CLEAN ENERGY MANUFACTURING ANALYSIS CENTER

CEMAC: Market Analysis of Biomass-Based Chemicals Substitutions

WBS NREL 6.3.0.5, PNNL 6.3.0.6, ANL 6.3.0.7

2017 BETO Peer Review

March 7, 2017

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Goal Statement of Project

Goal: To develop analyses and methodologies:

- To understand ***manufacturing costs and value-added along the supply chain,*** U.S.-specific competitive advantages, and potential market impacts of lignocellulosic-derived chemicals.
- That can be ***leveraged by decision-makers to inform investment strategies, policy, and other decisions*** to promote economic growth and competitiveness in the transition to a clean energy economy.

Relevance: Directly aligns with DOE BETO's strategic goals to provide an "analytical framework for bioproducts research" and to "develop bioproducts that enable biofuels". Goes beyond techno-economic considerations and includes market drivers and sustainability metrics in evaluation.

Outcome: Analyses of bioproduct production strategies that include economics, market assessments, and life cycle considerations. Detailed report that includes the results of the study. Development of new metrics to incorporate in analyses when producing chemical from biomass.

Quad Chart Overview

Timeline

- Start Date: October 1, 2016
- End Date: March 31, 2017
- Completion: 95%

Barriers

- At-A: Comparable, Transparent, and Reproducible Analyses
- At-C: Data Availability across the Supply Chain
- Im-A: Inadequate Supply Chain Infrastructure

Budget

	Total Costs FY 12 –14	FY 15 Costs	FY 16 Costs	Total Planned Funding (FY 17-Project End Date)
DOE Funded	$0	$0	$245 (NREL) $25 (ANL) $25 (PNNL)	$168 (NREL) $25 (ANL) $75 (PNNL)

Partners

- NREL (76%)
- PNNL (14%)
- ANL (10%)

CEMAC Project Overview: *History*

CEMAC Clean Energy Manufacturing Analysis Center

Operated by the Joint Institute for Strategic Energy Analysis

The Clean Energy Manufacturing Analysis Center (CEMAC) provides **unique and high-impact analysis, benchmarking, and insights of supply chains and manufacturing for clean energy technologies that can be leveraged by decision makers to inform research and development strategies,** and other policy and investment decisions. Housed at the National Renewable Energy Laboratory and operated by the Joint Institute for Strategic Energy Analysis, CEMAC engages the DOE national lab complex, DOE offices, U.S. federal agencies, universities, and industry to promote economic growth and competitiveness in the transition to a clean energy economy.

CEMAC was established in 2015 by the U.S. Department of Energy's Clean Energy Manufacturing Initiative.

CEMAC Overview: *Objective*
Create Partnerships and Bridge Strategic Gaps

Key questions

- What is the global & regional supply chain?
- What drives competitiveness?
- How is competitiveness changing?
- How does competitiveness align with roadmaps?

Clean Energy Manufacturing Analysis Program

- Transparent, consistent, validated methods?
- Regular update process
- Widely available reports and insights
- Protection of proprietary data

… a collaboration between organizations

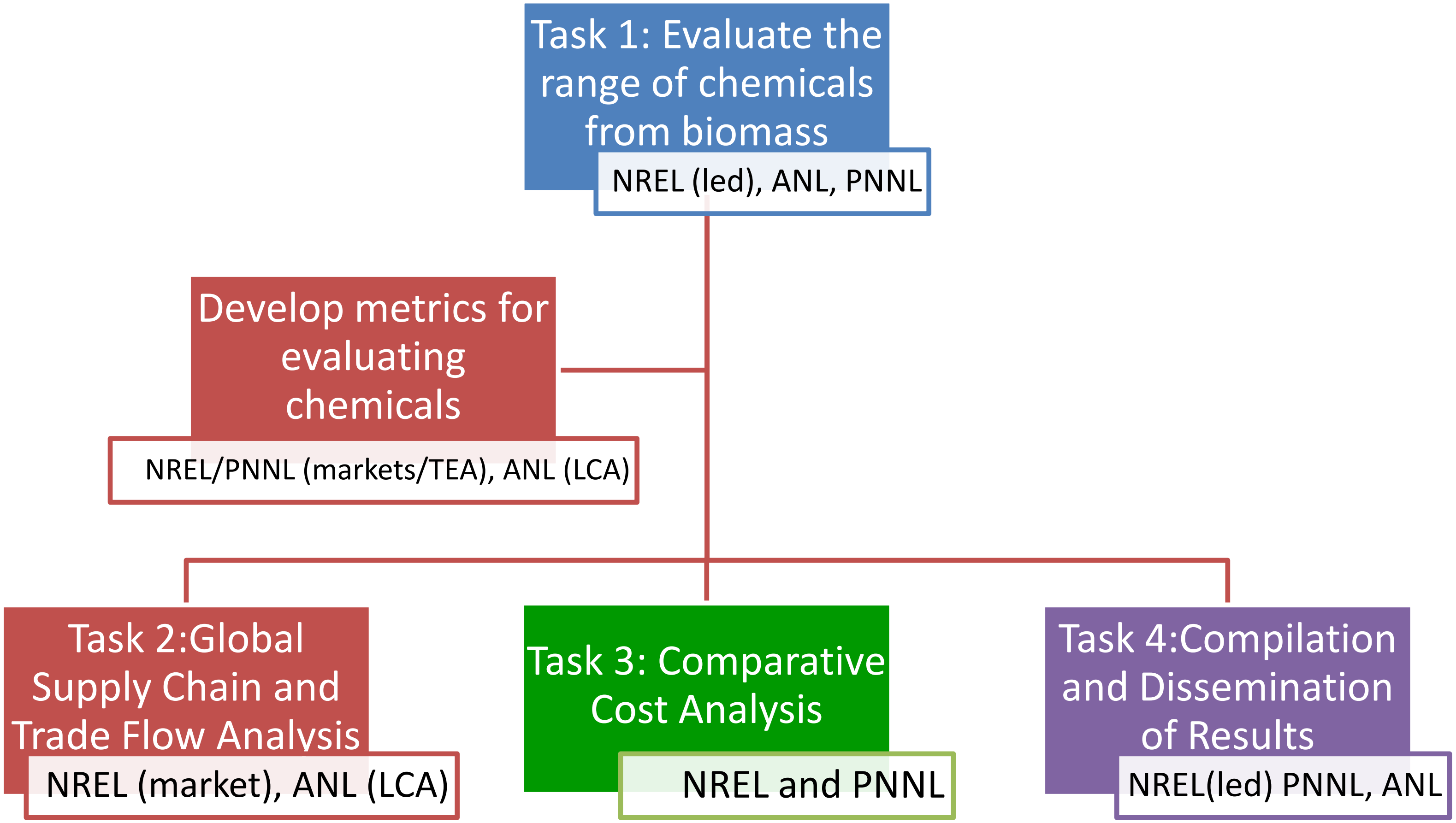
… a framework for world-leading strategy

… a hub to accelerate innovation

Key partners

- DOE Offices
- F500 Firms
- Startups
- State & local gov't
- National Labs
- Federal officials
- Academics

Project Approach: *Management*



- Monthly calls with entire team (including DOE) to discuss progress and next steps.
- Clear timeline on tasks/due date of deliverables and clear definition of responsibility.
- Yearly meeting with entire CEMAC team and external advisory board.
- Yearly CEMAC analyst day held at DOE to review project details.

Project Approach: *Technical*

Task 1: Selection of Biomass-Derived Chemicals and Products for Evaluation

- Evaluate a broad range of chemicals with a focus on platform chemicals
- Develop metrics for screening and reviewing impacts of producing biomass-derived chemicals

Task 2: Global Supply Chain and Trade Flow Analysis

- Collect data that will define the current and expected global supply chain and trade flow

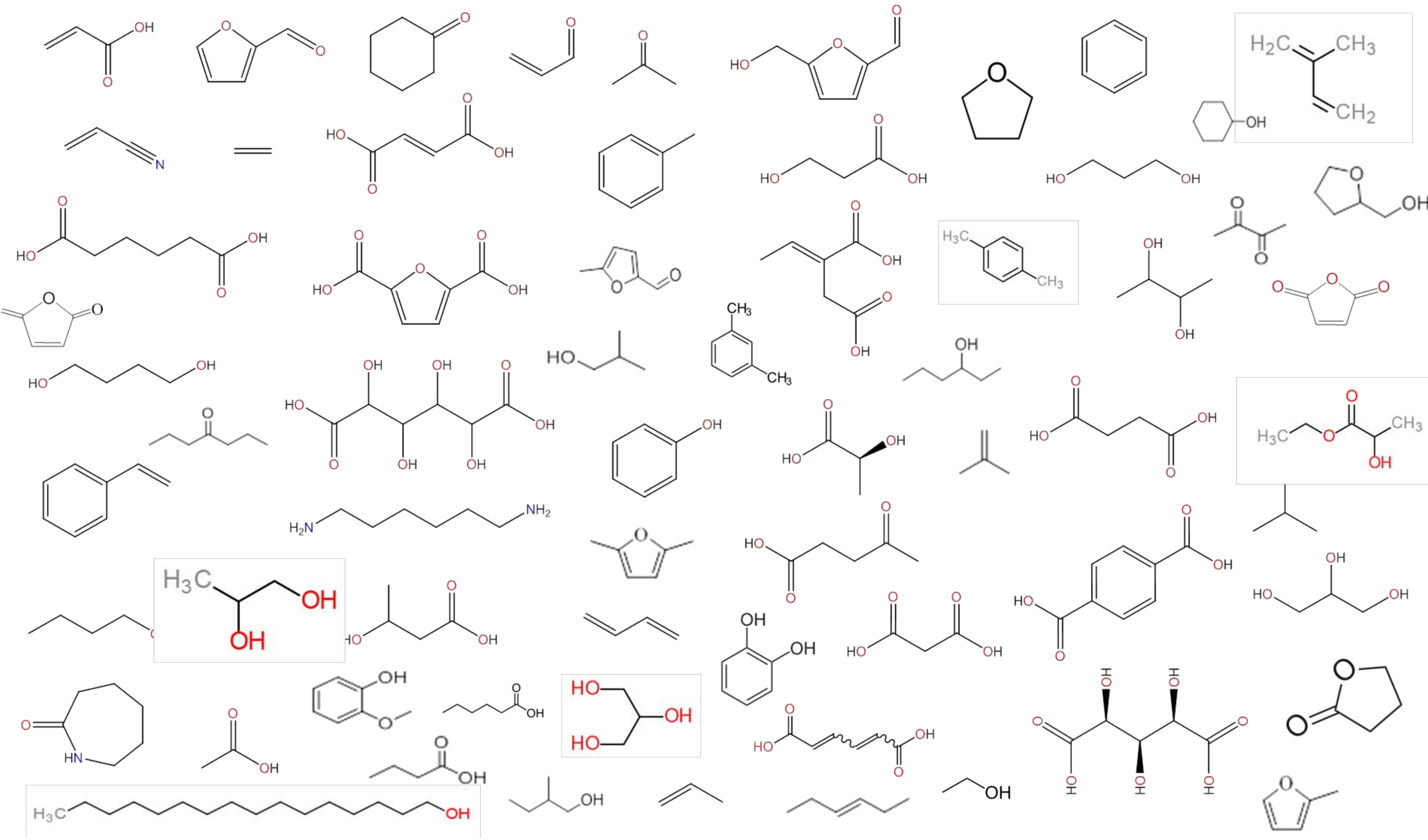
Task 3: Comparative Cost Analysis

- Adapt existing techno-economic analyses to calculate the cost of synthesis of a small (2-3) subset of important biomass-derived chemicals and products

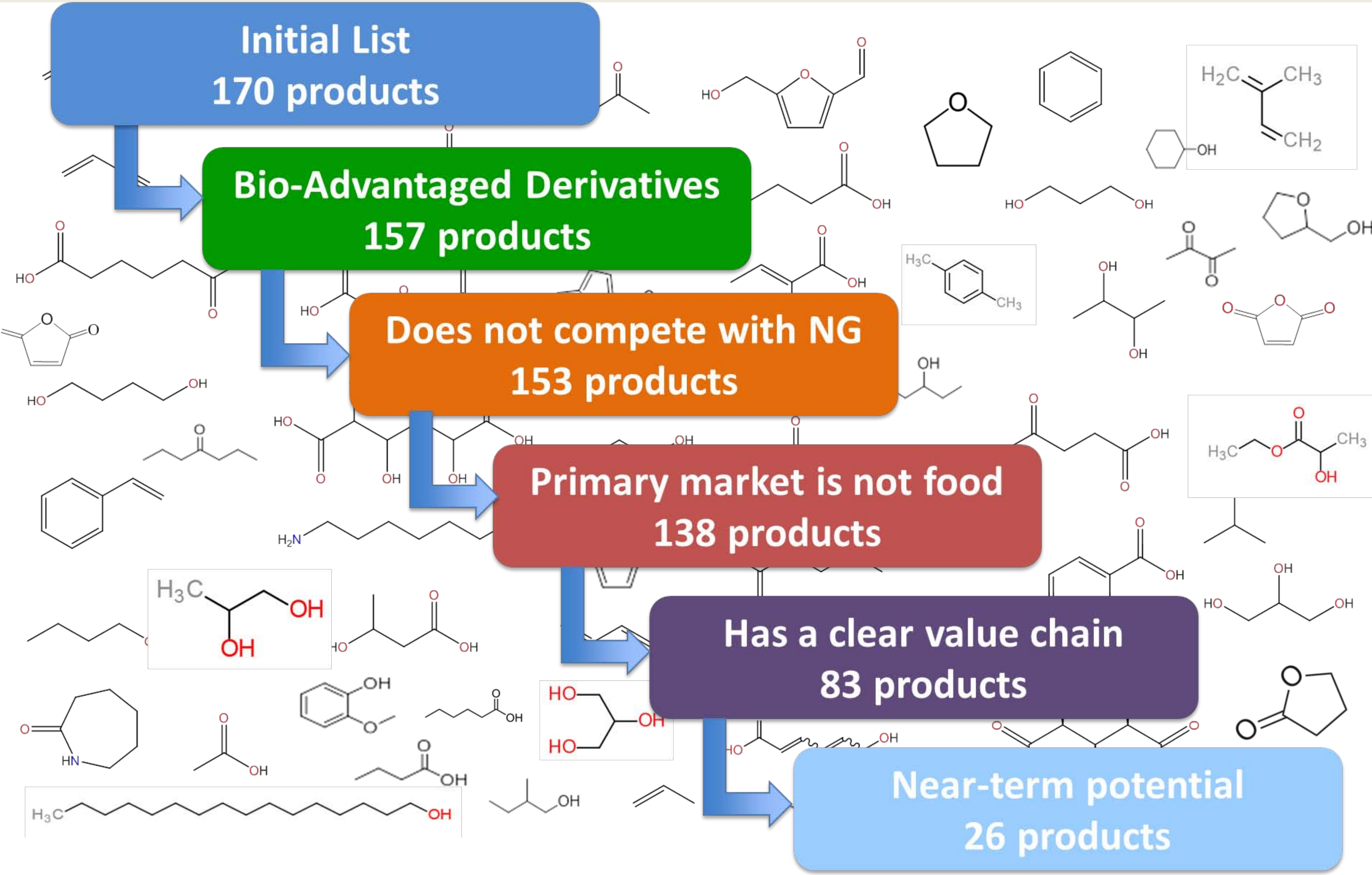
Task 4: Compilation and Dissemination of Results

Critical Success Factor: Data quality and availability.

Screening of biomass-derived chemicals: *Accomplishments*



Screening of biomass-derived chemicals: *Accomplishments*



Selection of biomass-derived chemicals and products for evaluation: *Accomplishments*

Product/Supply Chain Details

- Functional or direct replacement
- Expected end-use and end products
- Current production route from fossil
- Primary producers and consumers
- Captive or merchant market considerations

Conversion Processes

- Range of production platforms
- Estimated technical readiness level
- Data gaps/cost drivers/R&D needs
- Currently being pursued from commodity feedstocks? And from lignocellulosic biomass?

Market and Economics

- US and global consumption
- Projected growth of product and downstream products
- Current and historic average price
- US imports/exports (historic, current, projected estimates)

Sustainability

- Greenhouse Gas Emissions (GHG)
- Potential reduction versus fossil basis
- Key drivers in GHG impacts
- Water footprint
- Non-GHG drivers/reasons to replace the chemical from biomass

Selection of biomass-derived chemicals and products for evaluation: *Accomplishments*

Address Key Questions:

- Can a business case be made for this bioproduct? (Why?)
- Does the bioproduct make sense for CEMAC considerations?
- Does the bioproduct align with the DOE Bioenergy Technologies Office goals?
- What is DOE's motivation for the bioproduct?

LCA considerations: *Accomplishments*

Chemical compounds	Could offer significant benefits	Unlikely to offer significant benefit	Not enough information to know whether will offer a benefit	Notes	Sources		
					GREET	Peer-reviewed article	Industry or company website
Acrylic acid	X			55% GHG reduction (Cradle to grave)	X		
Acrylonitrile	X			29% GHG reduction (Cradle to grave)		[1]	
Adipic acid	X			85% GHG reduction (Cradle to grave)	X	[2]	
Butanediol (1,4-)	X			50% GHG reduction (Cradle to grave)	X		
Butanediol (2,3-)			X	LanzaTech is the ... known compan... to commercia... using indust... CO as feed... there are so... on ethanol ... none has been ... 2,3-BDO.			

Preliminary LCA reviewed by ANL showed that 20 of the products could offer significant benefits. Not enough data for other components

1. Lammens TM, Potting J, Sanders JP, De Boer IJ. Environmental comparison of bio-based chemicals from glutamic acid with their petrochemical equivalents. International Sugar Journal. 2012;114(1358):83-90.
2. Hermann, B. G.; Blok, K.; Patel, M. K. Producing bio-based bulk chemicals using industrial biotechnology saves energy and combats climate change. Environ. Sci. Technol. 2007, 41, 7915−7921.

Paring down list of 26 for case studies: *Accomplishments*

Initial list of 26 chemicals

- Acrylic Acid
- Acrylonitrile
- Adipic Acid
- 1,4-Butanediol
- 2,3-Butanediol
- N-Butanol
- Caprolactam
- Cyclohexanone
- Glucaric acid
- Fumaric acid
- 2, 5-Furandicarboxylic acid
- Hexamethylenediamine
- 3-Hydroxybutyric acid
- 5-Hydroxymethyl furfural
- Hydroxypropionic acid
- Iso-Propanol
- Itaconic acid
- Lactic acid
- Levulinic acid
- Malonic acid
- Muconic Acid
- Phenol
- 1,3-Propanediol
- Succinic Acid
- Terephthalic acid
- Xylaric Acid

Paring down list of 26 for case studies: *Accomplishments*

Being evaluated in other BETO supported projects

- Acrylic Acid
- Acrylonitrile
- Adipic Acid
- 1,4-Butanediol
- 2,3-Butanediol
- N-Butanol
- Caprolactam
- Cyclohexanone
- Glucaric acid
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- 2, 5-Furandicarboxylic acid
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- Phenol
- 1,3-Propanediol
- Succinic Acid
- Terephthalic acid
- Xylaric Acid

Paring down list of 26 for case studies: *Accomplishments*

Market analysis already exists

- Acrylic Acid
- Acrylonitrile
- Adipic Acid
- 1,4-Butanediol
- 2,3-Butanediol
- N-Butanol
- Caprolactam
- Cyclohexanone
- Glucaric acid
- Fumaric acid
- 2, 5-Furandicarboxylic acid
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- Muconic Acid
- Phenol
- 1,3-Propanediol
- Succinic Acid
- Terephthalic acid
- Xylaric Acid

Paring down list of 26 for case studies: *Accomplishments*

Near-term deployment unclear

- Acrylic Acid
- Acrylonitrile
- Adipic Acid
- 1,4-Butanediol
- 2,3-Butanediol
- N-Butanol
- Caprolactam
- Cyclohexanone
- Glucaric acid
- Fumaric acid
- 2, 5-Furandicarboxylic acid
- Hexamethylenediamine
- 3-Hydroxybutyric acid
- 5-Hydroxymethyl furfural
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- Itaconic acid
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- Levulinic acid
- Malonic acid
- Muconic Acid
- Phenol
- 1,3-Propanediol
- Succinic Acid
- Terephthalic acid
- Xylaric Acid

Paring down list of 26 for case studies: *Accomplishments*

Potential downstream product of proposed chemical

- Acrylic Acid
- Acrylonitrile
- Adipic Acid
- 1,4-Butanediol
- 2,3-Butanediol
- N-Butanol
- Caprolactam
- Cyclohexanone
- Glucaric acid
- Fumaric acid
- 2, 5-Furandicarboxylic acid
- Hexamethylenediamine
- 3-Hydroxybutyric acid
- 5-Hydroxymethyl furfural
- Hydroxypropionic acid
- Iso-Propanol
- Itaconic acid
- Lactic acid
- Levulinic acid
- Malonic acid
- Muconic Acid
- Phenol
- 1,3-Propanediol
- Succinic Acid
- Terephthalic acid
- Xylaric Acid

On-going case studies: *Accomplishments*

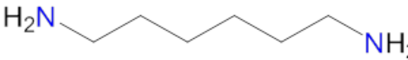
3-Hydroxypropionic Acid

Analysis focus on platform chemical

- Acrylic acid is primarily produced via propylene oxidation – shale gas impacts the price of feedstock.
- Potential feedstock for acrylic acid (5 MM MT/yr).
- Other markets include propanediol, acrylamide, acrylonitrile, acrolien, and malonic acid.

On-going case studies: *Accomplishments*

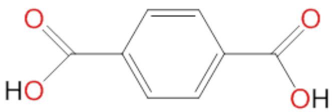
Hexamethylenediamine



Analysis focus on synergism with other BETO conversion focused R&D

- HMDA is part of the Nylon-6,6 value chain
- Fossil production through butadiene which has cost instability (due to shale gas)
- Completes the picture of renewable Nylon-6,6 with on-going support by BETO for renewable adipic acid production
  - Worldwide market is ~ 1.3 MM Metric tons/year
  - US produces ~60% of world demand and exports ~35% of what is produced
- Key sustainability drivers for fossil routes which utilize HCN as a catalyst

Purified Terephthalic Acid

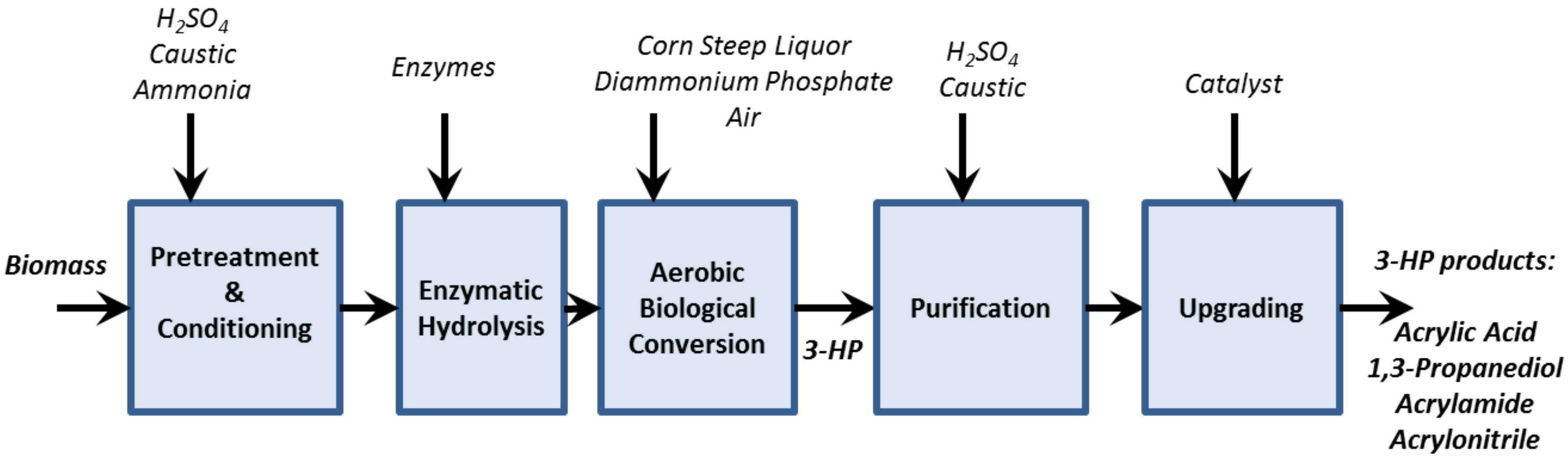


Analysis focus on large scale chemical production

- PTA is a feedstock for PET production.
  - PTA has a ~50 MM Metric ton/year market.
  - US produces ~6% of the world's PTA and imports ~15% of what is consumed
  - Understand value chain and market incentives for expanded production in the United States
- PET is a 60 MM metric tons/year market
  - US produces ~6% of world demand and imports ~1.1 MM metric tons/year. Production of PET has been reduced by ~1-2%/year over the last 5 years in the US.

TEA for 3-hydroxypropionic acid: *Results*

Developed preliminary TEA for 3-HP platform chemical and range of downstream products

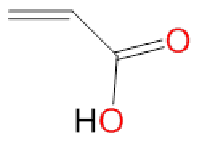


Investigated upgrading pathways to coproducts using patents/publications:

- Acrylic acid - Based on Cargill patent and consistent with recent ANL study
- 1,3-propanediol - Based on Cargill patent and consistent with recent ANL study
- Acrylamide - Based on Cargill patent; variation on acrylic acid production (via different catalyst)
- Acrylonitrile - Based on Cargill patent; upgraded from acyrlamide

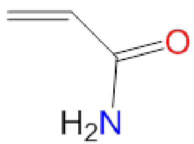
Preliminary TEA: Results

Estimate of current minimum selling price and comparison to recent price of fossil-equivalent

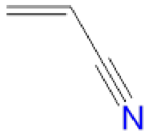


Acrylic Acid

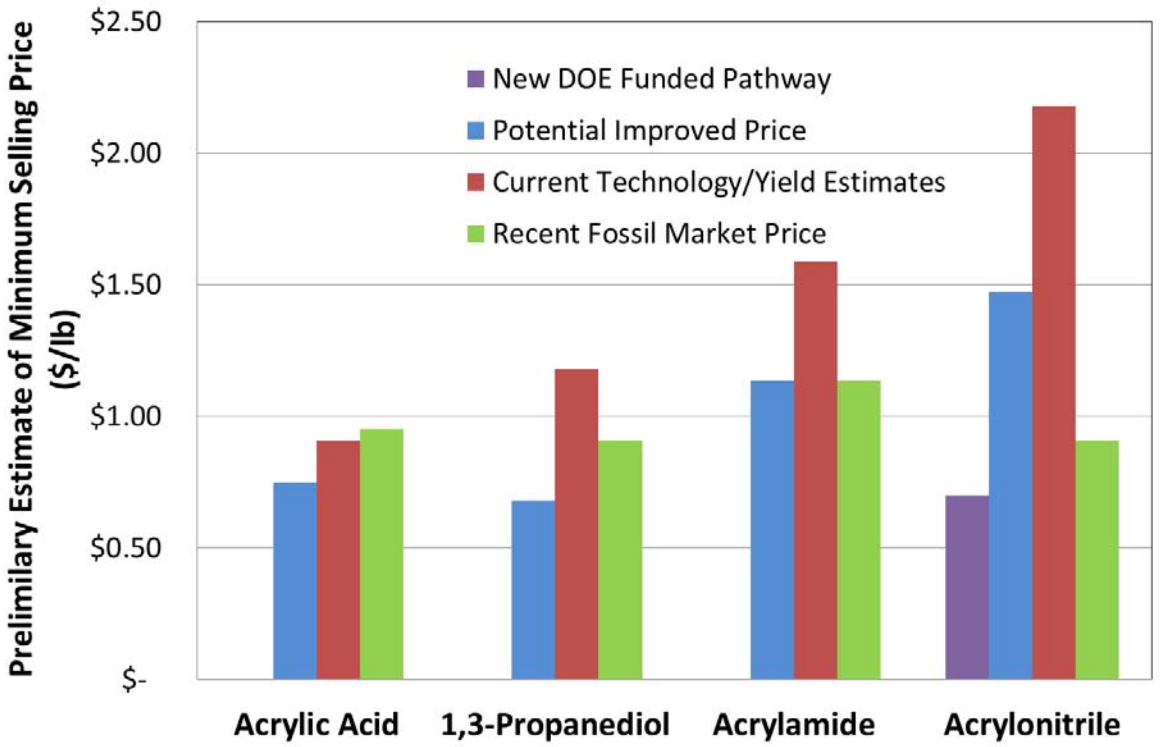
1,3-Propanediol



Acrylamide



Acrylonitrile



- Yield is the key driver for improving economics.
- BETO has supported alternative acrylonitrile pathway to lower cost.

US supply chain considerations:
Results

Investigated potential for bio-derived chemicals to integrate into existing fossil supply chain due to location and market availability

Acrylic Acid

US Production 1.5 MM metric tons/yr
Number of Biorefineries Required 7

1,3-Propanediol

US Production 0.045 MM metric tons/yr
Number of Biorefineries Required 0.3

Acrylamide

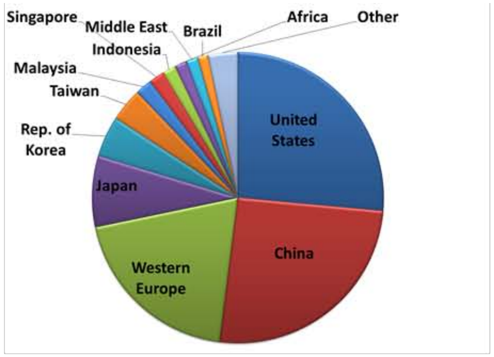
US Production 0.150 MM metric tons/yr
Number of Biorefineries Required 1.3

Acrylonitrile

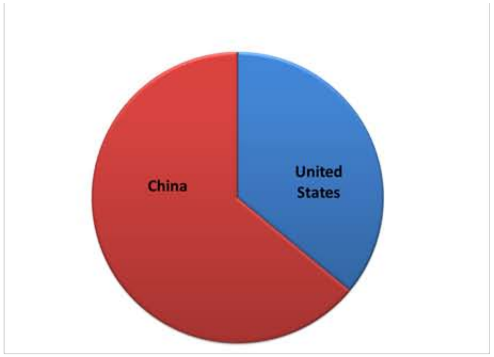
US Production 1 MM metric tons/yr
Number of Biorefineries Required 12

Global supply chain considerations: *Results*

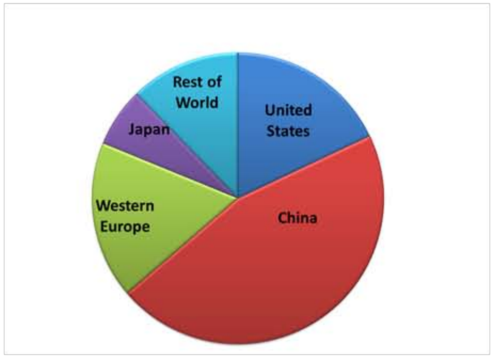
Investigated potential for bio-derived chemicals to integrate into existing fossil supply chain due to location and market availability



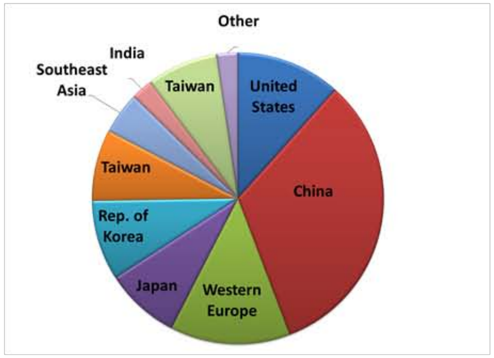
Acrylic Acid
World Consumption 5 MM metric tons/yr
Number of Biorefineries Required 27



1,3-Propanediol
World Consumption 0.125 MM metric tons/yr
Number of Biorefineries Required 0.8



Acrylamide
World Consumption 0.83 MM metric tons/yr
Number of Biorefineries Required 7.5



Acrylonitrile
World Consumption 5.6 MM metric tons/yr
Number of Biorefineries Required 67

Global supply chain considerations:
Results

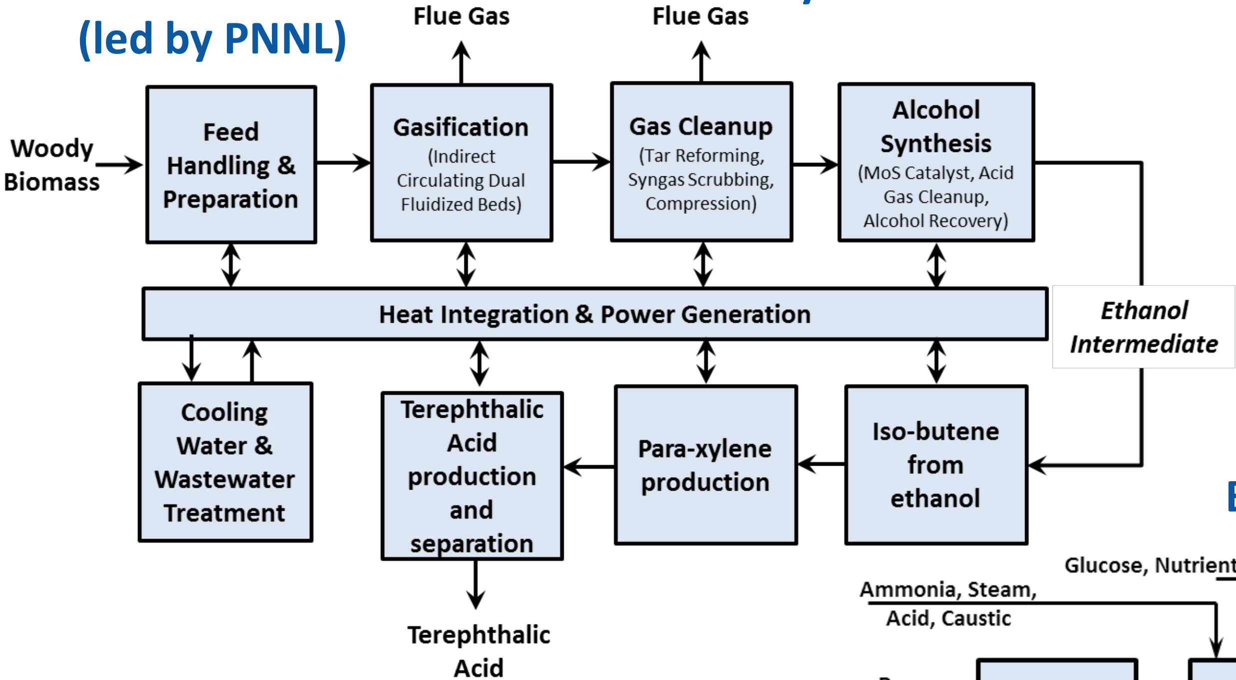
Understand risk due to raw materials required to meet global demand

Primary Raw Materials	Acrylic Acid	1,3-Propandiol	Acrylamide	Acrylonitrile	Total
Production per biorefinery (Mmton/yr)	0.18	0.15	0.11	0.08	
Number of Biorefineries	27	0.8	7.5	67	102
Percentage of total world production required					
Sulfuric Acid	0.4%	0.1%	0.1%	1%	1.6%
Sodium Hydroxide (Caustic soda)	1%	0.3%	0.3%	2.4%	4%
Ammonia	0%	0%	0%	0.1%	~0.1%
Enzymes					
Phosphoric Acid	0.01%	0%	0%	0%	0.01%
Ruthenium	0%	13%	0%	0%	5%
Methylamine	0%	0%	30%	**300%**	330%

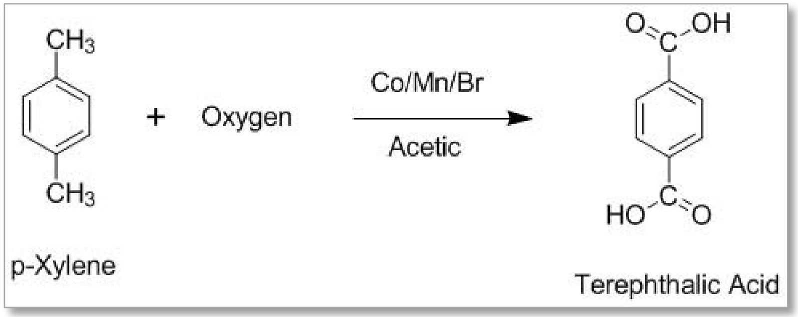
Limited on the methylamine for production of acrylonitrile in patented route.

Comparative TEA for terephthalic acid: *Results*

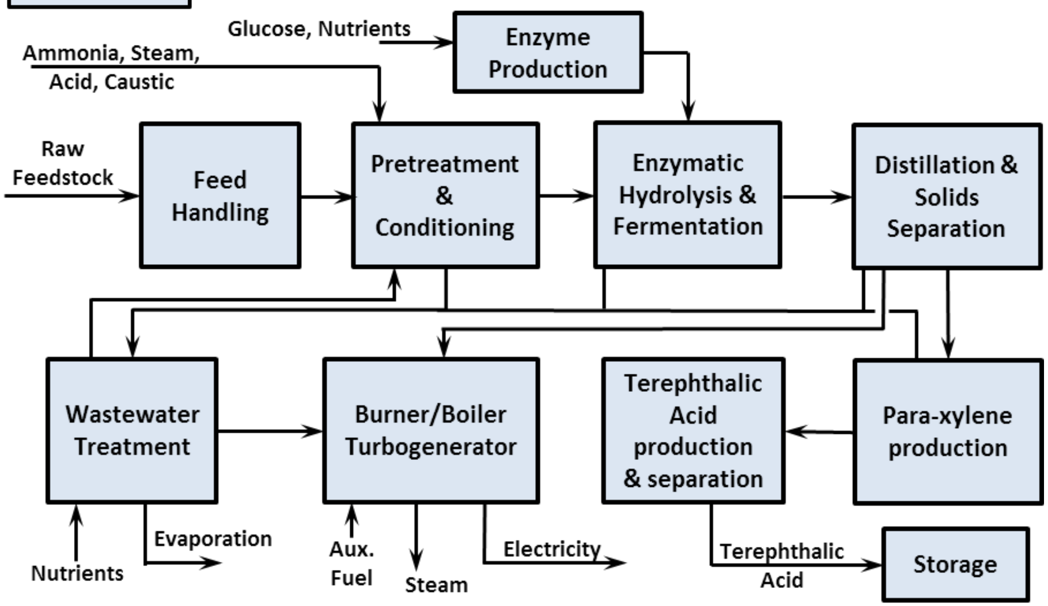
Thermochemical Production Pathway (led by PNNL)



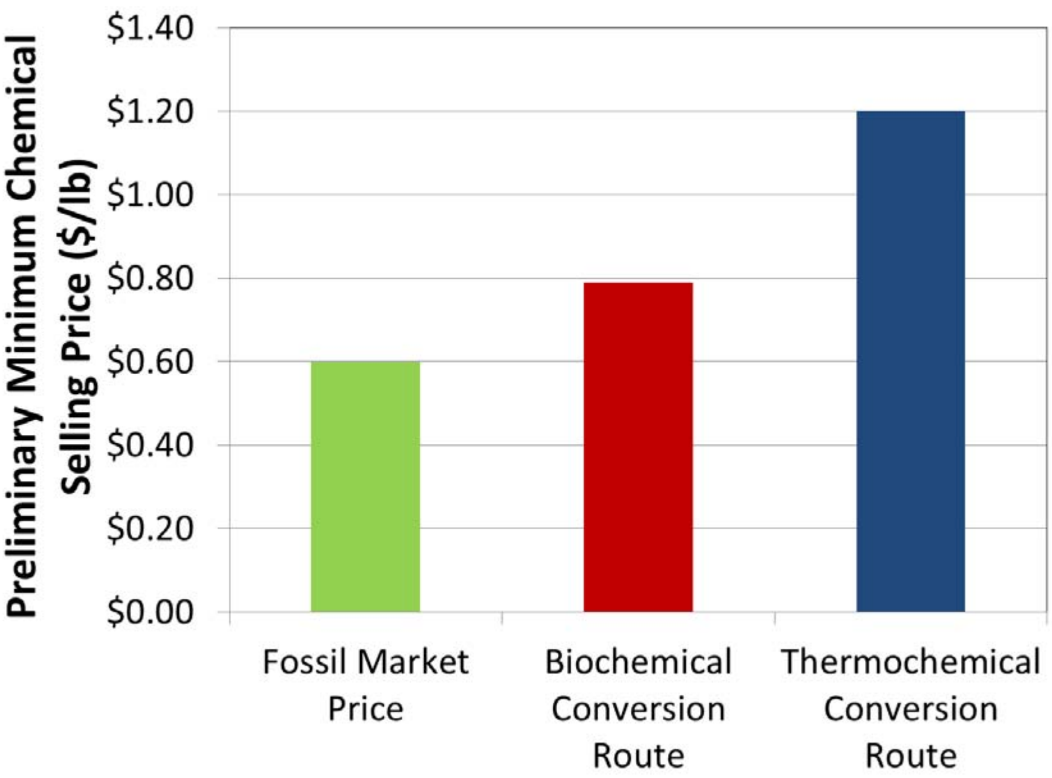
Compared 2 pathways for production of terephthalic acid via a butene intermediate



Biochemical Production Pathway



Comparative TEA for terephthalic acid: *Results*



Terephthalic Acid

US production = 3 MM metric tons/yr

Location based on end user needs

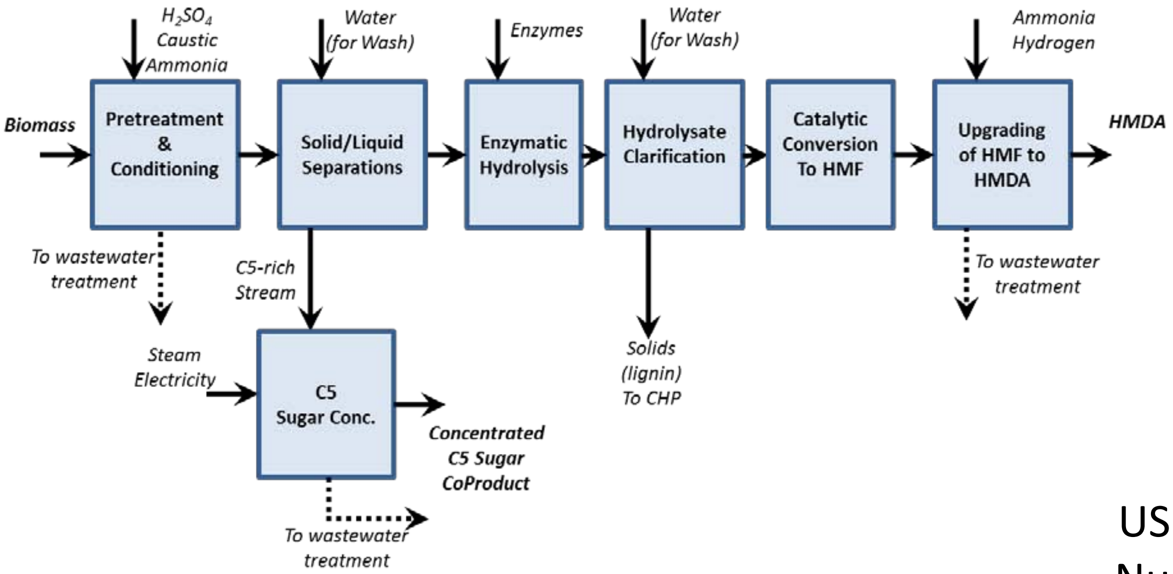
Number of biorefineries required =

Thermochemical: 48

Biochemical: 31

- Yield is a key cost driver and is the difference between 2 cases.
- Additional sensitivity cases are being performed to consider the impact of design variations.

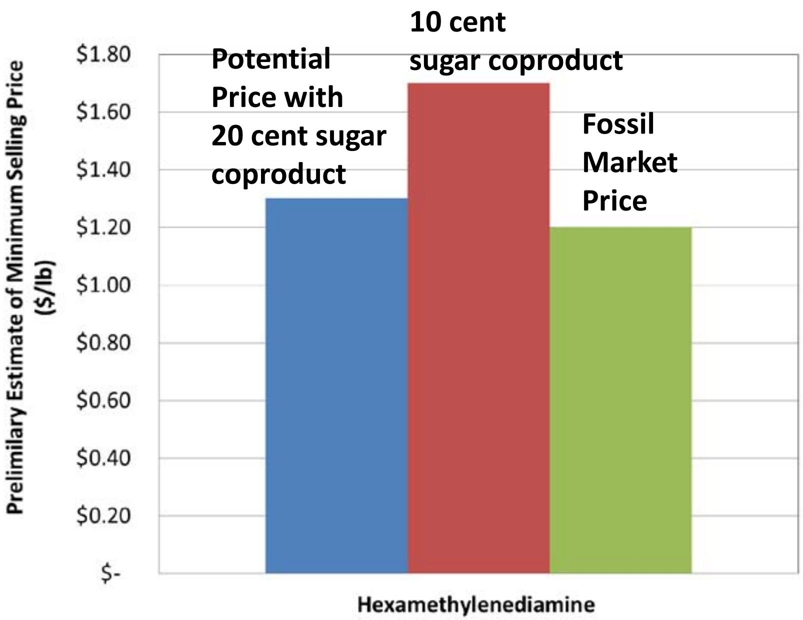
Comparative TEA for hexamethylenediamine: *Results*



Hexamethylenediamine

US production = 0.5 MM metric tons/yr

Number of biorefineries required = 14



- Assumes improved yield for HMDA production.
- Cost driver for conversion/selling price of C5-rich sugar.
- Alternative strategies could consider C6-rich production routes.

Review of Results

- Developed a methodology and key metrics for evaluating chemicals from biomass.
  - Sustainability evaluation identifies which chemicals would benefit by replacement wiith a bio-derived route.
- Developed preliminary TEA that identifies which products have the potential to compete with fossil-derived products.
  - Outlines key R&D required to reduce costs and scale-up risk.
- Market analysis considers which products have accessible supply chains both from business and logistical considerations.

Relevance

- Project directly supports BETO's Strategic Plan to "Provide an Analytical Framework for Bioproducts Research" and by 2020 "provide an analytical framework for bioproducts research by publishing market and life-cycle analyses, roadmaps, and/or reports."
- Per 2016 BETO MYPP "Technological developments in renewable chemicals can accelerate the commercial development of advanced biofuels by improving economics and diversifying market risks".
  - **Project focused on understanding diverse market, cost and sustainability drivers** for a broad range of chemicals **with results supporting both BETO and stakeholders.**

Relevance

- Outcome of this work is to expand current analysis methodologies when evaluating chemical coproducts
  - Approach being adopted in Agile Biofoundry project and expected to provide key metrics for future conversion target considerations.
  - Assess **sustainability drivers** including GHGs and social impact considerations.
  - Investigate **demands and resources** needed to move to larger scales.
  - Evaluate **value proposition** for moving products to market.
  - Focus on **market drivers and potential** for both US and global economy.

Future work

- On-going effort to finalize techno-economic and sustainability evaluations for 3 representative chemicals.
- Global supply chain and trade flow analysis.
  - Key questions asked during the supply chain analysis include:
    - What raw materials are required for the synthesis of biomass-derived chemicals?
    - Where are these raw materials sourced? Are there potential supply constraints?
    - What is the market for any coproducts? Are these captive or merchant markets?
    - What companies are currently involved in the manufacture of the chemicals being studied?
    - What are the competing synthetic processes for the bio-derived chemicals and products?
- Document results of study.
  - The project report will be submitted for publication in a peer-reviewed journal.
  - Results of this project will be included in the annual CEMAC summary report and summarized on the CEMAC website.
  - Present results at bioproducts conference.
- Multi-metric (market, cost, sustainability) evaluation being adopted in other BETO support projects for analysis of biochemicals.

Summary

Approach

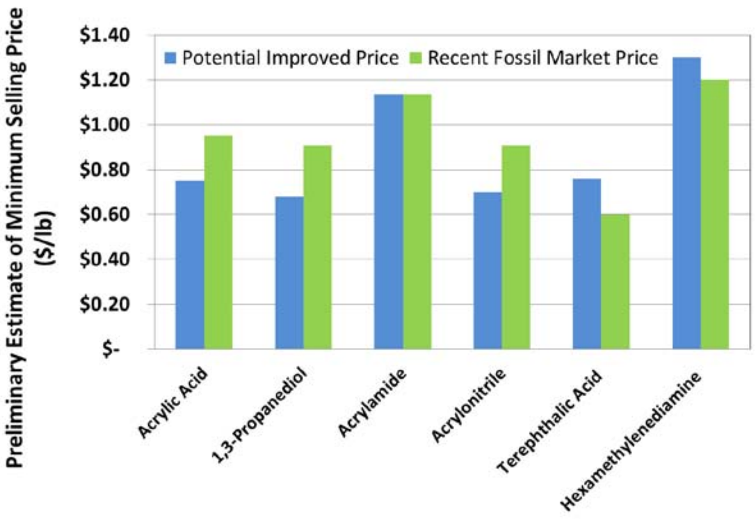
- Multi-lab, collaborative project to evaluate the production of chemicals from biomass.
- Evaluate production of chemicals from biomass consistent with CEMAC supply chain evaluation.
- Strong team of targeted partners from academia, national labs, and industry.

Technical accomplishments

- Evaluated over 170 different bioproducts on a range of metrics including economics, markets, and sustainability drivers.
- Developed a set of screening metrics to evaluate products.
- Developed case studies to evaluate economics, US and global markets, and supply chain needs.

Relevance

- Aligns with BETO Strategic Goals to develop a deeper understanding of bioproduct markets, economics, and sustainability.
- Methodologies to consider a range of metrics beyond costs are being adopted in other programs and projects.



Future work

- Publication of final report.

Acknowledgements

Thank you to …

- DOE Bioenergy Technologies Office
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- DOE Clean Energy Manufacturing Initiative
  - Brian Walker
- Collaborative team
  - Maggie Mann, Jennifer Markham, Christopher Scarlata (NREL)
  - Jennifer Dunn, Felix Adom, Pahola Thathiana Benavides Gallego (ANL)
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