysis (LCA)/sustainability metrics
- Technology focus:
  - 2001-2012: cellulosic ethanol
  - 2013+: hydrocarbon biofuels, bioproducts
Approach (Technical)

- Process model in Aspen Plus based on NREL research data (where available), published literature (when necessary)
- Assumes $n^{th}$-plant project cost factors and financing (ignores first-of-a-kind risks)
- Discounted cash-flow ROR calculation determines minimum fuel selling price (MFSP)
- Credibility of analysis supported by vendor-based cost estimates, thorough vetting with industry and research stakeholders
- Research advances $\rightarrow$ Higher modeled conversion $\rightarrow$ Lower MFSP
Approach (Management)

- Project management tracked using milestones
- Activities are highly integrated with research efforts, assist in go/no-go decisions for R&D
  - Example – FY14 TEA assessment for PHB catalysis to fuels; no-go decision on the research pathway due to challenging cost potential

- Critical success factors:
  - Leverage process design to highlight barriers for scale-up/commercialization in under-researched areas
  - Conduct sensitivity analysis to find biggest “bang for the buck” items for targeted improvement
  - Critical to maintain credible engineering analyses that are transparent and unbiased – Work with engineering subcontractors to reduce uncertainty, subject design reports to thorough external peer review

- Challenges:
  - New technology pathways for hydrocarbon biofuels = lack of public data availability on key process steps, more modeling uncertainty
  - TEA shows that economics are more challenging for long-chain hydrocarbon pathways vs ethanol; requires rigorous process optimization, maximizing carbon yields, considering coproduct opportunities

<table>
<thead>
<tr>
<th>Project Milestones/Activities</th>
<th>FY14</th>
<th>FY15</th>
<th>FY16 (not yet set)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Biological conversion pathway</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water use/WWT optimization in 2013 design case</td>
<td>▲</td>
<td>▲</td>
<td></td>
</tr>
<tr>
<td>Biological conversion R&amp;D out-year targets</td>
<td></td>
<td></td>
<td>▲</td>
</tr>
<tr>
<td>Lignin co-product modeling</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SOT assessment/out-year targeting updates</td>
<td></td>
<td></td>
<td>▲ ▲</td>
</tr>
<tr>
<td>Engineering design/alternative scenario studies</td>
<td></td>
<td></td>
<td>▲ ▲ ▲ ▼</td>
</tr>
<tr>
<td><strong>Catalytic conversion pathway</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Catalytic conversion design report</td>
<td></td>
<td></td>
<td>▲ ▲</td>
</tr>
<tr>
<td>SOT assessment/out-year targeting updates</td>
<td></td>
<td></td>
<td>▲</td>
</tr>
<tr>
<td>Alternative catalytic processing scenarios</td>
<td></td>
<td></td>
<td>▲ ▼</td>
</tr>
</tbody>
</table>

▲ = Milestone, ▲ = Quarterly progress measure, ▼ = Go/no-go decision
Technical Accomplishments/Progress/Results: 2013 Biological Pathway Design Report

- TEA detailed modeling focused on near-term ("2017") goal of $5/GGE selling price for renewable diesel blendstock
- Represents intermediate target on path to ultimate 2022 goal of $3/GGE, but allows for high transparency of process/design details
- Vendor quotes provided for all new operations via engineering contractor
- Thoroughly vetted through 15 industry peer reviewers
- Baseline pathway derived from ethanol process: whole-hydrolysate conversion of C5 + C6 sugars to diesel-range fatty acid intermediate
  - Aggressive targets for yield + productivity
  - Assumed generic organism with fatty acid secretion capability

http://www.nrel.gov/docs/fy14osti/60223.pdf
## 2013 Hydrocarbon Design Report Results – Contrasted Against 2011 Ethanol Design Report

<table>
<thead>
<tr>
<th>Minimum Fuel Selling Price ($/GGE, 2011$)</th>
<th>2012 Target</th>
<th>2017 HC Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3.61</td>
<td>$5.10</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Feedstock Contribution ($/GGE, 2011$)</th>
<th>2012 Target</th>
<th>2017 HC Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.13</td>
<td>$1.76</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Enzyme Contribution ($/GGE, 2011$)</th>
<th>2012 Target</th>
<th>2017 HC Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0.60</td>
<td>$0.37</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Non-Enzyme Conversion Contribution ($/GGE, 2011$)</th>
<th>2012 Target</th>
<th>2017 HC Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.88</td>
<td>$2.96</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Yield (GGE/dry ton)</th>
<th>2012 Target</th>
<th>2017 HC Target</th>
</tr>
</thead>
<tbody>
<tr>
<td>52</td>
<td>45</td>
<td></td>
</tr>
</tbody>
</table>

**Feedstock**

- **Feedstock Cost ($/dry ton)**: $58.50 vs $80.00

**Pretreatment**

- **Solids Loading (wt%)**: 30% vs 30%
- **Xylan to Xylose (including enzymatic)**: 90% vs 90%
- **Xylan to Degradation Products**: 5% vs 5%

**Conditioning**

- **Ammonia Loading (g per L hydrolysate liquor)**: 4.8 vs 1.6
- **Hydrolysate solid-liquid separation**: No vs No
- **Xylose Sugar Loss**: 1% vs 0%
- **Glucose Sugar Loss**: 0% vs 0%

**Enzymes**

- **Enzyme Loading (mg/g cellulose)**: 20 vs 10

**Enzymatic Hydrolysis & Bioconversion**

- **Total Solids Loading (wt%)**: 20% vs 20%
- **Combined Saccharification & Conversion Time (d)**: 5 vs 6.5
- **Corn Steep Liquor Loading (wt%)**: 0.25% vs 0.25%
- **Combined $cellulose$-to-$glucose \times glucose$-to-product$*: 86% vs 86%
- **Xylose to Product**: 85% vs 85%
- **Arabinose to Product**: 85% vs 85%
- **Metabolic Yield (total sugar-to-product)**: 0.44 vs 0.28

- **Theoretical metabolic energy yield limited to ~91% vs EtOH**
- **Cost increase consistent with targets at INL**
- **Reflects 5 more years of commercial enzyme progress**
- **TCI = $583 MM vs $471 MM**
- **Facility on-line time = 90% vs 96%**

---

More information:


*Does not include losses to contamination or cell growth*
Update to Biological Design Case

- While 2013 design case targets are plausible, subsequent R&D benchmark data showed large hurdles to overcome in short time
  - Low C5 conversion with whole hydrolysate
  - Low productivity
  - Best performance seen with yeast (requires extraction of intracellular lipids, not simple secretion of FAs)

- FY14 SOT modifies the process to add C5 sugar separation, conversion to chemical co-product (succinic acid), extraction of lipids from C6 train
  - Allows for more achievable targets by 2017 while maintaining MFSP

<table>
<thead>
<tr>
<th>Bioconversion Metrics – C6 Train to Fuel</th>
<th>Design Report Basis</th>
<th>New Schematic</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bioconversion Volumetric Productivity (g/L-hr)</td>
<td>1.3</td>
<td>0.4</td>
</tr>
<tr>
<td>Glucose to Product [total glucose utilization]</td>
<td>87% [95%]</td>
<td>78% [100%]</td>
</tr>
<tr>
<td>Xylose to Product [total xylose utilization]</td>
<td>82% [86%]</td>
<td>76% [98%]</td>
</tr>
<tr>
<td>Arabinose to Product [total arabinose utilization]</td>
<td>85% [85%]</td>
<td>-</td>
</tr>
<tr>
<td>Intermediate Product Recovery</td>
<td>97%</td>
<td>90%</td>
</tr>
<tr>
<td>Carbon Yield to RDB from Biomass</td>
<td>26.2%</td>
<td>12.5%</td>
</tr>
<tr>
<td>Carbon Yield to Succinic Acid from Biomass</td>
<td>n/a</td>
<td>12.2%</td>
</tr>
</tbody>
</table>
## Out-Year Targeting for R&D

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Minimum Fuel Selling Price ($/GGE, 2011$)</strong></td>
<td>$5.10$</td>
<td>$12.97$</td>
<td>$10.14$</td>
<td>$7.43$</td>
</tr>
<tr>
<td>Feedstock Contribution ($/GGE, 2011$)</td>
<td>$1.76$</td>
<td>$3.88$</td>
<td>$3.20$&lt;sup&gt;1&lt;/sup&gt;</td>
<td>$2.47$</td>
</tr>
<tr>
<td><strong>Conversion Contribution ($/GGE, 2011$)</strong></td>
<td>$3.33$</td>
<td>$9.09$</td>
<td>$6.93$&lt;sup&gt;1&lt;/sup&gt;</td>
<td>$4.97$&lt;sup&gt;1&lt;/sup&gt;</td>
</tr>
<tr>
<td>RDB Fuel Yield (GGE/dry ton)</td>
<td>45</td>
<td>18</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Succinic Acid Yield (lb/dry ton)</td>
<td>NA</td>
<td>197</td>
<td>206</td>
<td>232</td>
</tr>
</tbody>
</table>

### Feedstock
- **Feedstock Cost ($/dry ton)**
  - SOT: $80
  - 2015 Projection: $130
  - 2016 Projection: $115
  - New 2017 Target: $95

### Pretreatment/Separation
- **Xylan to Xylose (including conversion in C5 train)**
  - SOT: 30%<sup>1</sup>
  - 2015 Projection: 30%
  - 2016 Projection: 30%
  - New 2017 Target: 30%

### Enzymes
- **Enzyme Loading (mg/g cellulose)**
  - SOT: 10
  - 2015 Projection: 14
  - 2016 Projection: 12
  - New 2017 Target: 10

### Enzymatic Hydrolysis & Bioconversion – C6 Train
- **Total Solids Loading to Hydrolysis (wt%)**
  - SOT: 20%
  - 2015 Projection: 15%
  - 2016 Projection: 15%
  - New 2017 Target: 17.5%
- **Enzymatic Hydrolysis Time (d)**
  - SOT: 3.5
  - 2015 Projection: 3.5
  - 2016 Projection: 3.5
  - New 2017 Target: 3.5
- **Hydrolysis Glucan to Glucose**
  - SOT: 90%
  - 2015 Projection: 77%
  - 2016 Projection: 85%
  - New 2017 Target: 85%
- **Hydrolysis Residual Xylan to Xylose**
  - SOT: >30%
  - 2015 Projection: 30%
  - 2016 Projection: 30%
  - New 2017 Target: 30%
- **Glucose Sugar Loss** (into solid lignin stream after EH separation)
  - SOT: 1%
  - 2015 Projection: 5%
  - 2016 Projection: 4%
  - New 2017 Target: 2.5%

### Experiment Expt’l bioconversion scale/method
- SOT: NA
- 2015 Projection: Bench scale/Batch
- 2016 Projection: Bench scale/Fed-batch
- New 2017 Target: Bench scale/Fed-batch

### Enzymatic Hydrolysis & Bioconversion
- **Bioconversion Volumetric Productivity (g/L-hr)**
  - SOT: 1.3
  - 2015 Projection: 0.29
  - 2016 Projection: 0.35
  - New 2017 Target: 0.4
- **Lipid Content (wt%)**
  - SOT: NA
  - 2015 Projection: 57%
  - 2016 Projection: 60%
  - New 2017 Target: 60%
- **Glucose to Product [total glucose utilization]**
  - SOT: 87% [95%]
  - 2015 Projection: 75% [100%]
  - 2016 Projection: 78% [100%]
  - New 2017 Target: 78% [100%]
- **Xylose to Product [total xylose utilization]**
  - SOT: 82% [86%]
  - 2015 Projection: 74% [98%]
  - 2016 Projection: 76% [98%]
  - New 2017 Target: 76% [98%]
- **C6 Train Bioconversion Metabolic Yield (Process Yield) (g/g sugars)**
  - SOT: 0.34 (0.28)
  - 2015 Projection: 0.26 (0.26)
  - 2016 Projection: 0.27 (0.27)
  - New 2017 Target: 0.27 (0.27)
- **Carbon Yield to RDB from Biomass**
  - SOT: 26.2%
  - 2015 Projection: 10.4%
  - 2016 Projection: 11.4%
  - New 2017 Target: 11.8%

### Coproduct Production Performance – C5 Train
- **Bioconversion Volumetric Productivity (g/L-hr)**
  - SOT: NA
  - 2015 Projection: 0.3
  - 2016 Projection: 1.5
  - New 2017 Target: 2.0
- **C5 Train Bioconversion Metabolic Yield (Process Yield) (g/g sugars)**
  - SOT: 0.63 (0.59)
  - 2015 Projection: 0.64 (0.60)
  - 2016 Projection: 0.66 (0.65)
  - New 2017 Target: 0.795 (0.74)
- **Succinic Acid Recovery Efficiency**
  - SOT: NA
  - 2015 Projection: 80%
  - 2016 Projection: 80%
  - New 2017 Target: 80%
- **Carbon Yield to Succinic Acid from Biomass**
  - SOT: NA
  - 2015 Projection: 8.9%
  - 2016 Projection: 9.3%
  - New 2017 Target: 10.5%

1. Cost breakdowns to feedstock vs conversion cost contributions are allocated in new target case according to carbon efficiency to RDB fuel vs succinic acid
2. Feedstock costs based on a 5% “ash equivalent” basis for all years considered, consistent with values provided by INL ash “dockage” costs
3. First number represents sugar conversion to desired product (FFA), values in parentheses indicate total sugar utilization

---

SOT demonstrated at NREL; projections based on BETO R&D targets

Recovery yields targeted to be demonstrated by 2017 (2014-2016 fixed constant prior to 2017 demo)
## Conversion Stage Sustainability Metrics - Biological

<table>
<thead>
<tr>
<th>Sustainability Metric ¹</th>
<th>2014 SOT</th>
<th>2015 Projection</th>
<th>2016 Projection</th>
<th>2017 Design Case</th>
<th>2022 Projection ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>GHGs (g CO₂-e/MJ fuel) (fossil emissions)</td>
<td>-63.8</td>
<td>-58.0</td>
<td>-72.0</td>
<td>-78.6</td>
<td>-301</td>
</tr>
<tr>
<td>Fossil Energy Consumption (MJ fossil energy/MJ fuel)</td>
<td>-0.9</td>
<td>-0.8</td>
<td>-1.0</td>
<td>-1.1</td>
<td>-1.3</td>
</tr>
<tr>
<td>Total Fuel Yield (GGE/dry ton)</td>
<td>18</td>
<td>20</td>
<td>20</td>
<td>22</td>
<td>44</td>
</tr>
<tr>
<td>Biomass Carbon-to-Fuel Efficiency (C in fuel/C in biomass)</td>
<td>10%</td>
<td>11%</td>
<td>12%</td>
<td>13%</td>
<td>26%</td>
</tr>
<tr>
<td>Biomass Carbon-to-Coproduct Efficiency (C in succinic acid coproduct/C in biomass)</td>
<td>9%</td>
<td>9%</td>
<td>11%</td>
<td>12%</td>
<td>NA ²</td>
</tr>
<tr>
<td>Water Consumption (m³/day; gal/GGE fuel) ¹</td>
<td>6,294 m³/day (42 gal/GGE)</td>
<td>6,146 m³/day (48 gal/GGE)</td>
<td>5,817 m³/day (45 gal/GGE)</td>
<td>5,773 m³/day (42 gal/GGE)</td>
<td>4,553 m³/day (12 gal/GGE)</td>
</tr>
<tr>
<td>Net Electricity Import (KWh/GGE)</td>
<td>19.9</td>
<td>19.8</td>
<td>21.1</td>
<td>24.0</td>
<td>0.3</td>
</tr>
</tbody>
</table>

¹ Note, gal/GGE water metric is fully allocated to fuel product (not distributed to coproduct train), thus appears high in this format

² 2022 projection represents one possible scenario based on converting a fraction of lignin to adipic acid co-product; pathway reverts back to whole-hydrolysate conversion to fuels, thus removes C5 sugars-to-succinic acid process train

- Project also tracks key sustainability metrics for biorefinery design cases
- Sustainability metrics above only consider conversion stage (not a full Well-to-Wheel LCA)
- Demonstrated improvements in GHG emissions alongside TEA costs when routing lignin to select coproduct options in support of 2022 targets for $3/GGE
Technical Accomplishments/Progress/Results: 2014 Catalytic Pathway Design Report

- Design pathway based on aqueous phase reforming ("APR") catalysis of hydrolysate
  - Potential for flexibility around conversion of multiple hydrolysate species beyond monomeric sugars, including oligomers, acetate, sugar degradation products, soluble lignin, etc.
  - Catalytic upgrading based on patent literature for commodity sugars with additional guidance from industry (engineering subcontractor, technology vendors, and external industry guidance)
  - Maintains consistent front-end assumptions for biomass deconstruction (deacetylation, PT, EH) as biological conversion pathway
- Followed similar approach as biological design report
  - Vendor/subcontractor inputs
  - Report vetted through 11 external peer reviewers


Key updates vs Biological conversion design
### Out-Year Targets: Catalytic Pathway

<table>
<thead>
<tr>
<th><strong>2014 SOT Estimate</strong></th>
<th><strong>2015</strong></th>
<th><strong>2016</strong></th>
<th><strong>2017 Design Case Targets</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Minimum Fuel Selling Price ($/GGE, 2011$)</strong></td>
<td>$7.29</td>
<td>$5.89</td>
<td>$4.83</td>
</tr>
<tr>
<td>Feedstock Contribution ($/GGE, 2011$)</td>
<td>$2.58</td>
<td>$1.95</td>
<td>$1.41</td>
</tr>
<tr>
<td><strong>Conversion Contribution ($/GGE, 2011$)</strong></td>
<td>$4.71</td>
<td>$3.94</td>
<td>$3.42</td>
</tr>
<tr>
<td>Yield (GGE/dry ton)</td>
<td>50.3</td>
<td>59.1</td>
<td>67.5</td>
</tr>
</tbody>
</table>

**Feedstock**
- Feedstock Cost ($/dry ton) | $130 | $115 | $95 | $80 |
- Feedstock Blend
  - Stover
  - Stover
  - Blend
  - Blend

**Pretreatment**
- Solids Loading (wt%) | 30% | 30% | 30% | 30% |
- Xylan to Xylose Conversion (overall) | 81% | 84% | 87% | 90% |

**Enzymatic Hydrolysis**
- Solids Loading (wt%) | 20% | 20% | 20% | 20% |
- Enzymatic Hydrolysis Time (d) | 3.5 | 3.5 | 3.5 | 3.5 |
- Glucan to Glucose Conversion | 77% | 85% | 85% | 90% |
- Enzyme Loading (mg/g cellulose) | 14 | 12 | 10 | 10 |

**Sugar Conditioning**
- Sugar Loss in S/L Separation (Belt Filter) | 5% | 4% | 2.5% | 1% |
- Microfiltration Soluble Retention Loss | 10% | 10% | 10% | 10% |

**Catalytic Conversion and Upgrading**
- Hydrogen Feed Molar Ratio (H₂: total APR feed) | 9.8 | 9.8 | 9.8 | 9.8 |
- Total Hydrogen Consumption (wt % vs APR feed) | 4.6% | 5.3% | 5.9% | 6.5% |
- Hydrogenation WHSV (h⁻¹) | 0.7 | 0.85 | 1.0 | 1.2 |
- APR WHSV (h⁻¹) | 0.7 | 0.8 | 0.9 | 1.0 |
- Condensation WHSV (h⁻¹) | 0.7 | 0.85 | 1.0 | 1.2 |
- Hydrogenation catalyst lifetime (years) | 0.5 | 0.6 | 0.8 | 1 |
- APR catalyst lifetime (years) | 1 | 1.3 | 1.6 | 2 |
- Condensation catalyst lifetime (years) | 1 | 1.3 | 1.6 | 2 |
- Overall C Yield to Fuels vs APR Feed Components | 64% | 70% | 78% | 86% |
- Overall C Yield to Fuels vs Biomass C (vs Total C) | 29% (25%) | 34% (28%) | 39% (32%) | 45% (36%) |

---

1. Feedstock costs shown here based on a 5% “ash equivalent” basis for all years considered, per discussion with INL.
2. Values represent glucan/xylan conversion to both monomeric and oligomeric sugars.

---

*SOT:*
- Based on patent literature (for corn syrup)
- Catalyst lifetime reduced by 50%, C yield to fuels reduced by 25% (assumptions)

*SOT demonstrated at NREL; projections based on BETO R&D targets*

*2015/2016:*
- Interpolated projections to meet 2017 design case targets

---

*All projections based on external SMR H₂ sourcing*
### Conversion Stage Sustainability Metrics - Catalytic

<table>
<thead>
<tr>
<th>Sustainability Metric ¹</th>
<th>2014 SOT</th>
<th>2015 Projection</th>
<th>2016 Projection</th>
<th>2017 Design Case</th>
<th>2022 Projection ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>GHGs (g CO₂-e/MJ fuel)</td>
<td>39.8</td>
<td>42.7</td>
<td>45.8</td>
<td>49.2</td>
<td>-69.4</td>
</tr>
<tr>
<td>Fossil Energy Consumption (MJ fossil energy/MJ fuel)</td>
<td>0.73</td>
<td>0.75</td>
<td>0.78</td>
<td>0.82</td>
<td>0.3</td>
</tr>
<tr>
<td>Total Fuel Yield (GGE/dry ton)</td>
<td>50</td>
<td>59</td>
<td>68</td>
<td>78</td>
<td>76</td>
</tr>
<tr>
<td>Biomass Carbon-to-Fuel Efficiency (C in fuel/C in biomass)</td>
<td>29%</td>
<td>34%</td>
<td>39%</td>
<td>45%</td>
<td>41%</td>
</tr>
<tr>
<td>Total Carbon-to-Fuel Efficiency (C in fuel/C in biomass + NG)</td>
<td>25%</td>
<td>28%</td>
<td>32%</td>
<td>36%</td>
<td>33%</td>
</tr>
<tr>
<td>Water Consumption (m³/day; gal/GGE fuel)</td>
<td>5,038 m³/day (12.0 gal/GGE)</td>
<td>4,635 m³/day (9.4 gal/GGE)</td>
<td>4,269 m³/day (7.6 gal/GGE)</td>
<td>3,817 m³/day (5.8 gal/GGE)</td>
<td>3,496 m³/day (5.3 gal/GGE)</td>
</tr>
<tr>
<td>Net Electricity Export (KWh/GGE)</td>
<td>4.9</td>
<td>3.6</td>
<td>2.6</td>
<td>1.7</td>
<td>0.6</td>
</tr>
</tbody>
</table>

¹ Note, all cases based on external SMR H₂ sourcing basis

² 2022 projection represents one possible scenario based on converting a fraction of lignin to adipic acid co-product

- Sustainability metrics above only consider conversion stage (not a full WTW LCA)
- Alternative H₂ scenarios in design report proved very useful in quantifying large differences between SMR H₂ sourcing and alternative scenarios via *in situ* reforming of sugars or biomass gasification
  - 3-6X lower GHG emissions from conversion stage for alternative (internal) H₂ scenarios vs SMR basis
**Alternative H₂ Sourcing Scenarios**

- **Base case** assumes large hydrogen import purchased from off-site natural gas SMR production (*ex situ*).

- **Alternative case** investigates producing hydrogen internally (*in situ*) via reforming reactions from a fraction of hydrolysate, or by diverting a fraction of feedstock biomass to gasification train.

  - Increases cost to $5.48/GGE (*in situ*), $4.95/GGE (gasification).

  - Requires large fractional diversion of hydrolysate (41%, *in situ*) or biomass (36%, gasification) to generate required H₂ = reduced fuel yield.

  - Although lower yield/higher cost, also tradeoffs in sustainability.
Biochemical Pathways: Path to $3/GGE

- Solid lines = biological pathway, potential for 2022
- Dashed lines = reference for catalytic pathway scenarios for purchased and in situ H₂

*Plot is based on % lignin conversion, vs 80% solubilized upstream in deconstruction via modified alkaline pretreatment

### Chemicals of Interest

<table>
<thead>
<tr>
<th>Product</th>
<th>World Production (thousand tons/year)</th>
<th>Price ($/ton)</th>
<th>Projected growth rate</th>
<th>Primary Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,3 Butadiene</td>
<td>&gt;12,000</td>
<td>3200</td>
<td>5%</td>
<td>Synthetic rubber</td>
</tr>
<tr>
<td>1,4 Butanediol</td>
<td>&gt;1,000</td>
<td>3170</td>
<td>5%</td>
<td>Tetrahydrofuran, specialty chemicals</td>
</tr>
<tr>
<td>Adipic Acid</td>
<td>&gt;3,000</td>
<td>1700</td>
<td>4-4.5%</td>
<td>Nylon-6,6</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>&gt;5,700</td>
<td>1000</td>
<td>2.5%</td>
<td>Nylon-6,6 precursors</td>
</tr>
</tbody>
</table>

- We selected a small subset of chemical coproducts among many more possibilities
- Some coproducts show the potential to achieve $3/GGE target, others do not
- Critical to consider market volume capacity for coproducts from a high-volume industry such as biofuels
  - >25k tons/yr world market volume = minimum cutoff applied here
- TEA is currently higher-level for this process, but will be focus for future work in support of 2022 targets
Relevance

TEA Progression Goals: Biological

TEA Progression Goals: Catalytic (in situ H2)

NREL TEA modeling is highly relevant to BETO goals:
• Helps guide R&D, DOE decisions, out-year target projections
  • Technical targets (yields, process performance, etc)
  • Cost targets (BETO MYPP goal: $3/GGE MFSP by 2022)
• Identifies key R&D directions (yields, coproduct opportunities, etc)
• Analysis can serve a wide variety of stakeholders
  • Industry (facilitate interaction between industry, NREL, DOE)
  • TEA helps to “de-risk” a technology during research stages, prior to commercialization
  • Research community, decision makers

Nov 2014 MYPP Performance Goal:
“By 2017, achieve an nth plant modeled conversion cost of $3.30/GGE via a biochemical or chemical conversion pathway. This contributes to an MFSP of $5.10/GGE, an interim target on the path to $3/GGE fuels.”
Future Work

• Design/engineering assessment:
  – Collaboration with NREL Pilot Scale Integration project to better understand optimal design and cost for commercial-scale aerobic bioreactor systems – Q2 milestone
  – Collaboration with NREL LCA team to consider recommendations for strategies to reduce air pollutant emissions from NREL’s biological pathway model – Q4 Quarterly Progress Measure

• Alternative scenario modeling development:
  – Publication of NREL technical report documenting new C5/C6 parallel conversion strategy (fuels + coproducts); report will incorporate any pertinent updates to refine prior design case model – Q3 milestone
  – Preliminary TEA for catalytic conversion of furans-to-hydrocarbons, in collaboration with NREL Catalytic Conversion of Sugars project – Q4 milestone

• 2015 State of Technology assessment for FY15 R&D data – Q4 milestone

• FY16 and beyond: TEA support for biochem platform in moving to 2022 target ($3/GGE)
  – Go/no go milestone to downselect TEA focus to at least 2 most promising R&D options for achievement of $3/GGE by 2022 – Q2 FY16 go/no go
  – Likely to require lignin conversion to coproducts (R&D currently in progress)
Summary

• Biochemical Analysis task has seen a tremendous amount of activity and achievements since FY13 peer review
  – FY13 biological pathway design report published, showing one path to intermediate $5/GGE target and another to 2022 $3/GGE target
  – Biological pathway subsequently revised to pursue parallel conversion of C6 sugars to fuels, C5 sugars to chemical coproducts
  – FY14 catalytic pathway design report published showing intermediate paths to $4-5/GGE dependent on H₂ source, further paths to $3/GGE
  – Established out-year targets through 2017 to begin guiding near-term R&D goals at NREL, priorities at BETO (including MYPP projections)
  – Quantification of sustainability metrics for both conversion pathways

• TEA work is highly relevant to supporting program directions for BETO, near- and long-term R&D for NREL

• Supports industry and research community via transparent models and design reports, communication with stakeholders

• Further efforts planned moving forward around engineering/design optimizations, model refinements to further improve rigor for complex hydrocarbon pathway models
Responses to Previous Reviewers’ Comments from 2013 Review

• This kind of work is worth doing, but it needs independent verification.
• One means of achieving this important step is the design case peer review process, which is undertaken by NREL’s design reports that document the details of established models prior to publication and the release of these reports. This process solicits feedback from stakeholders in industry, academia, and other national laboratories with representation that spans all technology areas covered in the given pathway model. In many cases, the models and resulting cost estimates are modified as a direct result of the peer review feedback received prior to publication of the final report. Additionally, NREL maintains working relationships with outside partners, and strives to capitalize on opportunities for additional modeling feedback, validation, and/or improvement through these channels, as we are able to incorporate such inputs in publicly available reports.

• Very important to be able to track costs and direct R&D efforts. On-site enzyme production is a questionable approach.
• As noted in recent design report documents, the primary intention for inclusion of on-site enzyme production is to improve transparency in determining the true cost of cellulase enzymes for large-scale production of cellulosic biofuels. The intent is not to imply a judgment call about whether or not the industry should align to this mode of enzyme distribution. Further rationale for this approach in the context of NREL’s integrated biochemical process models may be found in the pertinent design report documentation.
Publications, Patents, Presentations, Awards, and Commercialization

Backup Slides
TEA Cost Projections to 2017 – Catalytic Pathway

With Feedstock Cost Progression

With Feedstock Cost Progression (Detail)

<table>
<thead>
<tr>
<th></th>
<th>2014</th>
<th>2015</th>
<th>2016</th>
<th>2017</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feedstock Basis</td>
<td>Corn Stover</td>
<td>Corn Stover</td>
<td>Blend</td>
<td>Blend</td>
</tr>
<tr>
<td>Total feedstock cost to biorefinery at 5% ash equivalent ($/dry ton)</td>
<td>$130</td>
<td>$115</td>
<td>$95</td>
<td>$80</td>
</tr>
<tr>
<td>Ash dockage vs 5% baseline ($/dry ton)</td>
<td>$11.28</td>
<td>$8.70</td>
<td>$4.40</td>
<td>-</td>
</tr>
</tbody>
</table>

1 Ash dockage fee is included in the overall “cost to biorefinery” and accounts for variances in ash content above 5% projected by INL prior to 2017 (10.5% in 2014, 9% in 2015, 7% in 2016)
• Ethanol leverages decades of NREL R&D experience
• HC pathways are much newer given advances in metabolic engineering
• No single best pathway selected by NREL or DOE
• Intention here is to evaluate a **representative** “middle-of-the-road” product for TEA analysis of the general biological conversion technology pathway
• FFA pathway was selected here due to:
  a) Represents median energy yield of all HC pathways (good indicator of economics)
  b) FFA synthesis is a fundamental pathway extensively studied
     • Avoids selection of fuel product(s) targeted by industry

<table>
<thead>
<tr>
<th>Product</th>
<th>Theoretical yield (metabolic, wt%)</th>
<th>Theoretical carbon yield (metabolic)</th>
<th>Theoretical energy yield (metabolic)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>51%</td>
<td>67%</td>
<td>98%</td>
</tr>
<tr>
<td>Pentadecane</td>
<td>29%</td>
<td>62%</td>
<td>88%</td>
</tr>
<tr>
<td>Farnesene (DXP pathway)</td>
<td>29%</td>
<td>64%</td>
<td>85%</td>
</tr>
<tr>
<td>Farnesene (MVA pathway)</td>
<td>25%</td>
<td>56%</td>
<td>74%</td>
</tr>
<tr>
<td><strong>Fatty Acid (Palmitic acid)</strong></td>
<td>36%</td>
<td>67%</td>
<td>89%</td>
</tr>
<tr>
<td>FAEE (Ethyl palmitate)</td>
<td>35%</td>
<td>67%</td>
<td>90%</td>
</tr>
<tr>
<td>Fatty Alcohol (Hexadecanol)</td>
<td>34%</td>
<td>67%</td>
<td>93%</td>
</tr>
</tbody>
</table>

# 2013 Biological Design Report: Costs for Alternative Biological Pathways

## Pathway Costs and Yields

<table>
<thead>
<tr>
<th>Pathway</th>
<th>Theoretical metabolic mass yield</th>
<th>Theoretical carbon efficiency</th>
<th>MFSP ($/gal)</th>
<th>MFSP ($/GGE)</th>
<th>Production (MMgal/yr)</th>
<th>Production yield (gal/dry ton biomass)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pentadecane</td>
<td>0.29</td>
<td>0.63</td>
<td>$5.19</td>
<td>$4.96</td>
<td>30.0</td>
<td>41.4</td>
</tr>
<tr>
<td>Farnesene (MVA)</td>
<td>0.25</td>
<td>0.56</td>
<td>$6.25</td>
<td>$5.97</td>
<td>27.0</td>
<td>37.3</td>
</tr>
<tr>
<td>Farnesene (DXP)</td>
<td>0.29</td>
<td>0.64</td>
<td>$5.44</td>
<td>$5.20</td>
<td>31.1</td>
<td>43.0</td>
</tr>
<tr>
<td>Farnesene (Anaerobic)</td>
<td>0.32</td>
<td>0.71</td>
<td>$4.61</td>
<td>$4.41</td>
<td>34.8</td>
<td>48.0</td>
</tr>
<tr>
<td>Fatty ester (palmitate ethyl ester)</td>
<td>0.35</td>
<td>0.67</td>
<td>$5.83</td>
<td>$5.55</td>
<td>28.9</td>
<td>40.0</td>
</tr>
<tr>
<td><strong>Fatty acid (palmitate, base case)</strong></td>
<td><strong>0.36</strong></td>
<td><strong>0.67</strong></td>
<td><strong>$5.35</strong></td>
<td><strong>$5.10</strong></td>
<td><strong>31.3</strong></td>
<td><strong>43.3</strong></td>
</tr>
<tr>
<td>Fatty alcohol (hexadecanol, anaerobic)</td>
<td>0.34</td>
<td>0.67</td>
<td>$4.94</td>
<td>$4.70</td>
<td>32.3</td>
<td>44.5</td>
</tr>
</tbody>
</table>
Overview of Catalytic Conversion Process

- Whole-hydrolysate conversion pathway, otherwise same targets as biological case for PT + EH
- Requires more extensive hydrolysate cleanup to remove SS fines (microfiltration), ions (IX) for catalyst protection

Conversion process:
- Hydrogenation + APR yields oxygenated intermediates <C7
- Condensation oligomerizes APR products to fuel-range paraffins and mono-oxygenates
- Mild hydrotreating to complete deoxygenation of condensation organic product phase
- Conversion yields, operating conditions based on patent literature
Framing the Analysis: Sensitivity Plots

**Biological Design Case**
- Xylose to FA conversion
- Bioconversion productivity
- TCI uncertainty

**Catalytic Design Case**
- C conversion efficiency
- TCI/ catalytic conversion capex
- Cellulose to glucose yield

Key Drivers:
- CONV xylose to FA 90%:85%:50%
- CONV productivity 3:1:3:0.4 g/L/hr
- Total capital investment -25%:0%:+25%
- EH enzyme loading 5:10:20 mg/g
- EH cellulose to glucose 95:90:70%
- Catalytic upgrading capital -50%:0%:100%
- CONV Air 0.1:0.4:1 VVM
- Sugar loss in S/L 1%:5%

Carbon efficiency from hydrolysate 0.86:0.7
Total capital investment -25%:0%:+25%
Catalytic upgrading capital -50%:0%:+100%
EH cellulose to glucose 95:90:70%
H₂ price 1.2:1.6:2$/kg
EH enzyme loading 5:10:20 mg/g
Total H₂ feed molar ratio 6:9:8:15
Microfilter Recycle Purge 0%:50%:100%
Microfilter Retentate loss 5%:10%:15%
Sugar loss in S/L 1%:5%
Disc refining option Disc refining: Acid PT
Deacetylation xylan loss 0%:2%:10%
WHSV-APR-1 2:1.2:0.7
PT residence time 2m:5m:10m
PT xylan to xylose 95:90:80%
S/L capital -50%:0%:+50%
PT reactor metallurgy Stainless steel:High alloy
EH % solids 25:20:17.5%
A400 capital -50%:0%:+50%
IX capital -50%:0%:+50%
Belt filter replacement Incl. in maint.:replace every 2 yr
PT acid loading 5:9:20 mg/g
EH time 2:3:5:5 d
PT glucose to glucose 12:10:6%
WHSV-Condensation 2:1.2:0.7
PT temperature 150:158:170°C
PT xylan to furfural 2:5:8%
WHSV-APR-2 2:1:0.7

ΔMFSP ($/GGE)
Base case $4.05
# Succinic Acid

![Diagram of Succinic Acid and its derivatives]

<table>
<thead>
<tr>
<th>Product</th>
<th>World Production (thousand tons/year)</th>
<th>Price ($/ton)</th>
<th>Projected growth rate</th>
<th>Primary Usage</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,4 Butanediol</td>
<td>&gt;1,000</td>
<td>3170</td>
<td>5%</td>
<td>Tetrahydrofuran, specialty chemicals</td>
</tr>
<tr>
<td>Maleic Anhydride</td>
<td>&gt;2,000</td>
<td>1240</td>
<td>5%</td>
<td>Polyster resin, BDO, Fumaric Acid</td>
</tr>
<tr>
<td>Tetrahydrofuran</td>
<td>&gt;1,500</td>
<td>2300</td>
<td>5%</td>
<td>Polymers, solvents</td>
</tr>
<tr>
<td>Poly-butyl succinate</td>
<td>&gt;10-15</td>
<td></td>
<td></td>
<td>Polymer</td>
</tr>
<tr>
<td>Pyrrolidinones</td>
<td>&gt;500</td>
<td></td>
<td></td>
<td>Solvent</td>
</tr>
</tbody>
</table>