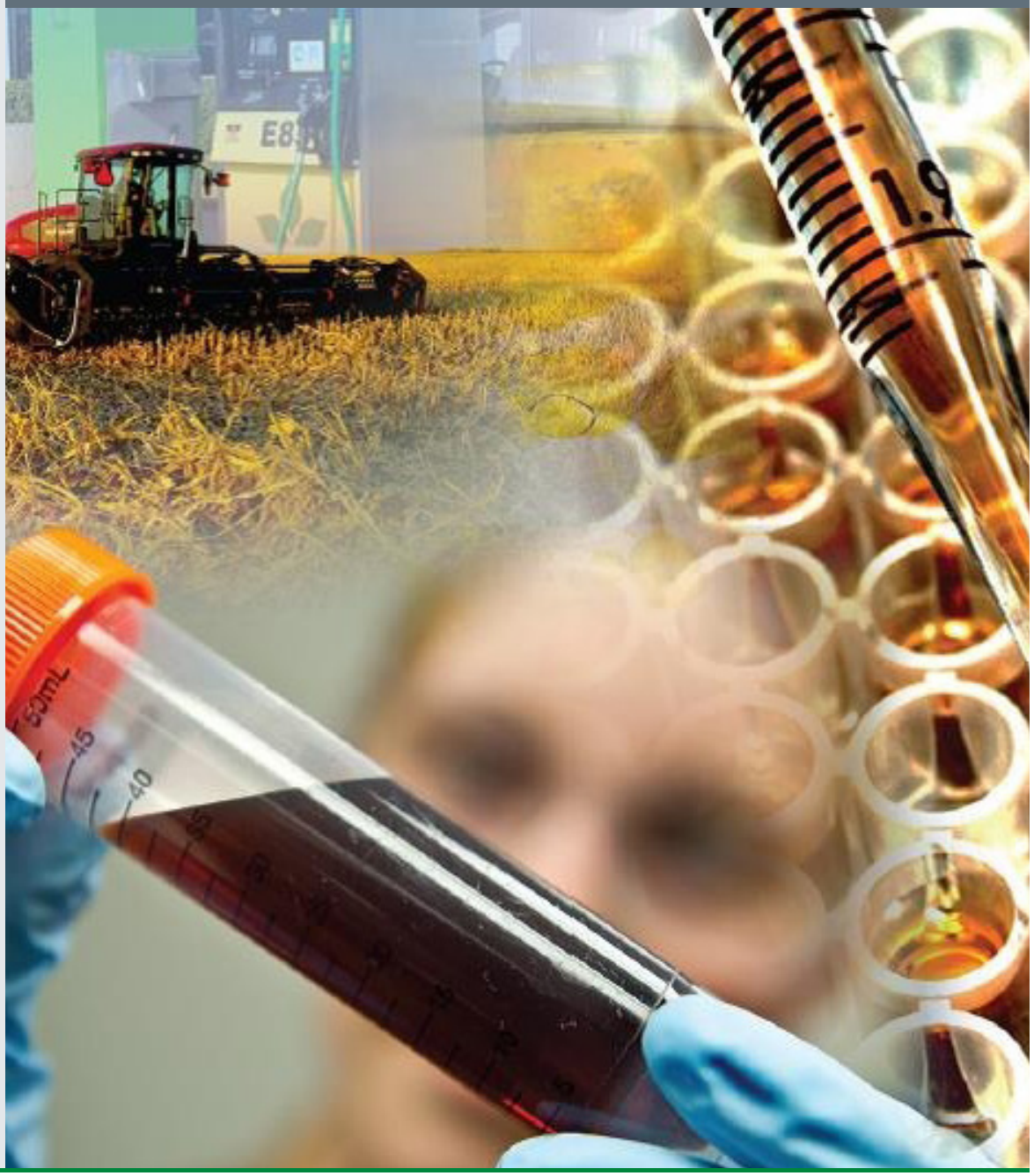
U.S. DEPARTMENT OF
ENERGY

Office of
ENERGY EFFICIENCY &
RENEWABLE ENERGY

Moving Beyond Drop-In Replacements: Performance-Advantaged Biobased Chemicals

Workshop Summary Report

June 2018



Summary report from the June 1, 2017 Workshop on Moving beyond Drop-In Replacements: Performance Advantaged Biobased Chemicals, held in Denver Colorado

Workshop and summary report sponsored by the

U.S. Department of Energy

Office of Energy Efficiency and Renewable Energy

Bioenergy Technologies Office

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Preface

The U.S. Department of Energy's (DOE's) Office of Energy Efficiency and Renewable Energy (EERE) invests in a diverse portfolio of energy technologies to achieve a stronger economy, a cleaner environment, more affordable and resilient domestic energy choices, and a more secure energy future for America. This report summarizes the results of a public workshop sponsored by DOE-EERE in Denver, Colorado on June 1, 2017.

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Introduction

The Bioenergy Technologies Office (BETO) funds early stage applied research and development (R&D) for a variety of technologies and processes to support domestic production of biofuels, biobased chemicals, and biopower. BETO focuses on reducing technology uncertainty, from feedstock supply and logistics through biorefinery technologies, to enable industry investment in technology deployment at scale. BETO has a successful track record of supporting R&D in cellulosic ethanol technologies, several of which are currently being deployed and commercialized. As cellulosic ethanol technologies mature, BETO has shifted its R&D support towards advancing technologies to create products that serve as drop-in replacements for fuels (such as renewable-gasoline, -diesel, and -jet fuel), performance-advantaged fuels through the Co-Optimization of Fuels and Engines effort, and chemicals that can supplement their fossil-derived counterparts or that may more easily be produced from biomass.

Why Bioproducts?

BETO funds research that supports the production of biomass-derived hydrocarbon fuels at the minimum fuel selling price (MFSP) of $3/gasoline gallon equivalent (GGE) or lower. Technoeconomic analysis suggests that to achieve an MFSP of $3/GGE or less, a value-added co-product must be sold to offset the cost of fuel. For example, analysis by the National Renewable Energy Laboratory has shown that for multiple biological pathways to hydrocarbon fuels, a lignin-based coproduct must be sold to reach an MFSP of $3/GGE (Figure 1).

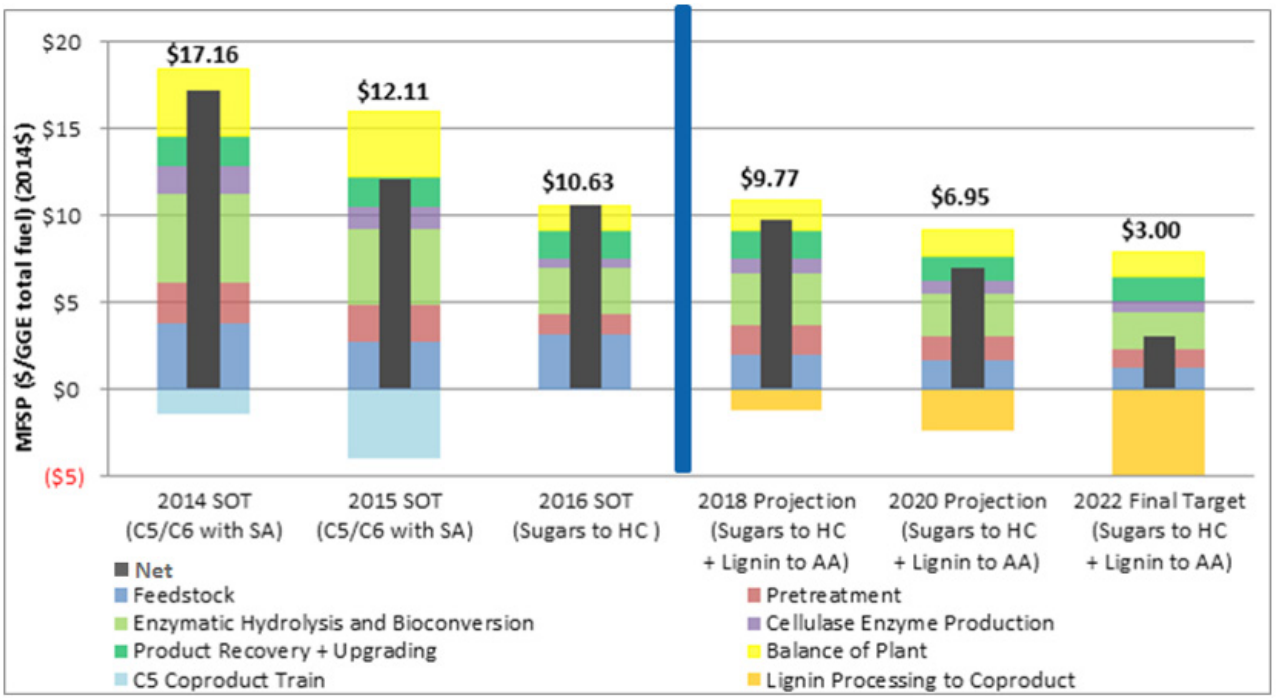

Figure 1. Cost projections for low-temperature deconstruction and catalytic upgrading of sugars pathway. To reach an MFSP of $3/GGE, the lignin waste stream must be converted into a value-added product (in this case, adipic acid)[1].

[1] Davis, Ryan. National Renewable Energy Laboratory - Biochemical Platform Analysis. Presentation at the 2017 Bioenergy Technologies Office Project Peer Review, Denver, CO, March 2017. Presentation available at: https://www.energy.gov/sites/prod/files/2017/05/f34/Biochemical%20Platform%20Analysis%20Project_0.pdf.

The strategy of producing bioproducts alongside biofuels is analogous to the petrochemical industry's approach to producing fuels and chemicals from the same crude oil feed. A major advantage of the petroleum industry is that its product slate is flexible and can be tuned to market demand. Furthermore, the petroleum industry takes advantage of the often higher margins commanded by chemicals as compared to fuels (Figure 2). As illustrated in Figure 2, approximately 76% of the volume of a barrel of crude oil goes towards making fuels, corresponding to $935 billion in revenue. In contrast, only 16% of the volume of a barrel of oil goes towards making petrochemicals; despite the much smaller volume, these chemicals produce almost as much revenue as fuels ($812 billion in revenue for chemicals). *To achieve a positive return on investment for a biorefinery that generates biofuels that are cost-competitive with their petroleum-derived counterparts, it could be necessary to flexibly co-produce bioproducts that can be sold at higher margins.*

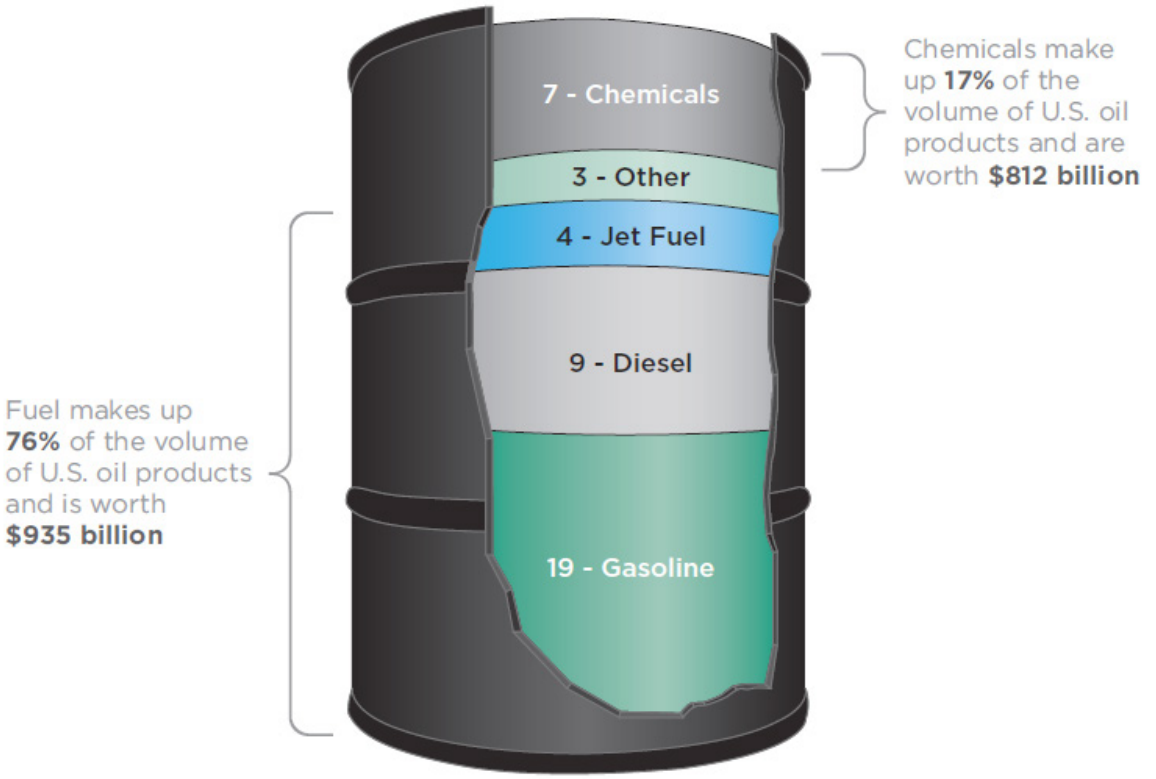

Figure 2. Products and revenue from a barrel of oil[2]

BETO invests in R&D to develop bio-derived products ("bioproducts") that have similar functions to petroleum-derived products, such as fuels and chemicals. Domestically produced bioproducts have several desirable qualities: they are made from American renewable, sustainable, resources while supporting the U.S. agricultural and bioprocessing industries; they can be manufactured in the U.S. to reduce imports and increase exports; and they can be designed to be easily recyclable and non-toxic.

Direct Replacements, Functional Replacements, and Novel Products

The relationship between a bioproduct and a petroleum-derived product can be categorized in one of three ways: bioproducts can be (1) *direct replacements* (i.e., the bio-derived product and the petroleum-derived product are chemically identical, also known as "drop-in" replacements); (2) *functional replacements* (i.e., the bio-derived product and petroleum-derived product are different chemically, but they have similar functions/properties); or (3) *novel products* (i.e., the bio-derived product does not resemble an existing petroleum-derived product in structure or function.) Because the molecular structure of a direct replacement is known, R&D targeted at developing direct

2 Bloomberg New Energy Finance, EIA, American Chemical Council. Bioproducts to Enable Biofuels Workshop Summary Report (U.S. Department of Energy, 2015), https://www.energy.gov/sites/prod/files/2015/12/f27/bioproducts_to_enable_biofuels_workshop_report.pdf

replacements is inherently simpler than targeting development of functional replacements or novel products. Biobased functional replacements and novel products represent an exciting and promising new area of R&D, but this research area is currently limited by the researcher's inability to identify target structures and structure-function relationships.

In 2004, the U.S. Department of Energy (DOE) released a report[3] listing the most promising chemicals that could be produced from biomass. This report, which focused on drop-in replacements, has served as a guiding document for the field and is widely cited by researchers working on technical challenges associated with producing these chemicals at commercial scale. Many from academia, government, and industry have requested an update to this report focusing on the emerging area of biobased functional replacements and novel compounds.[4] A strategy document on biobased novel compounds and functional replacements could take several forms, such as a description of the process for identifying targets or a list of promising biobased compounds. Regardless of the form, it will be difficult to produce a functional replacements/novel biobased compounds strategic plan without considerable R&D.

Moving Beyond Drop-in Replacements: Performance-Advantaged Biobased Chemicals

Due to the significant structural differences between petroleum-derived and bio-derived feedstocks, bioproducts also provide a platform to incorporate novel properties into existing materials. End users commonly struggle to replace chemicals that are toxic or pursue bioderived chemicals to provide new or improved performance attributes (for example, replacing bisphenol A[5]). Many manufacturers have an interest in introducing renewable, safe, cost-competitive compounds with highly desirable chemical properties to existing applications. While the search for existing petrochemical replacements that have enhanced properties or functionality has yielded few new opportunities, novel biobased alternatives remain largely unexplored. Performance advantaged biobased products are defined as novel products where the biobased product molecule does not resemble an existing petroleum-derived molecule in structure, butoffer a performance advantage over existing products.

Novel, performance-advantaged biobased products and functional replacements offer many benefits to the bioeconomy: they could enable biobased fuels—since bioproducts can be produced from biofuel process residues or at the same facility as biofuels—and they represent a new product slate that could increase consumer interest and performance advantages in biobased products. There are many challenges to pursuing R&D for performance-advantaged bioproducts and many possible ways to address those challenges; as a result, BETO hosted the Moving beyond Drop-In Replacements: Performance-Advantaged Biobased Chemicals Workshop in June 2017 to solicit stakeholder feedback to formulate a plan going forward. During this workshop, BETO sought responses to the following questions:

- What are the challenges in identifying and developing novel biobased chemicals?
- What are the solutions and strategies?
- If there was a concerted R&D effort in this area, what considerations do you think are most important?
- What is the best path towards
  - Producing a strategic plan for performance-advantaged biobased chemicals
  - Providing a repository of useful, fully characterized, biobased compounds with known properties for consumer use
  - Providing a publicly accessible, high-throughput screening facility for identifying biobased functional replacements and novel products?

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[3] T. Werpy and G. Petersen, eds., Top Value Added Chemicals from Biomass: Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas (U.S. Department of Energy, 2004), https://www.nrel.gov/docs/fy04osti/35523.pdf.

[4] An update was published in 2010: Bozell, J. J. and Petersen, G. R. Tehcnology development for the production of biobased products from biorefinery carbohydrates—the US Department of Energy's "Top 10" revisited. Green Chemistry 2010 12 539-554. DOI: 10.1039/b922014c

[5] For a description of how biobased isosorbide can be a performance advantaged replacement for bisphenol A, visit https://www.roquette.com/industries/performance-materials/polycarbonates/

Workshop Structure

Overview

BETO held the Moving beyond Drop-In Replacements: Performance-Advantaged Biobased Chemicals Workshop on June 1, 2017, in Denver, Colorado. Approximately 90 stakeholders attended, representing companies, national laboratories, government agencies, and academic institutions. A list of workshop attendees who agreed to share their contact information can be found in Appendix A. The breakdown of stakeholders is shown in Figure 3 below.

The day began with a keynote presentation from Nichole Fitzgerald of BETO to give participants an overview of the Office's current work on functional replacements, as well as to outline the goals of the workshop. This was followed by two keynote presentations from industry representatives—Dale McIntyre (Behr Masco) and Michael Saltzberg (DuPont Industrial Biosciences)—on their current work with performance-enhanced biobased chemicals. Participants then attended two breakout sessions in smaller groups to provide feedback. In the afternoon, a third and final keynote—given by Dr. Brent Shanks (Center for Biorenewable Chemicals, Iowa State University)—covered potential strategies for targeting future research in this area, followed by a final breakout session on the same topic. A detailed agenda can be found in Appendix B.

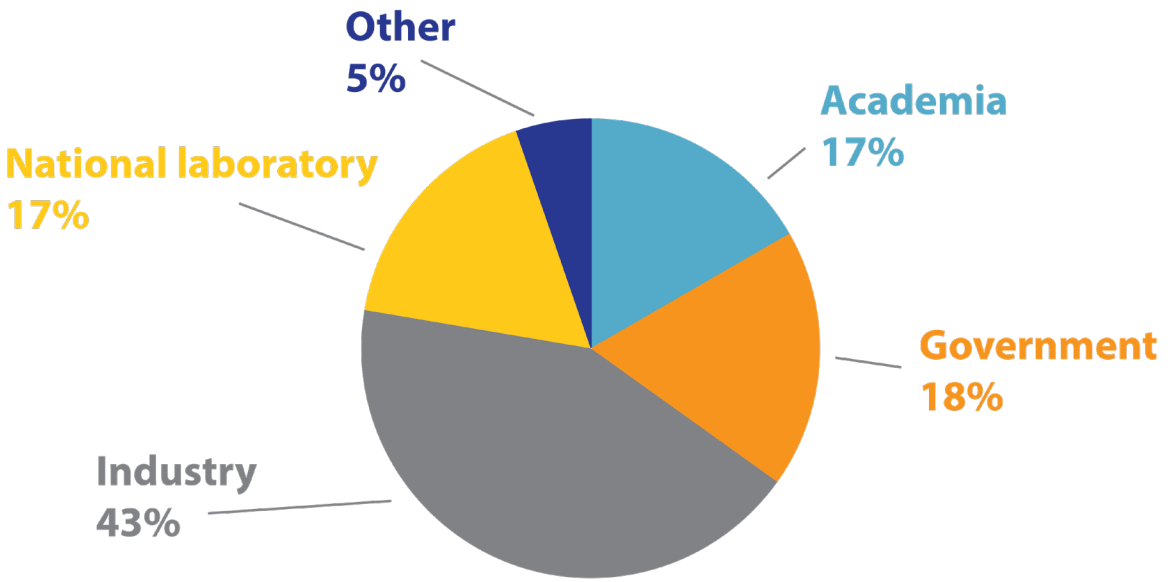

Figure 3. Workshop participants by sector

Breakout Session Structure

Participants were randomly assigned to one of four groups for the first breakout session to ensure an even distribution of stakeholder affiliations. Participants in each session were asked the same set of questions, focusing on why performance-advantaged biobased chemicals are of interest and the biggest challenges to identifying and developing these compounds. A full list of questions asked in each breakout session can be found in Appendix C.

At lunch, the facilitation team compiled the challenges identified in the first breakout session. At the end of the first session, each breakout group was asked to sort the challenges they identified into four broad categories described in more detail below. Participants could select which of these four options they were most interested in discussing further, which determined their group for the second breakout session. Each group was asked targeted questions about which challenges were top priorities for their category and how these challenges could be best addressed.

The third breakout session sought to identify strategies for organizing a cohesive R&D effort to facilitate the development and market acceptance of performance-advantaged biobased chemicals. This followed the same format as the first session, where participants were randomly assigned to one of the four groups and were all asked an identical set of questions.

For each breakout session, participants were seated in small groups of three to five people and were encouraged to discuss answers to each question among their table before responding in group discussion. Participants were also asked to write their answers on notecards, which were collected and recorded using ThinkTank software, ensuring that even comments that were not spoken were still recorded.

Participant Responses

Opportunities for Developing Performance-Advantaged Biobased Chemicals

As described above, each of the groups in the first breakout session first provided feedback on opportunities for developing performance-advantaged biobased chemicals. There was a general consensus that this area is of interest for stakeholders across sectors with potential for growth. Participants in all four groups identified benefits in three main areas as driving factors for this research: (1) generation of novel products, (2) economics, and (3) environmental impact. The top responses related to each area are identified in Figure 4 below.

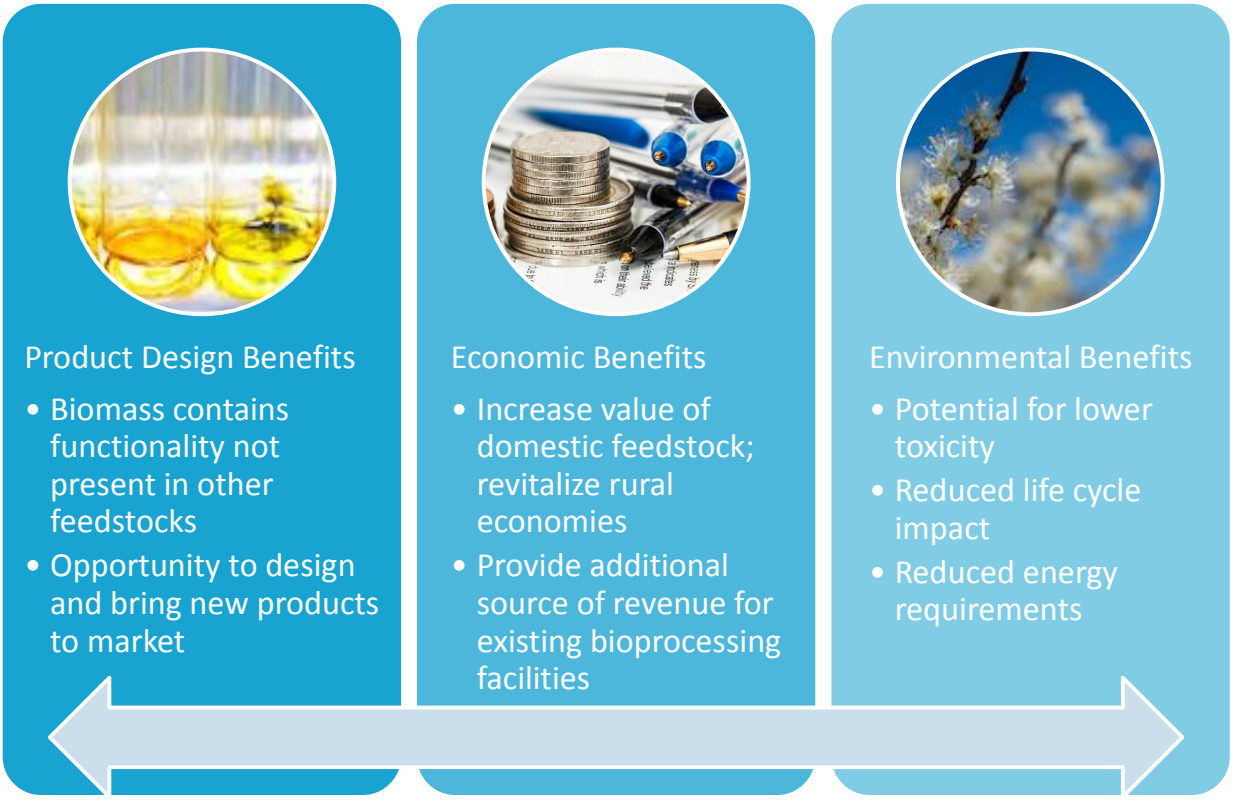

Figure 4. Opportunities for developing performance-advantaged biobased products

Generation of Novel Products

Responses in this topic related to product design highlighted the potential advantages of using a biomass feedstock, which offers novel molecular functionality when compared to traditional petrochemical processes. Biomass feedstocks contain large amounts of oxygen (up to 50 weight percent) and stereochemistry; these features would need to be introduced synthetically if using petroleum-based feedstocks. Starting with this functionality opens up new applications and opportunities in the chemicals industry. As Dr. Shanks noted in his keynote address, there is a great appetite for new performance attributes, but new petroleum-derived products have not been introduced since the 1990s. Several participants said that the potential for introducing new products to the market was a driver for interest in this area.

Conventional wisdom in the biomass industry has dictated that drop-in replacements, rather than novel chemicals, are the easiest products to produce from biomass because the product specifications, applications, and markets are already

established. Over the past decade or so, it has become apparent that producing chemicals from biomass that are already produced relatively cheaply from petroleum is often economically infeasible. It is also not trivial to meet product specifications when the starting feedstock changes so significantly – from a hydrocarbon to a carbohydrate. (A notable exception to this is succinic acid production.[6]) Those in the bioproducts arena have turned their attention to novel biobased chemicals that can be produced cheaply because they capitalize on the oxygenated and oxidized structure of biomass (i.e., additional reducing steps and reductants do not contribute to the process economics). As a result, many workshop participants indicated that new products and product design were a great opportunity for the biomass industry.

Economics

Because performance-advantaged biobased chemicals offer the opportunity to enter new markets, they offer a new source of revenue for existing biorefineries. This helps diversify these facilities' output and makes them more attractive to potential investors. Any process that increases the value of biomass also has the potential to strengthen rural economies and encourages investment in domestic resources.

By selecting a product that is well-suited for synthesis from biomass, such as a chemical that contains heteroatoms or stereochemistry already present in biomass, the production costs have the potential be lower than synthesizing the same product from petroleum-derived starting materials. It is important to realize that many of the products we use today are a result of over 100 years of process development by the petroleum industry. Many of these products are well-suited for synthesis from petroleum because, historically, that has been the starting material available. Similarly, many chemicals that can be made cheaply from biomass would be very expensive to make from petroleum.[7] There is great opportunity to develop novel, performance-advantaged products with inexpensive and comparatively efficient processes. Novel biobased chemicals may be a great market entry point for biorefiners.

Of note, however, many participants and keynote speakers did not believe there is much room for a "green premium" in the bioproducts arena. They felt strongly that consumers would not pay extra for a product simply because it has an improved environmental footprint. Indeed, the premise of this workshop was that producers would need to identify a *performance advantage* for a novel bioproduct.

Environmental Impact and Energy Efficiency

Utilizing biomass feedstocks can also potentially reduce the life-cycle impact of synthesis. Due to the relative lability of C¬O bonds, biobased chemicals could be designed to be biodegradable or have better recyclability than similar petroleum products, lowering the life-cycle cost of production. Participants also noted that biobased chemicals may offer reduced toxicity, which is an attractive feature for consumers for certain classes of products, such as personal care products or food packaging.[8]

Challenges and Potential Solutions

After discussing the opportunities above, participants were then asked to broadly identify the primary challenges for discovering and developing performance-advantaged biobased chemicals and for bringing those products to market. Initially, facilitators asked the participants in each group to identify challenges with no guidance on categories. After each group had been given the opportunity to list challenges, the first session finished with participants sorting the each previously identified challenge into one of four main categories that span the supply chain of chemical production: (1) target identification, (2) technology development, (3) end use, and (4) market acceptance (this category included challenges related to policy).

Facilitators had previously identified these four areas as likely major categories, but participants were also given the opportunity to come up with additional areas. Though this was an option, participants across all four rooms generally agreed that these four areas did cover most of the challenges, so they were used by the facilitators for the remainder of the workshop.

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[6] For a brief description of the success of succinic acid, see: http://www.biofuelsdigest.com/bdigest/2015/02/16/biofuels-digests-advanced-bioeconomy-awards-for-2015/

[7] For analysis of several compounds made from both biomass and petroleum feedstocks, see Mary J. Biddy, "CEMAC: Market Analysis of Biomass-Based Chemicals Substitutions" (presentation at the Bioenergy Technologies Office's 2017 Project Peer Review, Denver, Colorado, March 7, 2017), https://energy.gov/sites/prod/files/2017/05/f34/analysis_and_sustainability_biddy_6.3.0.5.pdf.

[8] For an example of the plastics industry employing the USDA BioPreferred labeling system, see https://www.plasticstoday.com/content/usda-biopreferred-label-program-growing-among-packaging-industry/35699489917212

For the second breakout session, the challenges from all four rooms were aggregated into a single set of feedback. Each breakout group in the second session worked with the collective feedback from session one for a single challenge category. For each group's area, participants were asked to prioritize what they viewed as the top 5–10 challenges from the first breakout session and then brainstorm potential solutions. Table 1 summarizes the top challenges identified by each group.

After reviewing each group's list of top challenges and potential solutions, four common themes emerged. These areas of challenges and potential solutions are presented below.

Table 1. Top Challenges as Identified by Participants

Technical Challenges	End-Use Challenges	Market Acceptance Challenges	Target Identification Challenges
Valorizing entire feedstock to functional molecules	Ability to rapidly scale production of new molecules	Informing the consumer of biobased alternatives and working with preconceptions about biobased materials	Relating structure to function: 1. Application identification 2. Modeling of physical properties 3. Structure property relationships
Technical uncertainty in combining technologies that are not well-established	Disconnect between technology and biochemical developers and end users/ formulators	Understanding where the biobased industry can provide opportunities	Developing high-throughput screening protocols and metrics to screen for, to identify performance-advantaged bioproducts
Low technical maturity when compared to petrochemical technologies	Difficult to determine which properties to screen for in pure streams because the properties might be distorted when introduced into formulations	Connecting partners to enable collaboration	Conflict between open communications and Intellectual Property (IP) protections
Separations technologies to deal with unique biomass-derived intermediate and product streams	Understanding the technical performance of new molecules in potential applications: 1. Identifying critical functional attributes 2. Connecting what can be made to what should be/ needs to be made for applications	Identifying criteria and specifications that will allow for market access and meet regulatory requirements	Disconnect between technology and biochemical developers and end users/ formulators

Table 1. Top Challenges as Identified by Participants (continued)

Technical Challenges	End-Use Challenges	Market Acceptance Challenges	Target Identification Challenges
Scaling processes and producing new materials at large enough quantities for testing by those manufacturing end products	Meeting commercial specifications	Working with supporting policies as well as government regulations	Unclear which novel biobased products are most useful to industry
Quantifying sustainability metrics related to biobased products		Competition with incumbent technologies and materials	Finding breakthrough opportunities where materials are limited
Relating molecular structure of biobased compounds to function in a variety of applications			
Developing catalytic methods for upgrading of biomass-derived intermediates			

The feedback presented below reflects stakeholder input only. BETO has not made a commitment to pursuing any of these strategies at this time or at any point in the future.

Lack of Communication between Relevant Stakeholders

The issue of poor communication channels between molecule producers and end-users appeared in some form as a top challenge in each of the areas identified above. Molecule producers cited issues with not knowing target commercial properties (where allowed by IP agreements) to screen for in potential molecules. End users felt there was a disconnect between the technology push from molecule producers and the market pull for biobased chemicals. In addition to communication issues between molecule producers and end users (both manufactures and consumers), some participants also cited issues with communication within those stakeholder groups as well.

Participants discussed a number of potential models for alleviating this problem. These included a centralized system to collect molecule performance specifications from industry, as well as a more organized structure, such as the Department of Energy's and National Science Foundation's I-Corps models, where end-market consumers are involved in validating the technology proof of concept. Most participants also agreed that addressing this issue would help lead to solutions for the other challenges that were identified.

Another potential benefit of increasing communication between the stakeholders involved in these processes is that it may help standardize metrics. Environmental sustainability was cited as one of the main drivers for pursuing performance-advantaged biobased chemicals, but without a consistent form of techno-economic analysis or life-cycle assessment or agreement on methods for calculating diffuse benefits such as ecosystem services, it can be difficult to quantify sustainability in a meaningful way. Performance metrics also need standardization; facilitating conversations between end users and producers would ensure that performance requirements were articulated clearly.

Moving forward, BETO is discussing internally what role DOE might play in facilitating these connections, as well as how BETO can better ensure that relevant stakeholders are aware of each other's work. Steps to improve communication between stakeholders can take place on a more rapid basis than many of the proposed solutions to other challenges and will be an important priority.

The following are some possible roles that workshop participants suggested BETO could play in facilitating communication between relevant stakeholders:

- Facilitate annual workshops or conferences that bring academic and national laboratory research scientists, small bioproducts companies, and end users together
- Sponsor BETO researchers to participate in I-Corps
- Act as a clearinghouse for performance-advantaged bioproduct technical challenges. BETO could collect lists of recommendations and technical challenges faced by private companies through an open submission process, obscure the attribution, and present the generic challenges in a funding opportunity announcement.
- Offer a challenge similar to the Green Chemistry and Commerce Council (GC3) preservative challenge, which connects scientists and end users by allowing applicants to submit solutions to problems related to conventional preservatives submitted by consumer product formulators, manufacturers, and suppliers[9]
- Gather stakeholder input to develop definitive lists of performance attributes to test for.

Not Enough Data for Effective Decision Making

Stakeholders from across sectors repeatedly cited a lack of data about the relationship between molecular structure and potential function as a major barrier to performance-advantaged biobased chemicals research. An inability to predict functionality means that scientists often produce a large number of potential molecules and find it difficult to test all of them or get feedback on which are the most attractive. Being able to better link structure to function would help researchers target fewer molecules and increase the potential for success.

While this was a major topic of discussion for the group discussing challenges related to target identification, it also emerged in several other groups. End users who are searching for a specific functionality, or even functionality related to a general class of products, also expressed that it was difficult for them to understand the potential performance of new molecules in target applications.

Across all breakout groups, participants' solutions to this issue primarily related to increasing access to high-throughput screening facilities. Participants suggested this could take place either by developing new facilities or by increasing awareness of existing ones. Such a facility would screen candidate molecules for a preselected set of properties and metrics. Aggregating data from high-throughput testing could help generate predictive models and, depending on the structure of the facility, could produce open databases of physical and chemical properties for researchers to use. In order to make a high-throughput center more effective, participants also suggested early efforts to identify high-priority target classes of molecules that would be most useful to screen.

Participants suggested the following possible ways that BETO could increase availability of data for effective decision making:

- Fund experimental research for identifying structure/function relationships for bioproducts
- Fund computational research for predicting structure/function relationships for bioproducts
- Fund market analysis for understanding the best opportunities for bioproducts
- Fund R&D for creative approaches to target bioproduct identification

[9] More information about the GC3 challenge can be found on GC3's website: http://www.greenchemistryandcommerce.org/projects/preservatives-project.

- Fund high-throughput screening of biobased chemicals and formulations to collect data on their performance attributes.

Low Technical Maturity of Technologies for Biobased Processes

Participants across all groups noted that biobased processes have a relatively low technical maturity and could benefit from additional early stage applied R&D. Participants in multiple groups identified challenges associated with separations, integration of biochemical and thermochemical processes, and scale-up as crucial barriers to progress. These challenges are not specific to the production of biobased chemicals, but they contribute to difficulties in the field. They also contribute to the difficulty some companies face when trying to attract potential investors.

Several stakeholders noted that scale-up was an area where the lack of data and equipment for biobased processes presents a specific challenge to developing performance-advantaged biobased chemicals. End users noted that, often, properties present in molecules that are tested at the lab and bench scale may be lost when scaling up to full production scale, or when combining into a finished formula at scale. Because production processes for many biobased molecules cannot be scaled rapidly, the risk associated with testing biobased replacements in formulas is increased.

To help reduce the risks/technology uncertainty associated with this area of challenges, participants primarily suggested more investment in research to better bridge the gap between breakthroughs at small scale to the larger scale technologies already available for end use. This could be in the form of pilot facilities specifically related to performance-advantaged biobased products, or could more generally involve investment in biorefineries and other bioenergy research facilities. In this way, improving individual unit operations, like separation steps, has the added advantage of positively affecting the rest of the bioeconomy as a whole.

Participants felt better processes for sharing lessons learned also need to accompany increased investment in technology development. Much like the previous challenges, participants felt that a perceived disconnect between molecule producers and end users may make it more difficult to overcome these issues.

Participants suggested the following possible ways that BETO could raise the technical maturity of biobased processes:[10]

- Provide researchers and small companies with access to large-scale demonstration facilities so that they can produce large quantities for end-use testing and demonstration
- Continue to fund research across the bioenergy supply chain, particularly in areas such as the following:[11]
  - Developing technologies for isolating, deconstructing, upgrading, and valorizing lignin and other biomass components
  - Developing separations technologies to address the unique challenges of biomass-derived intermediate streams
  - Developing catalytic methods for upgrading biomass-derived intermediates
  - Developing computational models for predicting structure-function relationships
  - Developing high-throughput screening methods for identifying structure-function relationships
  - Quantifying sustainability metrics related to biobased products
  - Ensure funding recipients make their findings available to the public to the maximum extent possible.

[10] The feedback presented below reflects stakeholder input only. BETO has not made a commitment to pursuing any of these strategies at this time or at any point in the future.

[11] Many of these areas can be addressed through existing BETO resources such as the Bioenergy Separations Consortium or the Chemical Catalysis for Bioenergy Consortium.

Difficulty Entering Product Markets

The final broad area of challenges relates to entering the market after product development and testing. This area covers issues related to both regulatory requirements for entering markets with new molecules and challenges to gaining consumer acceptance. While BETO does not work on regulatory issues, understanding stakeholder concerns in this area provides valuable information on how BETO can maximize the impact of research, and ensure that the data collected from R&D efforts is provided to regulatory agencies to help them make more informed decisions.

Participants indicated that it is currently difficult to predict the most impactful areas for which to develop performance-advantaged biobased chemicals. Targeting opportunities where petroleum-based materials are currently not meeting the needs of consumers would be ideal, but many participants did not feel like this information was available.[12] Even if these areas are identified and successful performance-advantaged alternatives can be produced, there were also concerns that the biobased products would struggle to break into established markets. This could be because consumers are not aware of the potential advantages of the product or of how biobased products may differ from traditional options.

Many of the issues with consumer acceptance are similar to the challenges identified above related to communication between stakeholders. In order to overcome these challenges, participants felt it would be useful to develop better methods for consumer feedback, in addition to developing structures for molecule producers and end users to better communicate. Information on the classes of products for which consumers would be most inclined to seek out a performance-advantaged biobased alternative would help end users and molecule producers target their research. Getting better feedback from potential consumers could also be accompanied by better consumer education initiatives to explain the advantages of biobased alternatives.

Participants suggested the following possible ways to reduce barriers to entry to product markets:

- Ensure representatives from consumer groups are part of any facilitated conversations between research scientists and end users
- Incorporate common consumer concerns into analysis when determining high-priority research targets
- Assist with the development of guidelines for educating consumers on biobased products
- Articulate potential regulatory and market entry hurdles to interested stakeholders so that they can design their R&D to address these challenges early on and ensure that relevant data is available to regulatory agencies.

Facilitating the Development of Performance-Advantaged Biobased Chemicals

After Dr. Shanks gave his keynote, participants were assigned randomly to one of four breakout sessions to discuss potential pathways towards overcoming the challenges identified in the previous session.

Many participants cited DOE's 2004 report, Top Value Added Chemicals from Biomass,[13] as a valuable resource that has been used and updated multiple times since its initial publication. They felt that another update specifically concerning performance-advantaged biobased chemicals would be a useful guiding document for R&D and would help focus efforts in this area.

The discussion in the earlier sessions had already touched on the idea of a scientifically-driven high-throughput testing facility that would both allow molecule producers and end users to connect and generate a large volume of data on molecular properties that could be used to better target future research. Participants were generally in favor of such a facility, but they had differing opinions on its exact structure and what it might contain. Some felt that there were existing facilities that this effort could adapt and add to in order to meet stakeholder needs. Others were

[12] The Green Chemistry Council has assembled a list of attributes needed in novel biobased chemicals: https://greenchemistryandcommerce.org/documents/GC3-Detailed-Tech-Needs.pdf

[13] T. Werpy and G. Petersen, eds., Top Value Added Chemicals from Biomass: Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas (U.S. Department of Energy, 2004), https://www.nrel.gov/docs/fy04osti/35523.pdf

Figure 5. Responses from across sectors indicated an interest both in a testing facility and in a structure that would better facilitate communication and collaboration.

more interested in the development of new structures specifically focused on performance-advantaged biobased chemicals.

Stakeholder Interest in a High-Throughput Testing Facility

At the conclusion of the third breakout session, participants discussed how they would use a potential facility that targeted the identification, synthesis, and testing of novel biobased compounds. A summary of the responses is shown in Figure 5 above.

The discussion responses indicate that, while participants were all interested in a testing facility, they differed in their opinions of what that facility should focus on. Not surprisingly, industry participants were interested in obtaining access to pilot facilities, whereas academics and national laboratory representatives were interested in earlier-stage research that focused on target identification.

DOE's Role in Addressing Challenges

As noted above, the challenges and solutions suggested by participants are reported here as a record of events only. This report does not represent a commitment by BETO to take specific action on any of these ideas now or at any point in the future. Some areas that participants suggested for increased funding or research are out of the scope of governmental involvement and would be better undertaken by private industry or other research institutions. Areas where BETO can play a role are highlighted below:

- Fund early stage research to develop fundamental resources that can be used to identify target performance advantaged biobased products. These resources could include roadmaps, market assessments, and computational models.
- Fund early stage research assessing structure/function relationships specifically for biobased molecules. Methods for assessing structure/function relationships could include computational studies and high-throughput property assessments.
- Fund early stage research for developing a repository of useful, fully characterized, biobased compounds with known properties relevant to consumer end-use.
- Fund early stage research for identifying and publishing performance attributes unique to biobased compounds along with example compounds that display those attributes.
- Fund computational and experimental research that will help link physical and chemical properties to different end use applications.

- Connect researchers in relevant areas across the nation to maximize communication and minimize redundant efforts.
- Communicate with agencies that would be responsible for regulating biobased products and can ensure that R&D projects share relevant data with these agencies so they can make informed decisions about how to structure potential regulations.

This workshop was intended to provide a broad overview of the current state of performance-advantaged biobased chemicals. One of the primary ways BETO can assist progress in this area is to continue the conversations that were started here and obtain additional detail for a more organized course of action moving forward. Many of the challenges articulated by participants would benefit from additional specificity before any action is taken to better target the tools used to address them.

Conclusions

Performance-advantaged biobased products present an important opportunity for the bioeconomy. The ideal novel biobased compound would achieve the following:

- Allow for new functionality in end products and generate new markets for manufacturers of biobased materials
- Increase the value of domestic biomass resources and provide a new revenue stream for biorefineries
- Reduce the environmental impact of some manufacturing processes

The focus of this workshop was to better understand current challenges to developing novel biobased compounds, discuss potential solutions, and determine the steps still necessary to generate a well-defined strategy for identifying and characterizing these compounds. While there was no single path forward, several themes emerged when discussing these topics:

- Work across the supply chain is often not as efficient or impactful as it could be due to difficulties facilitating communication between relevant stakeholders. More open communication is necessary to move forward.
  - Documents or other resources that identify potential target products are useful for standardizing communication across parties.
- In many cases, there are not enough data available on how molecular structure relates to potential function in formulated systems.
  - It would be useful to identify a finite set of metrics/properties/specifications for which a large number of candidate molecules could be screened.
  - A high-throughput testing facility that integrates computational modeling would be of use in solving these challenges.
- The low technical maturity of many technologies related to biomass conversion presents difficulties for advances in this area.
- Even with successful product development, there are a number of technology uncertainties associated with potential market acceptance of new chemicals.

DOE would like to thank workshop participants for their time and input on this topic. BETO will incorporate this feedback when developing programmatic plans for performance-advantaged biobased chemicals.

Appendix A: Registered Attendees

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Appendix B: Workshop Agenda

MOVING BEYOND DROP-IN REPLACEMENTS: PERFORMANCE-ADVANTAGED BIOBASED CHEMICALS

Hosted by the U.S. Department of Energy, Bioenergy Technologies Office
Embassy Suites by Hilton Denver International Airport
Denver, Colorado
June 1, 2017

Time	Event	Speaker
7:30 a.m.–8:15 a.m.	Registration	
8:15 a.m.–8:30 a.m.	Workshop Introduction	Nichole Fitzgerald, U.S. Department of Energy, Bioenergy Technologies Office
8:30 a.m.–8:50 a.m.	Assessing New Chemistry Options—A View from the Middle of the Supply Chain	Dale McIntyre, Behr Process Corporation
8:50 a.m.–9:10 a.m.	Reflections on Performance-Advantaged Biobased Chemicals	Michael Saltzberg, DuPont Industrial Biosciences
9:10 a.m.–9:20 a.m.	Break	
9:20 a.m.–10:50 a.m	Facilitated Breakout Session 1: Why Pursue Bio-Advantaged Chemicals and Functional Replacements? *Participants will be assigned to one of four sessions, all of which will discuss the same set of questions.	
10:50 a.m.–11:05 a.m.	Break	
11:05 a.m.–11:30 a.m.	Report Out from Breakout Session 1	
11:30 a.m.–12:30 p.m.	Lunch	
12:30 p.m.–2:00 p.m.	Facilitated Breakout Session 2: Addressing Challenges *Participants may select the breakout session topic of their choice. Topics will be based off answers to questions from Breakout Session 1.	
2:00 p.m.–2:15 p.m.	Break	
2:15 p.m.–2:45 p.m.	Report Out from Breakout Session 2	
2:45 p.m.–3:05 p.m.	Creating a General Strategy for the Development of Biobased Chemicals	Brent Shanks, Center for Biorenewable Chemicals, Iowa State University
3:05 p.m.–3:15 p.m.	Break	
3:15 p.m.–4:45 p.m	Facilitated Breakout Session 3: Next Steps *Participants will be assigned one of four sessions, all of which will discuss the same set of questions.	
4:45 p.m.–5:00 p.m.	Break	
5:00 p.m.–5:30 p.m.	Report Out from Breakout Session 3	
5:30 p.m.–5:45 p.m.	Concluding Remarks	Nichole Fitzgerald, U.S. Department of Energy, Bioenergy Technologies Office

Appendix C: Breakout Session Questions

Session 1: Motivations for Performance-Advantaged Biobased Chemicals

- Why pursue performance-advantaged biobased chemicals and functional replacements (e.g., industry motivations, new products, improved performance, sustainability)?
- How do you define "performance advantaged"? What specific properties or metrics would a biobased chemical need to have/achieve to be considered performance advantaged?
- What are the biggest challenges to identifying/developing novel compounds and functional replacements and bringing those products to market?

Session 2a: Technical Challenges

- What were the most important technical challenges that were identified in the morning session? What are possible solutions to those technical challenges?
- Are there challenges that need to be solved in an immediate (next 1–3 years) timeframe before other challenges can be addressed?
- What metrics are needed to determine if a chemical is a performance-advantaged bioproduct?
- Which qualities of biobased chemicals generate the most excitement for end users?
- Are there significant knowledge gaps in the current state of the art that, if filled, could increase the likelihood of identifying performance-advantaged bioproducts?
- If a facility were set up to do high-throughput identification of novel biobased products, what are the most critical properties to screen for when developing screening protocols?

Session 2b: End-Use Challenges

- What were the most important end-user challenges that were identified in the morning session? What are possible solutions to those challenges?
- Are there challenges that need to be solved in an immediate (next 1–3 years) timeframe before other challenges can be addressed?
- How commercially viable are novel biobased chemicals? Are there specific subsets of molecules that are more commercially promising?
- Which qualities of biobased chemicals generate the most excitement for end users?
- Which end-use sectors are most interested in introducing performance-advantaged biobased chemicals?
- How can BETO best bridge the gap between those producing novel biobased compounds and those who need novel compounds or replacements for their formulations?

Session 2c: Market Acceptance Challenges

- What were the most important market acceptance challenges that were identified in the morning session? What are possible solutions to those challenges?
- Are there challenges that need to be solved in an immediate (next 1–3 years) timeframe before other challenges can be addressed?
- What types of testing are needed for a novel compound to ensure its market acceptance?

- What are the regulatory challenges associated with bringing novel biobased compounds to market?
- How commercially viable are novel biobased chemicals? Are there specific subsets of molecules that are more commercially promising?
- Are there examples of successful introductions of novel biobased chemicals into the market on which future efforts should be based?

Session 2d: Target Identification Challenges

- What were the most important target identification challenges that were identified in the morning session? What are possible solutions to those challenges?
- Are there challenges that need to be solved in an immediate (next 1–3 years) timeframe before other challenges can be addressed?
- What metrics are needed to determine if a chemical is a performance-advantaged bioproduct?
- How can research be focused to better identify performance-advantaged chemicals? Partnerships? Research centers?
- Are there examples of models for this kind of effort that work particularly well?
- How do sustainability and life-cycle analysis factor in when determining which products to target?
- If a facility were set up to do high-throughput identification of novel biobased products, what are the most critical properties to screen for when developing screening protocols?
- Are there significant knowledge gaps in the current state of the art that, if filled, could increase the likelihood of identifying performance-advantaged bioproducts?

Session 3: Next Steps

- What types of resources would be useful for researchers and businesses to facilitate the development and market acceptance of performance-advantaged biobased chemicals? (Road maps? Research centers? Facilitated collaborations?)
- Are there examples of models for this kind of effort that work particularly well?
- If roadmaps/guiding documents are identified in the previous question, ask the following: What is the best strategy for developing biobased novel compounds and functional replacements guiding document? From your point of view, what information/metrics would it be critical that this document contain?
- If a research center is employed for identifying biobased novel compounds and functional replacements, what would that center look like?
- What elements would you like to see in a research center that was targeting the identification, synthesis, and testing of novel biobased compounds?
- What are possible intellectual property models for research centers and consortia?

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DOE/EE-1713 • June 2018