

Analysis in support of novel bio-based products and functional replacements WBS (2.1.0.500)

Performance Advantaged Bioproducts

DOE Bioenergy Technologies Office (BETO)

2019 Project Peer Review

March 5, 2019

Mary J. Bidy

National Renewable Energy Laboratory

Goal Statement

Goal: The goal of this project is to understand the value proposition for novel performance advantaged bioproducts. The result of this analysis will be a guiding document that can be used by industrial and academic researchers to focus their R&D on chemicals with the greatest potential to impact and grow the bioeconomy.

Outcome:

- **Year 1:** Develop peer reviewed draft paper outlining value proposition and pull for performance-advantaged products.
- **Year 2 and 3:** Develop top ten report for performance- advantaged products that is vetted by stakeholders.

Relevance: The result of this analysis will be a guiding document that can be used by industrial and academic researchers to focus their R&D on chemicals with the biggest potential to impact and grow the bioeconomy.

Quad Chart Overview

Timeline

- Start: FY2017
- Merit review cycle: FY2017-2019
- 50% complete of review cycle

	Total Costs Pre FY17	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19- Project End Date)
DOE Funded	\$0	\$0	\$200k	\$500k

Barriers addressed

Ct-J. Identification and Evaluation of Potential Bioproducts

At-A. Analysis to Inform Strategic Direction

At-D. Identifying New Market Opportunities for Bioenergy and Bioproducts

Objective

The outcome of this project is to understand the value proposition for novel performance advantaged bioproducts. The result of this analysis will be a guiding document that can be used by industrial and academic researchers to focus their R&D on chemicals with the greatest potential to impact and grow the bioeconomy.

End of Project Goal

Provide DOE BETO with a final draft of the top ten bio-advantaged products report. This draft will incorporate and address reviewer comments (from at least 10 external reviewers) and we will brief BETO on how this was completed. Work with BETO for final internal review and approval for final publication and release of report by end of 2020.

Project Overview

History: Building from Prior Work

- Focus of report is on products that will have near-term market impact. These are bio-derived chemicals that are currently being produced either at demonstration or commercial scales
- Assesses ways in which chemicals production can be leveraged to expand and accelerate the growth of biofuels

Range of drivers for bio-derived products:

- Supply/demand and market need (fossil replacements)
- Consumer demand
- Superior properties and potential lower costs

<http://www.nrel.gov/docs/fy16osti/65509.pdf>



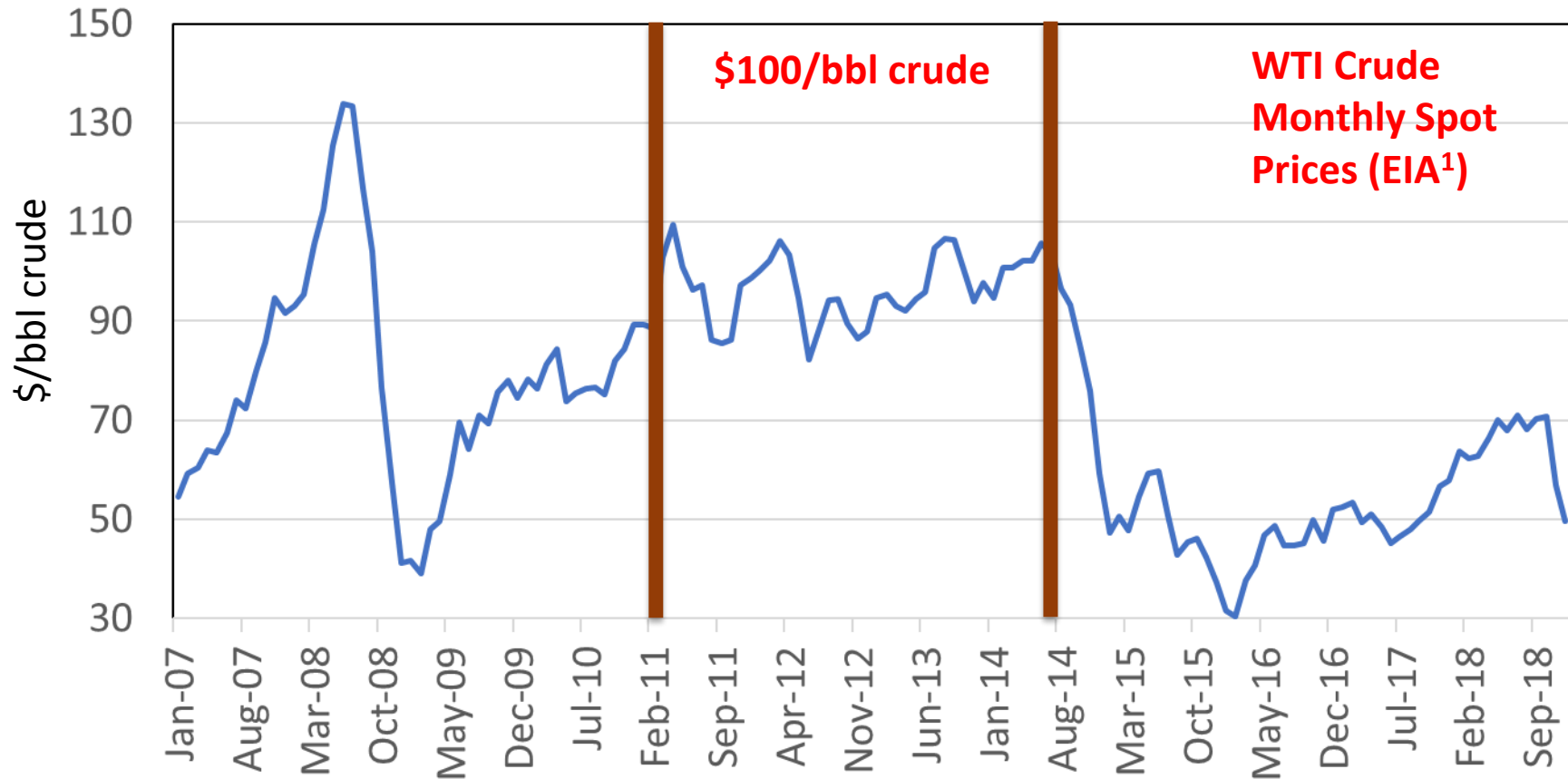
Chemicals from Biomass: A Market Assessment of Bioproducts with Near-Term Potential

Mary J. Bidy, Christopher Scarlata, and
Christopher Kinchin
National Renewable Energy Laboratory

NREL is a national laboratory of the U.S. Department of Energy
Office of Energy Efficiency & Renewable Energy



Project Overview – Background/Motivation



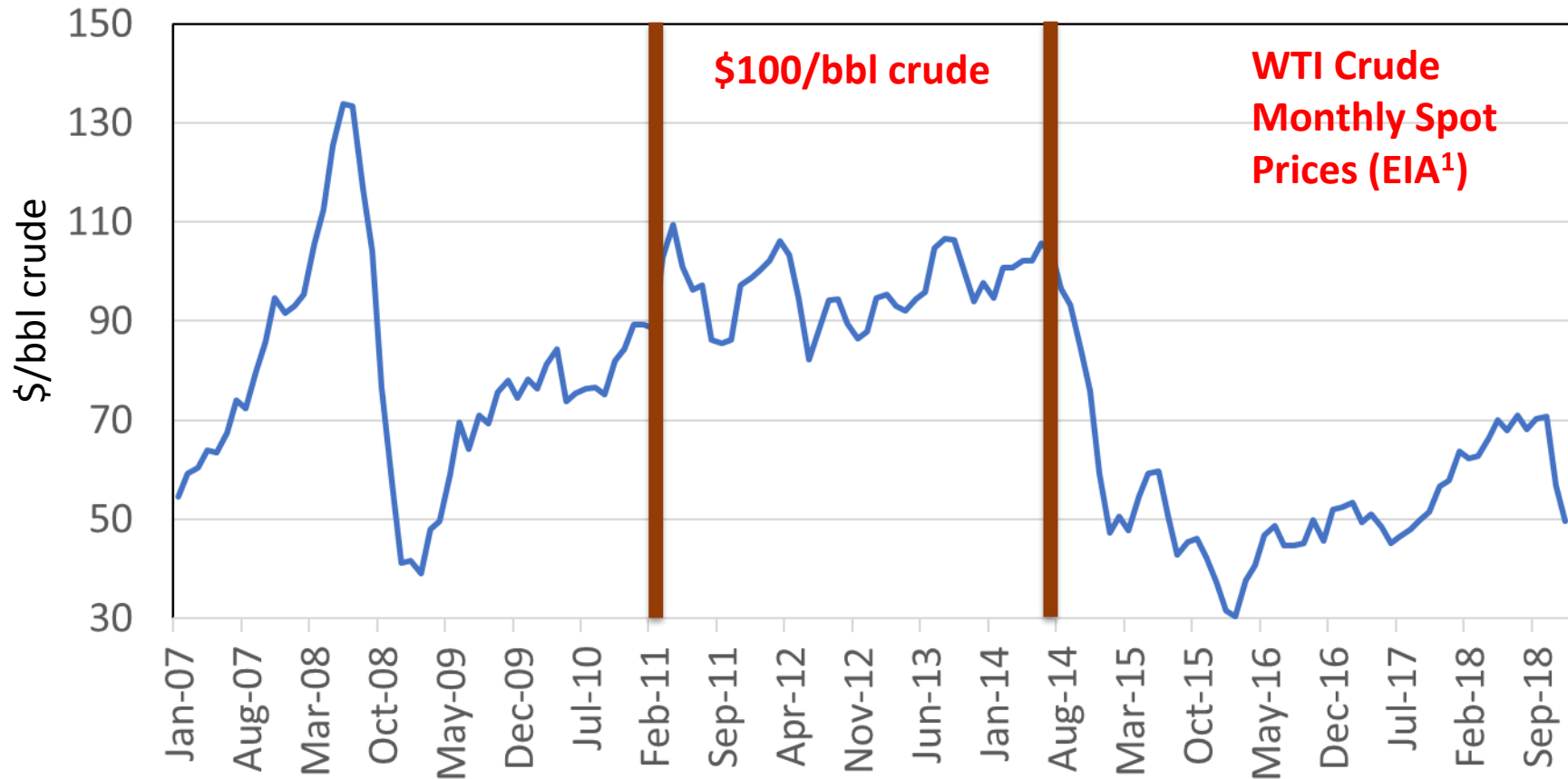
Lux reports that low oil prices are driving the VC shift their focus to biobased chemicals that offer improved performance

Roughly ~80% of VC investments in 2016 when compared to 46% from 2010 to 2015.²

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Project Overview – Background/Motivation



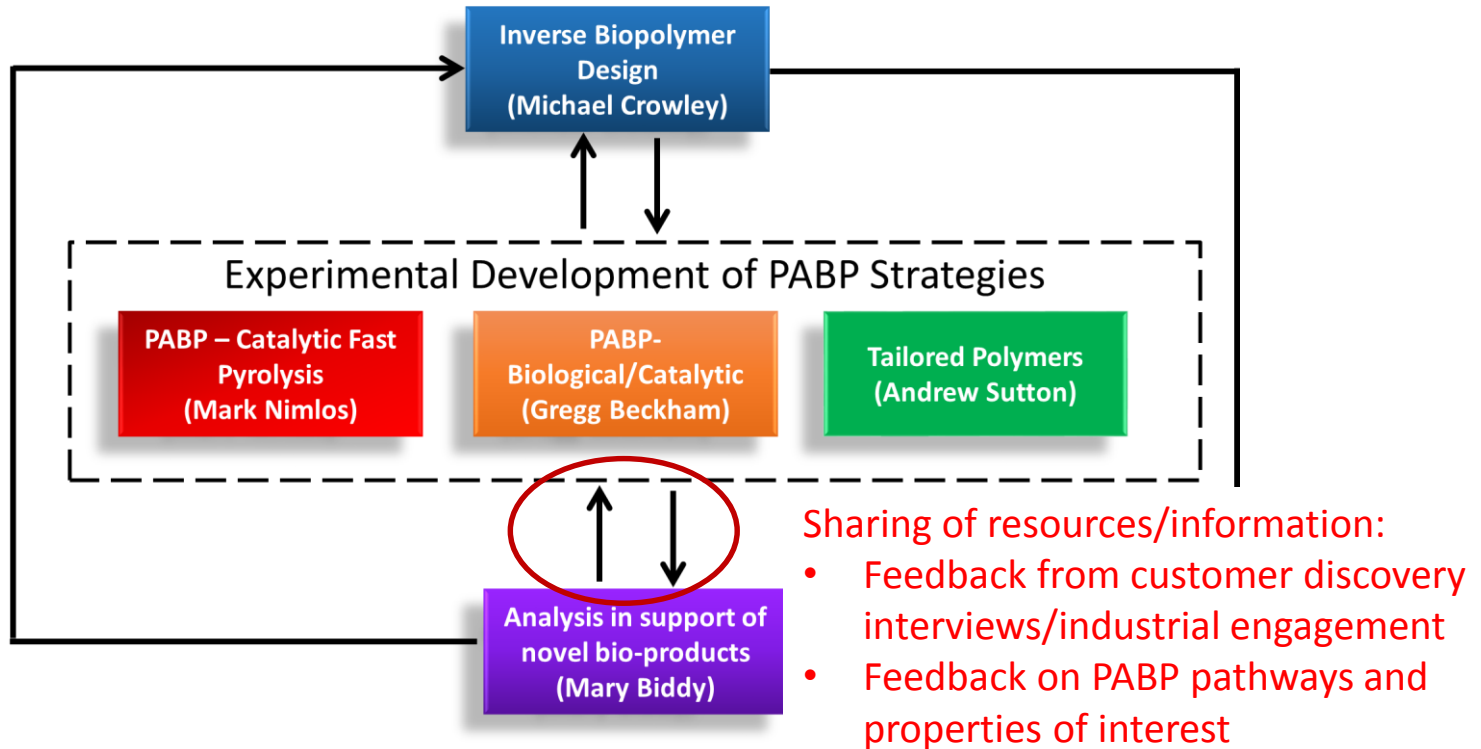
Evaluate what the opportunities are for performance advantaged bioproducts (PABPs)

- Provide analyses to support the strategic mission
- Understand the market drivers and needs for the various end-product sectors
- Provide a basis and rationale to identify a long-range vision for PABPs

1. <https://www.eia.gov/dnav/pet/hist/LeafHandler.ashx?n=pet&s=rwtc&f=a>

Approach - Management

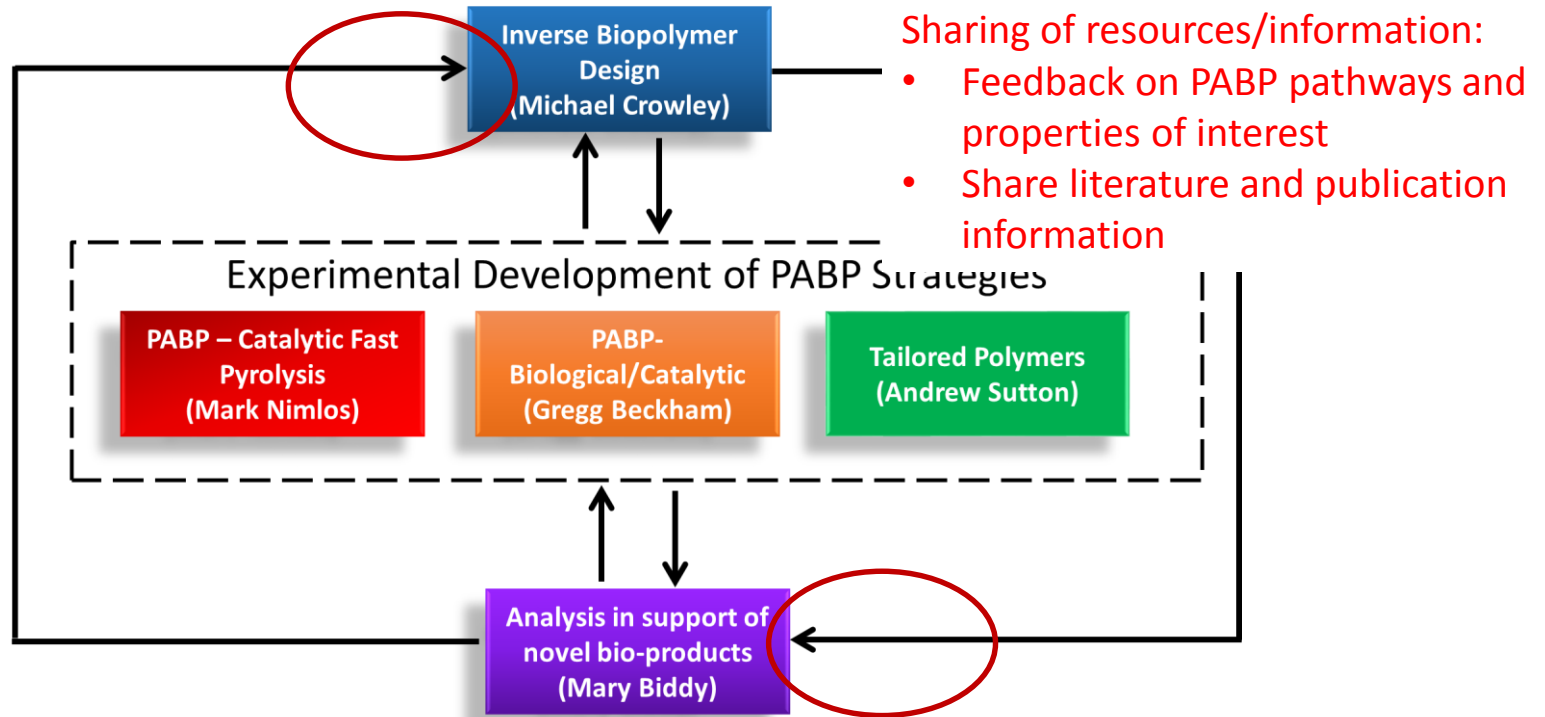
Integrated approach to share information/resources with entire PABP team



- Biweekly meetings among PABP BETO projects
- Monthly meetings with BETO Technology Manager
- AOP development with BETO Technology Manager
 - Quarterly progress measures to continuously update towards final end of year milestone

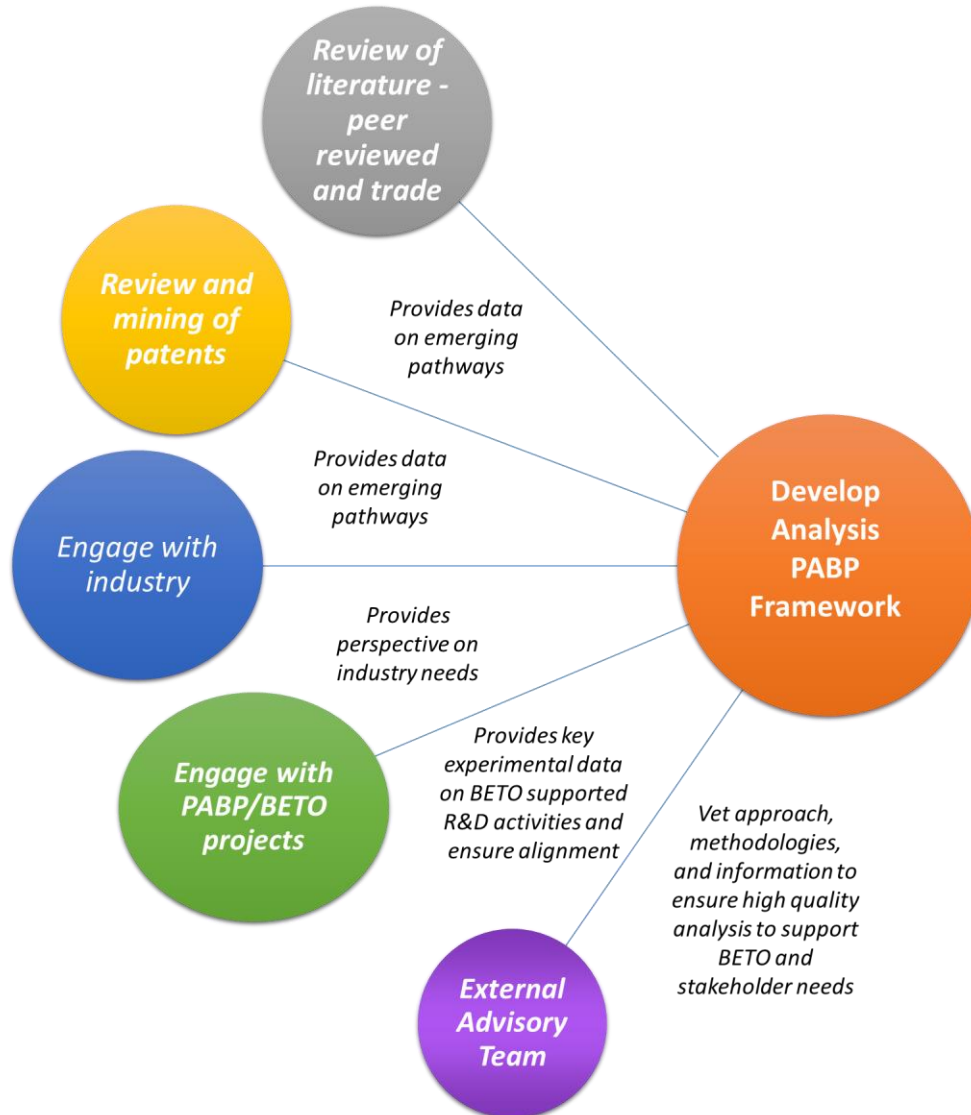
Approach - Management

Integrated approach to share information/resources with entire PABP team



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Approach - Technical



Approach:

- Data gathered from variety of sources to build an analysis focused PABP framework
- External Advisory Panel regular review of approach and information
 - Currently 11 advisors
 - Broad range of perspectives and experience in bioproducts
 - Development/inception
 - Scale-up
 - Market development/strategy
 - End-Use
 - Policy
 - Group includes members from academia, industry, and government agencies
 - Each have 20+ years expertise

Approach - Technical

Critical Success Factors	Challenges	Approach to overcome
Develop reliable results and outcomes.	Availability and quality of data.	<ul style="list-style-type: none"> • Work with BETO and stakeholders to provide missing information. • Stakeholder engagement to review results and approach.
Develop reliable results and outcomes.	Consistency of analyses and ensuring coordination.	<ul style="list-style-type: none"> • Collaboration with core PABP projects to ensure consistency in approach and assumptions. • Outline current approach to share data among products as well as external to PABP projects.
Applying the appropriate method to address questions.	A wide range of analysis approaches can be employed.	<ul style="list-style-type: none"> • Engage with BETO/stakeholder to review and vet approach.
Clearly defining critical questions to address.	Scope shift.	<ul style="list-style-type: none"> • Working closely with stakeholders (BETO) to define needs and key questions. • Outline plan to address questions in AOP and active project management/regular check-ins to keep project inline with goals.

Progress

Year 1 Goal: *Develop peer reviewed draft paper outlining value proposition and market pull for performance-advantaged products.*

How we started?

- Developed initial detailed outline of paper (5 pages)
- Provided draft to external advisory team for review.
- Provided key guidance questions on draft including:
 1. Are the market pull and value opportunities that are highlighted appropriate in the current market?
 - a. Does the report provide the proper level detail for these topic areas?
 - b. Are there any market pull and value opportunities that should be removed or modified in the report?
 - c. Are there additional market pull and value opportunities that are missing and should be included?
 2. While the draft highlights a few specific performance-advantaged products, are there additional products that the report should focus upon?
 3. Are there any other gaps or missing details that should be included in the write-up?

A Review of Market Drivers and Value Opportunities of Performance-Advantaged Products

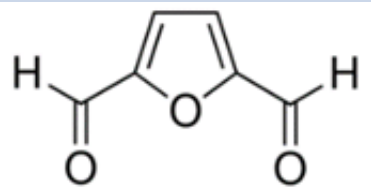
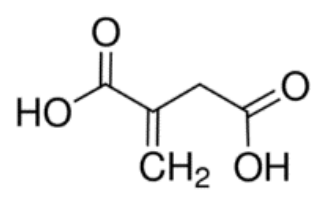
Mary J. Biddy
National Bioenergy Center, National Renewable Energy Laboratory, Golden, Colorado 80401

There are strong motivations for the production of bio-derived chemicals. Foremost, chemicals production is a major driver in the US economy, accounting for roughly 2% of the US GDP over the past several decades, and the U.S. Chemical Industry provides over 15% of the world's chemicals (ACC 2015, BETO 2016, Bureau of Economic Analysis 2016). Producing chemicals from biomass, therefore, can significantly impact the growth of the chemicals industry and the US economy overall. Moreover, the selective inclusion of oxygenated components into a hydrocarbon (fossil) backbone typically requires alternative processing which can be costly and can impact the production from energy, sustainability, and/or safety standpoints. These considerations often limit the development of oxygenated products from fossil feedstocks and provides new market opportunities that may be leveraged by chemicals derived directly from biomass. Due to the unique molecular formulation of biomass, which is rich in not only carbon but also oxygen, biomass-derived chemicals have a promising opportunity if the oxygenated components can be maintained and utilized for novel chemistries. Performance-advantaged bioproducts are chemicals, not traditional produced from fossil feedstocks, that have unique characteristics and properties. Such products from biomass could have a unique market pull and drivers for utilization to help move more products to market. This discussion will briefly review the potential market drivers and value propositions for performance-advantaged products at a holistic level and will identify specific areas where performance-advantaged products could fill a specific market need.

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Progress

Study begins by introducing a number of performance advantaged bioproducts that are either commercially scaled or are moving toward commercialization and understanding properties which help drive value-proposition.

Performance-Advantaged Product	Applications	Desirable properties
<p>2,5-Furandicarboxaldehyde</p>  <chem>O=Cc1cc(=O)oc1C=O</chem>	<p>A precursor to many polymers including polyesters, polyamides, and polyurethanes. Potential to replace PET in producing plastic bottles. Due to its unique nature, enables opportunities for new applications in packaging and light-weight materials.</p> <p>Current production capacity: At pilot scale</p>	<p>Improved barrier permeability properties compared to PET including up to 10-fold higher for O₂, up to 6-fold for CO₂, and 2-fold for H₂O.</p> <p>Moduli that are 1.6 times higher than PET which can allow for lighter bottles.</p> <p>Higher glass transition temperature which allows for hot fill applications.</p> <p>Lower melting temperature which can allow for energy reduction in processing</p>
<p>Itaconic Acid</p>  <chem>OC(=O)C=C(O)CC(=O)O</chem>	<p>Most utilized for polymeric applications. Utilized as cross-linking agent in production of superabsorbent polymers. Poly itaconic acid has the potential to replace sodium tripolyphosphate in detergents. Also utilized in UV-curable coatings in electronics industry.</p> <p>Current production capacity: 50,000 metric tons</p>	<p>Readily biodegrades in soil.</p> <p>Unique structure allows molecule to take part in addition polymerization.</p>

Progress

Based on feedback of reviewers, increased emphasis on end uses and specific performance needs and drivers to outline value proposition.

Transportation
Applications



Plastic
Packaging



Textiles



Paints and
Coatings



Personal Care
Products



Household
Cleaners



Progress

Based on feedback of reviewers, increased emphasis on end uses and specific performance needs and drivers to outline value proposition.

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Progress

Summary of applications for bioproducts in automobiles (sample of 20 reviewed)

Manufacturer and Make	Components
Honda Accord Hybrid and Plug-In Hybrid	Proprietary Bio-Fabric in seat covers. PTT carpeting. Plastics from bumpers produced at Honda plants in the U.S. and Canada reformulated to make mud and splash guards.
Kia Soul EV	Roughly 53 pounds of bioproducts are used to make 19 different interior parts including door panels, headliner, seat trim, roof pillars, and carpets. <i>UL certified based on bio-components.</i>
Lexus CT200 Hybrid	Bio-based PTT in carpeting and PET in luggage compartment liner.
Mazda MX-5	Bio-based plastics (from isosorbide) utilized in interior components. Bio-based fibers for carpet and upholstery (lactic acid-derived).
Nissan Leaf	Recycled PET based seats. Recycled clothes for sound insulation underneath the hood, and old electrical appliances such as refrigerators and washing machines find new life as the Leaf's center console.
Toyota Camry, Corolla, Prius, RAV4	Bio-based plastics utilized in seat cushions, upholstery, carpet, some trim pieces and air vent registers.

Progress

Most bioproducts and recycled materials utilized in interior and aesthetic components. Current expansion for use in automotive exteriors.

Frame

Must provide the strength to pass safety testing:

- High tensile strength
- High stiffness—bending, torsional, static, and dynamic
- Highly paintable, easy to design, smooth finish
- Targets of “light-weighting” but retain strength—critical for electric and hybrid vehicles due to increase weight of batteries
- Target materials that can be recycled.



Headlights and Reflectors

Requirements defined by SAE J576:

- Material thickness
- Heat resistance
- Outdoor weathering
- Luminous transmittance.



Bumper

The United States is expected to adhere to the standard 49 CFR Part 581 National Highway Traffic Safety Administration. Additional desirable properties include:

- High corrosion resistance
- Light weight
- Ease of design
- Greater amount of shock energy absorption
- Ease of manufacturing by use of injection molding.

Wheel Covers

Key property considerations:

- High resistance to corrosion
- High resistance to extreme environments (salt, chemicals, heat, or cold)
- Lightweight
- High dimensional stability
- Easily paintable
- Durability
- UV resistance.



Progress

Evaluating longer term strategies in the automotive industry (2 examples)

Longer-term strategies	Key needs	Desirable Properties
Electric and hybrid vehicles	Additional battery weight requires light weighting of vehicles to increase vehicles range	<ul style="list-style-type: none"> • Meet the required strength and safety requirements • Light weight materials • Can be easily and cheaply adopted into current manufacturing facility requirements • Material that can be recovered and recycled (per laws and mandates of the European Union, Japan, and South Korea)
Modular production of components and automobiles	Polymeric materials that can be utilized in 3 dimensional printing applications	<ul style="list-style-type: none"> • For 3D printing – low VOC, storage stability, ability to produce components at higher printer speed, and ease of processing (due to melt temperature) • For applications – will need to meet specific end use applications such as durability and strength

Progress

Based on feedback of reviewers, increased emphasis on end uses and specific performance needs and drivers to outline value proposition.

Transportation
Applications



Plastic
Packaging



Textiles



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Progress

Closing summary: The need and opportunity for research and development

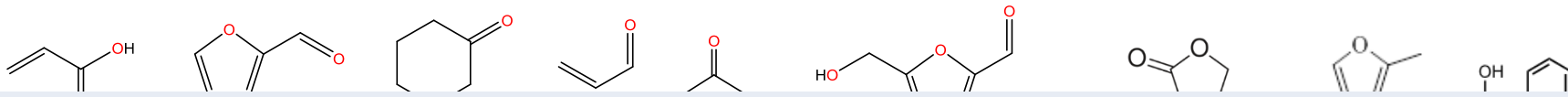
- Need to further explore the desirable properties, performance needs, and potential areas of growth for these bio-derived materials.
- Prior work tends to be either case studies, or focused on producing chemicals and identifying conversion pathways.
- Utilize informed rational design approach towards new and novel chemistries:
 - Systematic approach to understand how the basic, unique molecular structures available from biomass-derived chemicals (such as functionalized oxygen-containing molecules) can translate to performance-advantaged characteristics.
 - Link fundamental modeling with basic R&D for developing conversion pathways.
- Alongside the rational design of these new products, there must be an understanding of what the market will accept and will pay for such novel products.
- Detailed sustainability assessments to ensure that these products and processes are following the principles of green chemistry and to ensure no unintended consequences due the use of these new products.

Progress

Closing summary: The need and opportunity for research and development

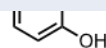
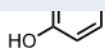
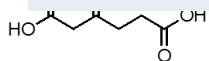
Discussion of this approach has been presented in 2018 ACS Green Chemistry Conferences, USDA/DOE BRDI Technical Advisory Meeting, and Advanced Energy and National Security Interagency Roundtable Meeting via invited talks by the PI.

Progress



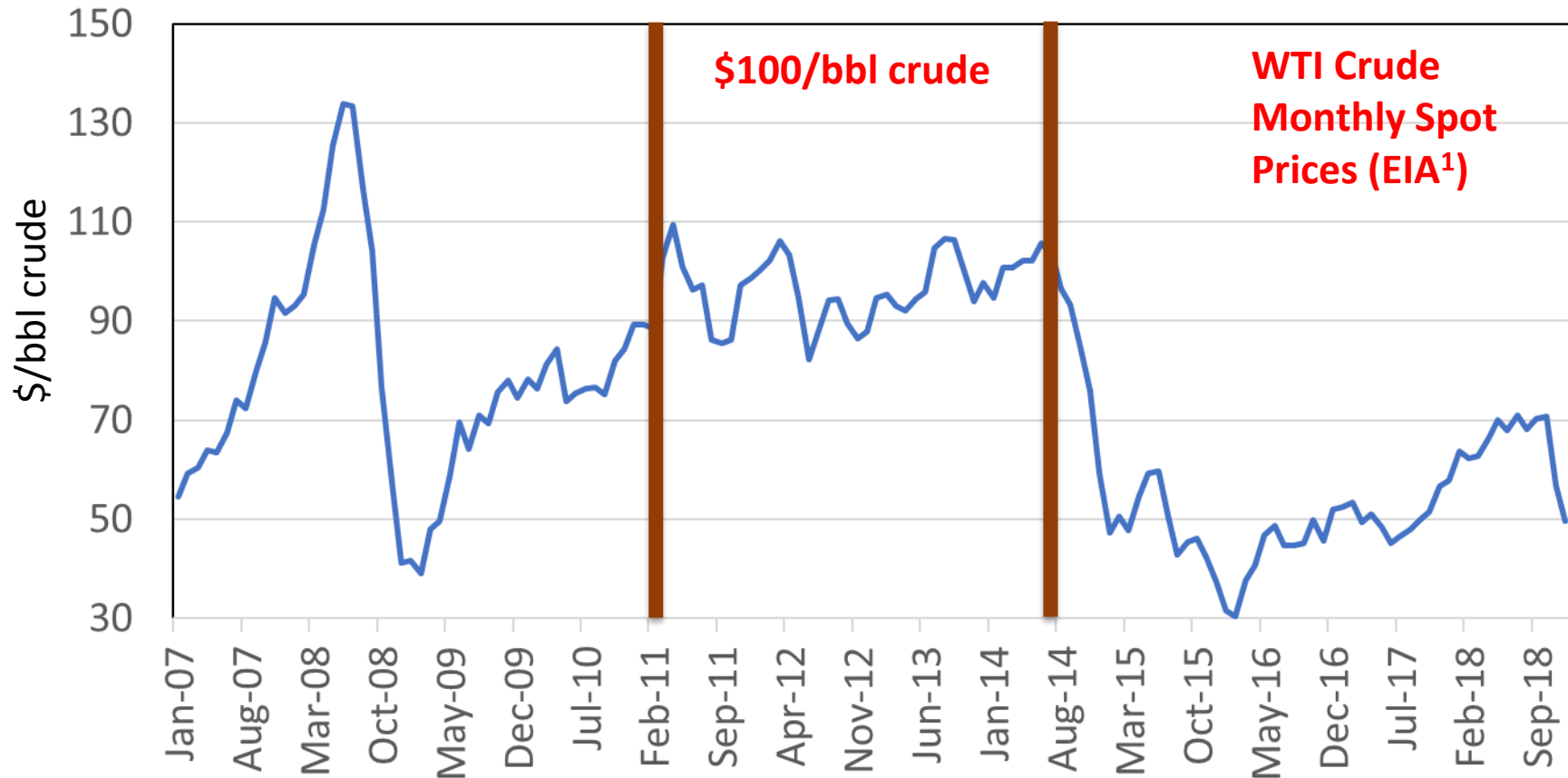
On-going work to develop PABP Analysis Framework:

- Based on review of literature, patents, industry engagement, and integration with PABP teams compiled at list of ***over 170 PABP molecules to data and continue to expand***
- **Working to characterize each PABP molecule based key metrics including:**
 - Potential end uses/market drivers
 - Properties and relationship to potential end products
 - Value proposition/potential market adoption
 - Biomass production route
 - Estimated market size (if known)
 - State of Technology Development
 - Estimated price (if known)
 - Key challenges in production route
 - Key players (potential producers and end users)
 - Sustainability drivers



Relevance

Goal: Understand the value proposition for novel performance advantaged bioproducts.



Lux reports that low oil prices are driving the VC shift their focus to biobased chemicals that offer improved performance

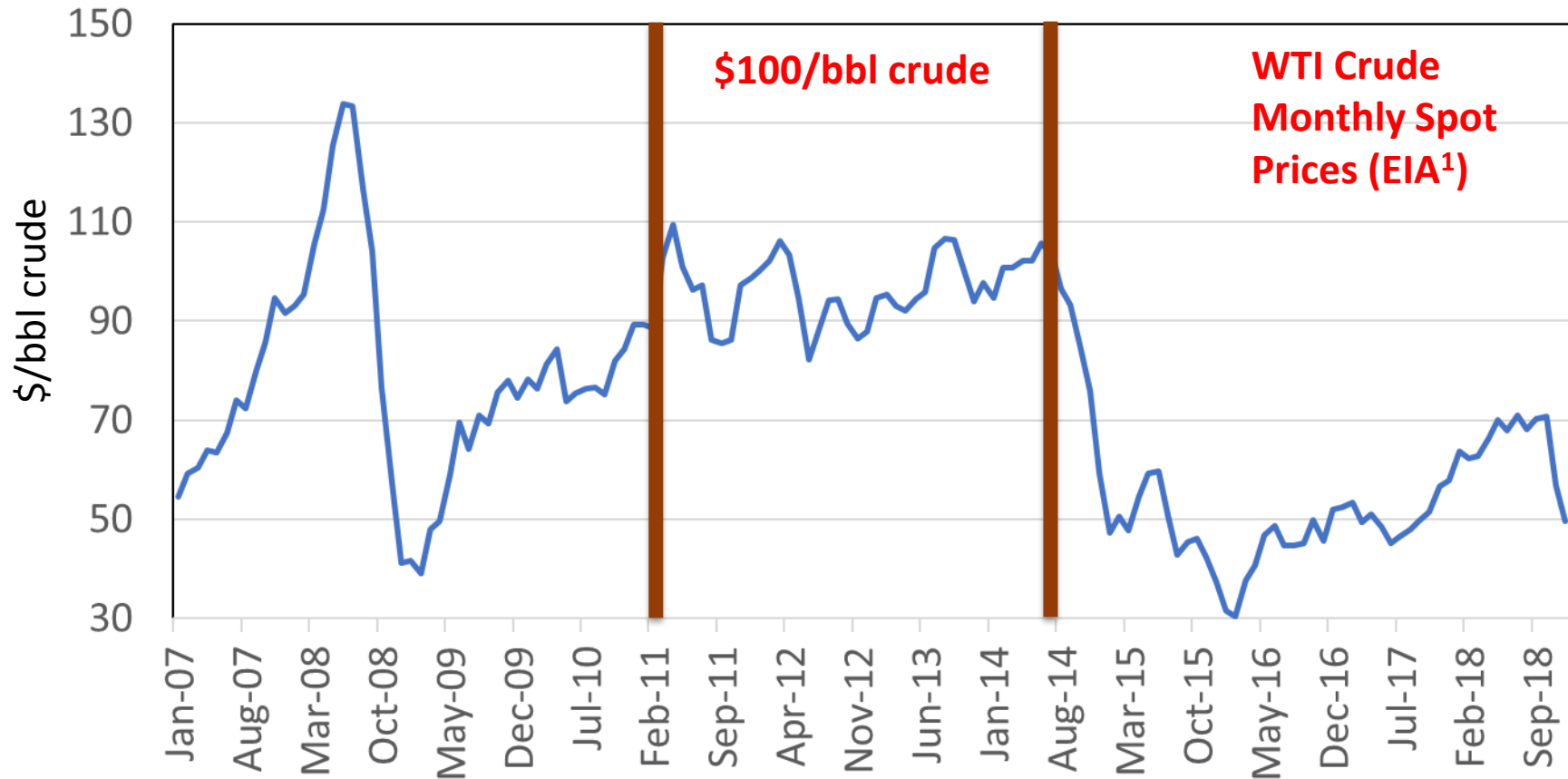
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Relevance

Goal: Understand the value proposition for novel performance advantaged bioproducts.



“Biobased chemicals are most commonly used today in high-value, low-volume specialty applications and finding success if they are needed to meet regulatory requirements or offer competitive or better performance and/or novel properties,” Doris de Guzman (Tecnon OrbiChem)

Companies must also ensure that any biobased raw materials they use do not interfere with the food supply.²

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Relevance

Working to Address Challenges Identified by Stakeholders

Moving Beyond Drop-In Replacements: Performance-Advantaged Biobased Chemicals Workshop Outcomes (Adopted from 2018 DOE BETO Workshop Report)

Top Challenges as Identified by Participants	Project Contributions to Address
<p>Target Identification: <i>Finding breakthrough opportunities where materials are limited</i></p> <p>Market Acceptance Challenges: <i>Identifying criteria and specifications that will allow for market access and meet regulatory requirements</i></p>	<p>Analyses are focused on forward looking, macro-trends in chemical sectors that have track-record of adopting bioproducts. Work has begun to outline specific properties needed for end-use applications.</p>
<p>Target Identification: <i>Unclear which novel biobased products are most useful to industry</i></p> <p>Market Acceptance Challenges: <i>Understanding where the biobased industry can provide opportunities</i></p>	<p>Initial review of a range of market sectors to identify specific drivers and outline value-proposition for the adoption of performance advantaged bioproducts. Analysis approach and methods reviewed by external advisors.</p>
<p>End-Use Challenges: <i>Understanding the technical performance of new molecules in potential applications:</i></p> <ol style="list-style-type: none">1. Identifying critical functional attributes2. Connecting what can be made to what should be/needs to be made for application	<p>PABP analysis framework tool will be a publicly available resource to outline the wide range of PABP molecules as well as critical properties and potential end-use applications.</p>

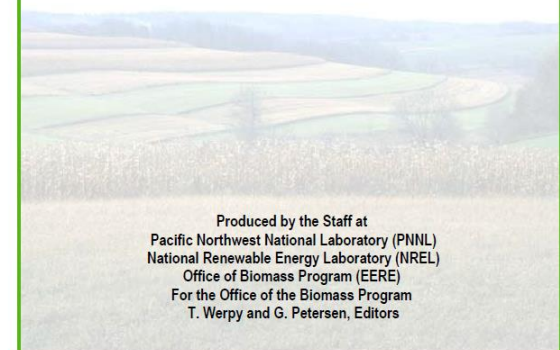
Future Work

Year 2 and 3: Develop top ten report for performance- advantaged products that is vetted by stakeholders.

- Populating key metrics of **PABP Analysis Framework** with over 170 PABP products
- **Supported by Go/No-Go:** Prior to providing suggested list of performance advantaged products for review by external stakeholders, ensure that enough data exists to summarize at least 20 bio-advantaged molecules and key metrics. Summarize in brief to DOE BETO.
 - Ensure that at least 20 performance advantaged molecules have been identified as potential candidates to consider in the study. Additionally, ensure the critical information to support key metrics for comparison of these products (including potential for scale-up, market and technical risk, social and sustainability drivers) is available.



Top Value Added Chemicals from Biomass Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas



Produced by the Staff at
Pacific Northwest National Laboratory (PNNL)
National Renewable Energy Laboratory (NREL)
Office of Biomass Program (EERE)
For the Office of the Biomass Program
T. Werpy and G. Petersen, Editors

<https://www.nrel.gov/docs/fy04osti/35523.pdf>

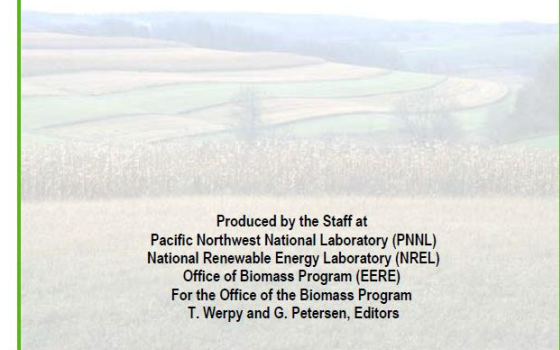
Future Work

Year 2 and 3: Develop top ten report for performance- advantaged products that is vetted by stakeholders.

- Following Go/No-Go approval, review data and selection with external review team to vet approach.
- Outline of data due to BETO in FY19 Q3.
- Sections of draft due to BETO as QPMs through FY19-FY20.
- Final draft to BETO by Q3FY20 with simultaneous review with external review team.
- Potential for a larger stakeholder briefing during project development – to be held at appropriate conference.
- Goal is for publication in Q4FY20.



Top Value Added Chemicals from Biomass Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas



<https://www.nrel.gov/docs/fy04osti/35523.pdf>

Summary

Overview: The goal of this project is to understand the value proposition for novel PABPs.

Approach:

- Close alignment with other PABP projects to enable and support goals of BETO.
- Regular project check-ins with projects to ensure coordination.
- **Externally advisory team** made up of **11 stakeholders** with experience across the value chain of bioproducts. Reviews methods and provides guidance to ensure sound approach

Technical Progress:

- Developed **draft paper** for peer reviewed publication **outlining value proposition** and market pull for performance-advantaged products.
- Approach reviewed by externally advisory team.
- Draft **outlines market needs** for transportation applications, plastic packaging, textiles, paintings and coatings, personal care products, and household cleaners.
- Focus on **macro trends and future projections for growing markets**. Outlines key property needs to meet these objectives.
- On-going work to develop **PABP analysis framework** including over 170 different products.

Relevance: Provide credible results to assist in strategic direction of PABP development. Works to outline key drivers and needs for additional market adoption.

Future Work:

- Develop **top ten report for PABP** that is vetted by stakeholders.
- **Go/no-go ensures enough data available** to develop guiding document on PABP products.
- Planned **stakeholder review** is part of project milestones and project strategy. Additional reviews with broader stakeholders will be performed, pending DOE feedback.

Acknowledgements

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NREL researchers:

- Zia Abdullah, Chris Kinchin, Jennifer Markham, Avantika Singh, Eric Tan, Ling Tao, Rick Elander, Tom Foust, and NREL technology platform researchers

Collaborators on BETO PABP projects

- Gregg, Beckham, Performance-Advantaged Bioproducts via Selective Biological and Catalytic Conversion
- Michael Crowley, Inverse Design of Polymers
- Mark Nimlos, Performance-Advantaged Bioproducts from Catalytic Fast Pyrolysis
- Andrew Sutton, Tailored Polymers Through Rational Monomer Development

Industrial, National Laboratory, and Academic Partners

External Advisory Team





Thank you

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Accomplishments – Milestone Chart

Milestone/QPM	Due Date	Progress
Summary slide deck for briefing to BETO that outlines on-going work in functional replacements. This will review previous work (by EPA, private industry and academia) on functional replacement efforts. Will summarize on-going efforts to reach out to stakeholders engagement. Outline at least 8 market pull and value proposition metrics to consider for bio-advantaged molecules. Provide summary to BETO to obtain feedback prior to sharing with external stakeholders for review and comment.	12/31/2017	Met on-time 
Review feedback from at least 10 external stakeholders on value proposition/market pull metrics to BETO. Make recommendation on which key metrics to move ahead with to support Q4 white paper based on stakeholder feedback and suggestions. feedback prior to sharing with external stakeholders for review and comment.	3/31/2018	Met on-time 
Provide BETO with an outline of the performance advantaged report as well as a brief introduction draft. Review with BETO to ensure content appropriate and study is appropriately supporting BETO R&D and strategic goals.	6/31/2018	Met on-time 
Report to BETO (with later publication upon BETO approval) that outlines at least 5 market pull and value proposition drivers for bio-advantaged molecules. This white paper will also include details on the challenges/barriers that must be overcome to enter into these markets. With BETO's approval, share with at least 10 external stakeholders for review.	9/31/2018	Met on-time 
Go/No-Go: Prior to providing suggested list of performance advantaged products for review by external stakeholders, ensure that enough data exists to summarize at least 20 bio-advantaged molecules and key metrics. Summarize in brief to DOE BETO.	3/31/2019	In progress
Provide BETO with draft report that includes at least 5 bio-advantaged production section write-ups for initial feedback. Report will be finalized by Q1 for review by at least 10 external stakeholders.	9/31/2019	In progress
Provide DOE BETO with a final draft of the top ten bio-advantaged products report. This draft will incorporate and address reviewer comments (from at least 10 external reviewers) and we will brief BETO on how this was completed. Work with BETO for final internal review and approval for final publication and release of report by end of 2020.	6/31/2020	In progress

Response to Reviewers' Comments 2017

This is a new project. *There were no reviewer comments from 2017.*

Presentations

- Invited Presentation: Mary J. Bidy “Performance-advantaged products from biomass: Market pull and drivers to support innovative products” 2019 ACS Green Chemistry Conference
- Invited Presentation: Mary J. Bidy “Performance-advantaged products from biomass: State of the market and opportunities for innovative products” USDA/DOE BRDI TAC Meeting
- Invited Presentation: Mary J. Bidy “Performance-advantaged products from biomass: State of the market and opportunities for innovative products” Energy Security Roundtable.