2.1.0.301 Analysis & Sustainability Interface

MARCH 6, 2017
CONVERSION

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Goal Statement

GOAL: Develop process models and performing techno-economic analysis:

- Direct researchers towards high impact results
- Complete annual state of research technology (SOT) for pyrolysis oil upgrading
- Provide analysis upon request for BETO

Outcome: Use analysis to enable R&D of sustainable, economic biomass conversion to liquid fuels and chemicals:

- Identify barriers and cost reduction strategies
- Assess sustainability impacts
- Set technical & cost targets
- Track R&D progress

Relevance: addresses BETO Strategic Goal “Provide context and justification for decisions at all levels by establishing quantitative metrics, tracking progress towards goals, and informing portfolio planning and management” (March 2016 MYPP)
Quad Chart Overview

Timeline

- October 1, 2012
- September 30, 2019
- Percent complete:
  - 100% for pre-merit review period
  - 17% for merit review period

Budget

<table>
<thead>
<tr>
<th></th>
<th>Total Costs FY 12–FY 14</th>
<th>FY 15 Costs</th>
<th>FY 16 Costs</th>
<th>Total Planned Funding FY 17-FY19</th>
</tr>
</thead>
<tbody>
<tr>
<td>DOE Funded</td>
<td>$1,245K</td>
<td>$783K</td>
<td>$837K</td>
<td>$2,775K</td>
</tr>
</tbody>
</table>

Addressing Evolving Research Needs

- FY12-14: Pyrolysis oil upgrading, syngas conversion to distillates
- FY15-16: Pyrolysis oil upgrading, syngas conversion to distillates and chemicals, sustainability, biochemical conversion
- FY17-19: Merit Reviewed Project

Barriers Addressed

- **Im-E: Cost of production**
  - Identify cost drivers and cost reduction strategies
  - Use results to direct research
- **St-C: Sustainability data across the supply chain**
  - Provide input to green-house-gas and water usage assessments
- **At-A: Comparable, transparent and reproducible analysis**
  - Publish analysis (e.g. pyrolysis oil upgrading design case and annual SOT)
  - Share results and details with external labs and entities

Partners

- Interactions/Collaborations:
  - ANL: life-cycle analysis
  - INL: feedstocks
  - NREL: techno-economics
  - NREL-SI: techno-economics
  - ORNL: experimentalists
  - PNNL: experimentalists
  - Paul Mathias - Fluor
Project Overview

- **Challenge:** develop **performance and cost models** that can be used to further understand biofuel development needs

- **Question:** how to **focus limited research** dollars towards greatest impact?

- **Context:** **Economic** and **sustainable** biofuel production

- **Project History:**
  - **FY09-14:**
    - Preliminary **pyrolysis upgrading design report** (updated in FY13)
    - Pyrolysis upgrading **SOT** published annually
    - TEA for conversion of **oxygenated intermediates** to distillates
  - **FY15:** **sustainability analysis** project combined
  - **FY16:** **fungal conversion** analysis project combined

- **Overall Objective:** Provide economic analysis for core research. Key FY17 objective: model experimental results at projected mature commercial scale to **support BETO’s 2017 Verification targets** and provide information for public use.
Approach (Management)

Approach Structure

- Annual Operating Plans (AOPS), Project Management Plans (PMPS) in place
- Quarterly reporting to BETO (written & regularly scheduled calls)
- BETO Merit Reviewed in FY16 for the FY17-19 timeframe
- Go/No-Go decision point in FY18
- Tech-to-market: publish analysis for use by stakeholders

Project Structure and Alignment with BETO Portfolio

A&S Interface

Task A: Pyrolysis & Upgrading (65%)
Task B: Oxygenated Intermediates (20%)
Task C: Fungal Conversion (15%)

INL Feedstock Logistics
PNNL Conversion Research Thermochemical Biochemical
ANL Supply Chain Sustainability

Models & Outputs
BETO supported analysis at other labs for 3 Consortiums
Approach (Technical)

Analysis Methodology

- Develop biorefinery models in Chemcad or AspenPlus
- Develop capital and operating costs for ISBL and OSBL*
- Perform discounted cash flow analysis
- Determine sustainability metrics
- Perform sensitivity analysis
- Use consistent assumptions across all BETO analysis

GOALS: Track Progress Reduce Costs

* ISBL = Inside Battery Limits; OSBL = Outside Battery Limits; TEA = Techno-economics; LCA = Life Cycle Analysis
Approach (Technical)

- **Critical Success Factors**
  - Work with PNNL, NREL and INL towards meeting the **FY17 Pyrolysis and Upgrading Verification** targets
    - Biweekly calls with BETO, INL, NREL and PNNL & data exchange
    - Analysts attend **PNNL weekly** conversion team **technical meeting**
    - Scheduled & as needed **analysis meetings** with PNNL researchers
  - Identify **gaps and opportunities**: where is research needed? What research has the greatest impact?
  - Make results **available for public use**

- **Technical Challenges**
  - **Data Transfer for FY17 Verification** (addressed by formal and informal meetings noted above)
  - **Limited Data** (particularly in the early stages of research)
    - Develop **flexible models** to quickly assess scenarios and sensitivities
    - Quantify **sustainability impacts** concurrently with TEA
    - Seek **review** and input from experts outside of PNNL
All annual **milestones** and progress measures **met** (see backup slides for details)
Technical Accomplishments
Task A: Pyrolysis Oil Upgrading

Design Cases are a means for “Prioritizing Conversion Research and Development Barriers” (MYPP)

- **Design cases** include major cost drivers, how future targets can be achieved.
- **Detailed** equipment sizing, costs and heat and material balances
- Seven conversion design cases (NREL, PNNL)
- **Standard assumptions** agreed upon with BETO, ensures consistency and transparency
- Reports receive extensive external review from experts in the field
- **This project directly supports the Pyrolysis and Upgrading pathway towards meeting the 2017 BETO target.**

“By 2017, validate an nth plant modeled minimum fuel selling price (MFSP) of $3/GGE (2014$) via a conversion pathway to hydrocarbon biofuel with GHG emissions reduction of 50% or more compared to petroleum-derived fuel.” (March 2016 MYPP)
Technical Progress
Task A: Pyrolysis Oil Upgrading

Conceptual commercial scale cost and performance models

BETO research is largely **focused on the hydrotreating steps**

- Fast pyrolysis systems are commercially available
- Hydrotreating research supported by this project
Technical Progress
Task A: Pyrolysis Oil Upgrading

Scenario Analysis Informs Research Focus

- **Scenarios are combinations of effects** that acting together can meet the target costs.
- **Key scenario parameters**
  - Reactor space velocity
  - Reactor temperature
  - Reactor pressure
  - Reactor configurations
  - Catalyst cost
  - Catalyst life
  - Catalyst type
  - Catalyst regeneration methods
  - Integrated hydrocracking

- **Design case and research up through FY14** based on 3 reactor system with analysis & research focus on last bed.
- **FY15-16** first two reactors combine into single “deep stabilizer”
- **Scenarios now focus on “deep stabilizer”**

![Graph showing conversion rate with different years and SOT (stages of technology)]
Technical Progress
Task A: Pyrolysis Oil Upgrading

Example of How Scenario Analysis Informs Research

Cases D+E+F combined can reach 2017 target

Individual scenarios are extensions of existing research
Feedstock-Conversion Interface Consortium (FCIC)

- **FCIC Goal**: reduce costs and risks of producing biofuels by including low-cost, diverse feedstocks into the supply chain.

- **Analysis Goal**: model process performance, assess economics and greenhouse gas (GHG) emissions
  - Identify blendstock formulations that reduce fuel production costs
  - Assess sustainability impacts (in backup slides)
  - Understand relationship between feed type and conversion performance

Supports BETO key Activity (MYPP): “Understand relationship between feedstock quality and conversion”
Technical Progress
Task A: Pyrolysis Oil Upgrading

TEA results from 1st TEA publication* shown here combined with results from 2nd publication draft

Technical Progress Task B: Oxygenated Intermediates Conversion

Problem: Multiple catalytic conversion routes from oxygenates to distillates and products being pursued experimentally

Solution: Compare relative economics to identify gaps and opportunities to help narrow research focus

<table>
<thead>
<tr>
<th>Conversion Routes to fuels and co-products*</th>
<th>Co-Product Analysis Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol → n-octanol + 2-ethylhexanol → fuels</td>
<td>$3/gge achievable with co-product</td>
</tr>
<tr>
<td>Ethanol → n-butanol → fuels</td>
<td>$3/gge achievable with co-product</td>
</tr>
<tr>
<td>Ethanol → 1,3-butadiene → fuels</td>
<td>$3/gge may be achievable with co-product</td>
</tr>
<tr>
<td>Ethanol → i-butene → fuels</td>
<td>1 mole CO₂ produced / mole butene; butene value won’t offset yield loss</td>
</tr>
<tr>
<td>Syngas → light olefins → fuels</td>
<td>ethylene &amp; propylene recovery cost &gt; added revenue</td>
</tr>
</tbody>
</table>

Joint NREL-PNNL analysis completed Q4 FY15 (published FY16) helped eliminate pathways that co-form CO₂ (Tan et al, 2016)

Co-product analysis at PNNL also informed decision making
Technical Accomplishments Task B: Oxygenated Intermediates Conversion

► **Result:** Focused catalyst research on three most promising catalytic routes (gray boxes are eliminated routes)

► **Next step:** work with researchers to further narrow focus

► **In Addition:** working with Paul Mathias (Fluor) to improve modeling of non-ideal separations

Using analysis to support researchers Go/No-Go decisions towards focusing on the most impactful catalyst research
**Problem:** need higher fuel yields to meet 2022 targets

**Solution:** Investigate hybrid biological / thermochemical processing

- Sugar conversion to lipids using **oleaginuous yeasts**
- Hydrothermal Liquefaction (HTL) to convert lipid reactor effluent carbon (e.g. lipids, organism, unconverted sugars) and lignin to fuel precursors
- Hydrotreat (HT) HTL biocrude to distillate fuel

**Goal:** Use analysis to direct biochemical research towards meeting the BETO 2022 target costs
Technical Progress
Task C: Biochemical Conversion

- Determined **SOT MFSP** to serve a basis for tracking future research
- Performed sensitivity analysis to **ID research gaps** and opportunities
- Preparing **TEA draft** for submission to peer reviewed journal (first-of-a-kind research and analysis)

**PROCESS CONFIGURATION**

<table>
<thead>
<tr>
<th>Feedstock Cost</th>
<th>FEEDSTOCK COST</th>
</tr>
</thead>
<tbody>
<tr>
<td>$120/ton</td>
<td>Feedstock cost, $120/ton</td>
</tr>
<tr>
<td>$60/ton</td>
<td>Feedstock cost, $60/ton</td>
</tr>
</tbody>
</table>

**CAPITAL**

| Bioreactor (seed and lipid production) area installed cost, +25% |
| Bioreactor (seed and lipid production) area installed cost, -50% |

**YIELDS**

- Hydrothermal liquefaction yield after separation, 50% wt per dry feed
- Hydrothermal liquefaction yield after separation, 60% wt per dry feed
- Hydrotreating yield after separation, 80% wt per dry feed
- Hydrotreating yield after separation, 90% wt per dry feed
- Annual production yield, 80 MMgge per year
- Annual production yield, 105 MMgge per year

**OPERATING PARAMETERS**

- Lipid production tank retention time, 72 hrs
- Lipid production tank retention time, 30 hrs
- Seed tank retention time, 48 hrs
- Seed tank retention time, 24 hrs
- Aeration rate, 0.6vvm
- Aeration rate, 0.2vvm
- Hydrogen consumption for hydrotreating, 4.2% g/g dry feed
- Hydrogen consumption for hydrotreating, 3.2% g/g dry feed

**CATALYSTS & CHEMICALS**

- Chemical cost, +100%
- Chemical cost, -100%
- Nutrient cost, +100%
- Nutrient cost, -100%
- Catalyst cost (HTL and HT catalysts), +100%
- Catalyst cost (HTL and HT catalysts), -100%

**MFSP range is $3/gge to $7/gge**
**Technical Progress**

**Task C: Biochemical Conversion**

- **Opportunities for Fungal Processing**
  - FY15 white paper reviewed
    - potential fuel precursors
    - finishing requirements to gasoline, diesel and jet
  - Completing draft for journal submission

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"Conversion technologies that produce renewable diesel and...jet can fill the need for biomass-based alternatives for these...markets" (MYPP March 2016)
PROJECT GOAL: Develop cost and performance models to enable R&D of sustainable, economic biomass conversion to liquid fuels and chemicals

Why project is important

- Develops experimentally-based modeled production costs indicating high impact research areas for conversion
- Assists researchers in defining targeted research
- Makes best use of limited research funding

BETO Analysis & Sustainability Strategic Goals: “Provide context and justification for decisions at all levels by establishing quantitative metrics, tracking progress towards goals, and informing portfolio planning and management” (MYPP)
Relevance to Meeting Platform Goals and Objectives of the BETO Multi-Year Program Plan

► Task A (Pyrolysis Upgrading) directly supports: “By 2017, validate an nth plant modeled minimum fuel selling price (MFSP) of $3/GGE (2014$) via a conversion pathway to hydrocarbon biofuel with GHG emissions reduction of 50% or more compared to petroleum-derived fuel.” (March 2016 MYPP)

► Metrics and technical targets are TEA driven

► Enabled focused catalyst research to reduces costs
  - Longer life
  - Less expensive catalysts
  - Regeneration protocols

► Tasks B and C provide analysis input to researchers indicating cost-reduction opportunities for gasoline, jet & diesel supporting: “By 2022, validate an nth plant modeled MFSP of $3/GGE (2014$) for two additional conversion pathways to hydrocarbon biofuel with GHG emissions reduction of 50% or more compared to petroleum-derived fuel” (March 2016 MYPP)
Relevance

Relevance to Advancing State of Technology

- Supporting BETO funded projects at other DOE laboratories
  - Input (from PNNL process models) to ANL Supply Chain Sustainability Analysis and GREET Model for pyrolysis pathway
  - Input and review for the NREL’s Biomass Scenario Model and JEDI (Jobs) model
  - TEA for ORNL hydrotreating catalyst development

- Supporting BETO consortia
  - Direct support for
    - Feedstock-Conversion Interface Consortium (major)
    - Consortium for Computational Physics and Chemistry (minor)
  - Models leveraged for other multi-lab consortia projects
    - Fuel and Engine Co-Optimization
    - Separations Consortium
Technology Transfer & Relevance to Bioenergy Industry

► Publications
- Pyrolysis Upgrading Design Case contains detailed process inputs and results available for use by stakeholders (industry, universities, other research organizations)
- Pyrolysis upgrading SOT annual publication
  - Details of improvements underlying the cost reductions reported in the MYPP
  - Industry and university advances
  - Less expensive catalysts
- Journal publications, presentations and other lab reports are listed in backup slides

► Information Dissemination & Use
- Energy Information Agency: shared example pyrolysis & upgrading process models
- Biomass Technology Group (BTG) The Netherlands: shared example pyrolysis upgrading stoichiometric calculations
- Universities: field faculty and student analysis & modeling related questions
Future Work (next 18 months)

- **Task A: Support Pyrolysis & Upgrading Verification**
  - Complete analysis related to FY17 Verification
  - Leverage all scales of experimental work (bench, pilot, demo)
  - Complete reporting of all FY17 Verification analysis for publication
  - Complete draft report of pure and blended feedstocks for submission to peer reviewed journal
  - Present results at FY18-19 conferences

- **Task B: Support Oxygenated Intermediates Upgrading**
  - Assist catalyst researchers to find best focus for distillate fuels and chemicals production
  - Investigate fuel/products scenarios leading to cost reductions and taking into account fuel/chemical market size
Future Work (next 18 months)

► **Task C: Support Biochemical Conversion**
  - Assist fungal researchers with identifying promising routes to fuels and chemicals
  - Submit BC/HTL TEA draft and Fungal Conversion paper to peer reviewed journals
  - Leverage upgrading strategies from related work (e.g. thermochemical research)

► **Sustainability** integrate sustainability metrics with economics to understand the tradeoffs

► **Key milestones and deliverables**
  - 2017 Pyrolysis and Upgrading FY17 Verification TEA (9/2017)
  - **FY18 Go/No-Go**: continuation of project in present form or divide into subtasks under respective research tasks
Summary

Guide Research - Track Progress - Reduce Costs

- **Approach** closely coupled analysis and research
- **Technical Accomplishments/Progress/Results**
  - Identified sustainable cost reduction strategies
  - Enabled impactful, focused research
  - Published results for use by stakeholders
- **Relevance** directly supports BETO’s 2017 and 2022 goals
- **Future work**
  - Analysis support for 2017 Verification and SOT reporting (FY17 & 18)
  - Submit 3 manuscripts to peer reviewed journals (FY17)
  - Go/No-Go (mid-FY18)
- **Status since 2015 Review**: expanded collaborations with other labs
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ANL
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Z. Wang
Felix Adom

INL
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Damon Hartley
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Tyler Westover
Erin Searcy
Additional Slides

- Milestones and Quarterly Progress Measures
- Response to comments from 2013 Review
- Publications & Presentations
- List of abbreviations
### Technical Accomplishments: Milestones Since FY15 Review

<table>
<thead>
<tr>
<th>Description (QPM=quarterly progress measure)</th>
<th>Due Date</th>
<th>Completed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Completed pyrolysis SOT report detailing technical accomplishment completed to meet the 2014 targets, including sustainability metric update (Annual Milestone)</td>
<td>Mar-15</td>
<td>completed</td>
</tr>
<tr>
<td>Draft oxygenates to distillates design case completed for external review (with NREL), including sustainability metrics (QPM)</td>
<td>Jun-15</td>
<td>completed</td>
</tr>
<tr>
<td>Complete a manuscript draft to be submitted to a peer-reviewed journal on integrated TEA/sustainability analysis that will focus on key uncertainties/sensitivities around bio oil based fuel production processes and identify trade-offs and/or synergies among economics and sustainability metrics. This will facilitate better informed biorefinery design decisions for optimized cost and sustainability performance. (Stretch Milestone)</td>
<td>Sep-15</td>
<td>Stretch milestone moved and completed in FY16</td>
</tr>
<tr>
<td>Deliver to BETO an updated pyrolysis and upgrading target table showing FY15 progress towards the performance goal of $3/gge, including sustainability metrics</td>
<td>Dec-15</td>
<td>completed</td>
</tr>
<tr>
<td>Publish completed pyrolysis and upgrading SOT report detailing technical accomplishments completed to meet the FY15 targets, including updated sustainability metrics and industry and university accomplishments.</td>
<td>Mar-16</td>
<td>completed</td>
</tr>
<tr>
<td>Complete TEA and summarize in a brief the co-product opportunities related to the fuel only production pathways developed in FY15</td>
<td>Jun-16</td>
<td>completed</td>
</tr>
<tr>
<td>Complete TEA and brief researchers on results from updating the fungal lipid &amp; isoprenoid/polyketide biorefinery process models and costs with data from literature and FY15 and early FY16 research</td>
<td>Jun-16</td>
<td>completed</td>
</tr>
<tr>
<td>Deliver to BETO an updated pyrolysis and upgrading target table showing FY16 progress towards the performance goal of $3/gge, including sustainability metrics.</td>
<td>Sep-16</td>
<td>completed</td>
</tr>
<tr>
<td>Complete TE and sustainability analysis for the newest set of blended feed data from the INL/NREL/PNNL feedstock interface experimental project, compare to the projected goal of $3/gge, include sensitivity analysis and summarize the TEA &amp; LCA results in a brief to BETO. (QPM)</td>
<td>Dec-16</td>
<td>completed</td>
</tr>
<tr>
<td>Complete baseline TEA and projected improvements for conversion of ethanol to C4 linear olefins using a one step process, review results with the researchers for use in the experimental project 2.3.1.304/2.3.1.305 Q2 milestone and summarize in a brief to BETO. (QPM)</td>
<td>Mar-17</td>
<td></td>
</tr>
<tr>
<td>Complete updated fungal biochemical conversion model with the most recent experimental data, including co-product opportunities, review results with researcher and summarize in a draft to BETO that can be submitted to a peer reviewed journal. (QPM)</td>
<td>Jun-17</td>
<td></td>
</tr>
<tr>
<td>Complete (1) draft manuscript of economic and sustainability and sensitivity impacts from fast pyrolysis and upgrading of blended feedstocks for submission to a peer reviewed journal. (QPM)</td>
<td>Jun-17</td>
<td></td>
</tr>
<tr>
<td>Evaluation of the 2017 pyrolysis demonstration: Produce the updated pyrolysis 2017 SOT analysis, based on the experimental data from the demonstration, showing the progression towards the goal of $3/gge, and the associated sustainability metrics. This will be delivered to BETO in the form of a spreadsheet containing the water fall charts and sustainability tables for input to the MYPP. A summary brief will also be delivered to BETO. (ANNUAL)</td>
<td>Sep-17</td>
<td></td>
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</table>
Responses to Previous Reviewers’ Comments

Reviewer Comments

- Great work on looking beyond GHG, such as water, etc. Good attempt at striving for detail in OSBL (such as hydrogen production, waste water, etc). This is typically the weak link and requires site specific information and the experience on an EPC contractor. ISBL falls out with Aspen and costing techniques, although most likely based on Gulf Coast economics so be careful. Need to make sure that everyone within National Lab system that is using Aspen costing are calibrated. A TEA user group would help here to join up on assumptions and physical properties, which may already exist. Can the Aspen tool be developed in a way that it can be readily applied (and not abused) in the hands of the researcher?

- This project is making good progress and provides useful insights to researchers about where opportunities to reduce costs exist. There is good coordination with related analyses at other labs. Like other DOE Design Cases dealing with Nth plants, this one does not provide economics relevant to early adopters for the first several plants where costs will me much higher. First plants will require much greater capital and contingency expenditures, for example, and the present analyses do not adequately address these. DOE should consider other types of analyses to assist with early commercial adoption of emerging technologies.

- The work is well planned and executed. It would benefit by the inclusion of creation of simple spreadsheet-based tools that could be distributed to researchers, allowing them to quickly assess the impact of their work and set firm targets for performance improvements.

- Much needed economic analysis that needs to standardize the metrics that projects are evaluated by. This project demonstrates good progress and clear reporting. As an 'interfacing" activity it should also drive toward achieving 2017 objectives, and not just an approach to see how it turns out.

PI Response: Thank you for your review. We agree that standard assumptions and methods are vital with regard to analysis. BETO meets monthly with the labs in a regularly scheduled meeting to ensure that design cases, MYPP updates and overall assumptions are aligned. Aspen and related software does tend to require experience to make it useful, and consideration should be given to how best to make these methods and results more generally available for use by all stakeholders. While Nth plant assumptions are useful for tracking the effects of research improvements, we agree that it does not address first-of-a-kind plants. That is being addressed, for example, with NREL’s Biomass Scenarios Model.

We also agree that merely modeling the research results at the end of each year is insufficient in terms of assisting research directions. Hence, a key aspect of this project is the ongoing dialogue between the researchers and the analysts throughout the year, meeting several times per month. New experimental results are incorporated into the models, and the analysts provide feedback to the researchers on the resulting cost impacts as well providing cost reduction scenarios that are used to plan future experiments.
Publications since 2015 Peer Review


Publications & Presentations

Publications since 2015 Peer Review, cont.


Presentations since 2015 Peer Review


Technical Progress
Task A: Pyrolysis & Oil Upgrading

- **Key finding:** Yields, costs and GHG reduction do not necessarily trend in the same direction (e.g. compare switchgrass fuel production costs to conversion GHGs)
- Important to **assess Cost and Sustainability together**

**Conversion GHGs**

- Natural Gas
- Electricity
- Catalyst
- Infrastructure
- Waste Disposal

Assess blendstocks and their processing to understand sustainability impacts

**Methodology**
- GHG emissions evaluated with SimaPro software, the GREET model, and the EcoInvent database.
- Feedstock and end use analysis underway
Abbreviations and Acronyms

- ANL: Argonne National Laboratory
- AOP: annual operating plan
- BC: Biochemical Conversion
- BETO: Bioenergy Technologies Office
- GGE: gasoline gallon equivalent
- HTL: hydrothermal liquefaction
- INL: Idaho National Laboratory
- LCA: life-cycle analysis
- MFSP: minimum fuel selling price
- MYPP: multi-year program plan
- NREL: National Renewable Energy Laboratory
- ORNL: Oak Ridge National Laboratory
- PMP: Project Management Plan
- PNNL: Pacific Northwest National Laboratory
- SCSA: supply chain sustainability analysis
- SOT: state of research technology
- TEA: techno-economic analysis