PERFORMANCE-ADVANTAGED BIOPRODUCTS AND SEPARATIONS

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Performance-Advantaged Bioproducts and Separations (PABP/SEPS) Technology Area is one of 14 related technology areas that were reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review, which took place on March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 14 projects were reviewed in the Performance-Advantaged Bioproducts and Separations session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $25,459,273 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 3% of the BETO portfolio reviewed during the 2019 Peer Review. During the project peer review meeting, the principal investigator (PI) for each project was given 30–35 minutes (depending primarily on the funding level) to deliver a presentation and respond to questions from the review panel.

Projects were evaluated and scored for their project approach, technical progress and accomplishments, relevance to BETO goals, and future plans. This section of the report contains the results of the project review, including full scoring information for each project, summary comments from each reviewer, and any public response provided by the PI. Overview information on the PABP/SEPS Technology Area, full scoring results and analysis, the Review Panel Summary Report, and the Technology Area Programmatic Response are also included in this section.

BETO designated Ms. Andrea Bailey as the Performance-Advantaged Bioproducts and Separations Technology Area Review Lead, with contractor support from Jessica Phillips (Allegheny Science & Technology). In this capacity, Ms. Bailey was responsible for all aspects of review planning and implementation.

PABP/SEPS OVERVIEW

The PABP/SEPS session covered projects in two areas:

1. Projects identifying promising novel bio-based molecules that could offer a performance advantage over existing products, and that are not currently produced through any process.
2. Projects that are part of the DOE national lab-led Bioprocessing Separations Consortium (BioSep) that are developing cost-effective, high-performing separations technologies in biochemical and thermochemical processes.

These two areas were combined into a single review session due to the similarities in technology types that were reviewed.

PERFORMANCE-ADVANTAGED BIOPRODUCTS

Because bioproducts can be produced from biofuel process residues or at the same facility as biofuels and represent a new revenue stream that could increase consumer and investor interest in bio-based processes, research on bio-based products helps enable bio-based fuels production. BETO funds bioproducts research on both direct replacements, which are identical to products produced through existing processes, and on novel products, which may have potential performance advantages. Projects reviewed in this session focus specifically on these novel products, which are referred to as performance-advantaged bioproducts (PABP). This work involves both predictive modeling of platform molecules and experimental synthesis of the most promising candidates.

BETO’s work on PABP spans both independent competitive awards and national lab projects, and a national lab-led consortium of projects working on combining capabilities to identify new products and test their performance attributes.

BIOPROCESSING SEPARATIONS CONSORTIUM

Developing cost-competitive biofuels and bioproducts requires proven technologies to separate process streams. Today, the cost of separation can represent up to 70% of processing costs. BETO currently funds research and development (R&D) to address these needs through the national lab-led BioSep.

BioSep addresses separations challenges such as impurities in intermediates impeding downstream biological and chemical catalysts, the need for low-cost purification technologies, and recovery and conversion of dilute carbon. The consortium is organized around the two primary process types: biochemical conversion and thermochemical conversion. There is also a crosscutting analysis team, integrated with the two research teams, which conducts techno-economic analysis (TEA) and life cycle assessment (LCA) to inform and prioritize research directions.

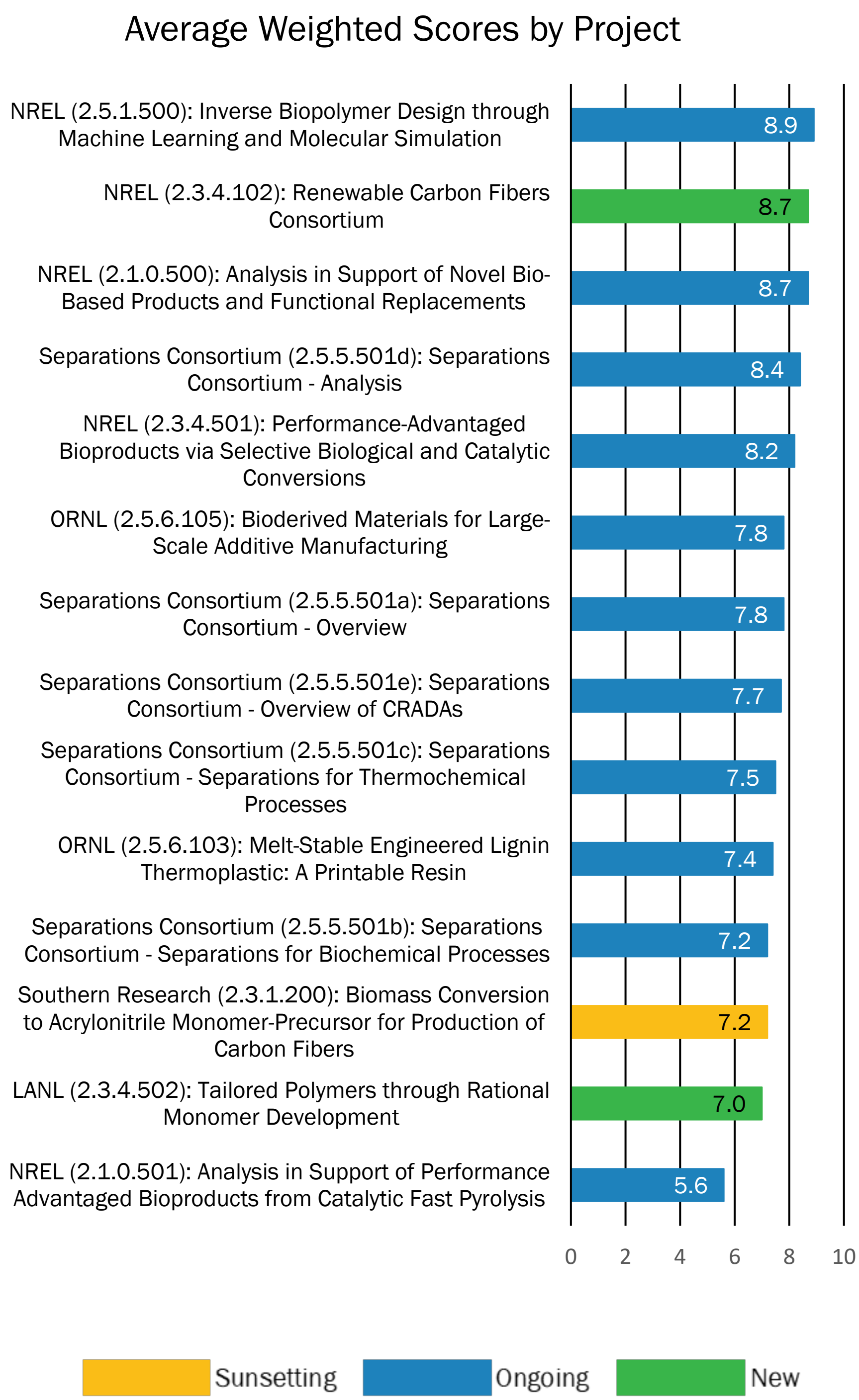
PABP/SEPS REVIEW PANEL

The following external experts served as reviewers for the PABP/SEPS Technology Area during the 2019 Project Peer Review.

Name	Affiliation
Joseph Bozell*	University of Tennessee
Matthew Tobin	Matthew B. Tobin Consulting
Jeff Scheibel	J. J. Scheibel Consulting LLC
Melissa Klembara	DOE's Advanced Manufacturing Office
Peter Keeling	Purdue University

*Lead Reviewer

TECHNOLOGY AREA SCORE RESULTS



PABP/SEPS REVIEW PANEL SUMMARY REPORT

Prepared by the PABP/SEPS Review Panel

Given the space demands of the final report, this write-up can be, at best, only a summary of critical highlights and high-level comments resulting from the panel review. Much more detailed and project-specific information was distributed to the PIs.

Differentiation of the projects resulted primarily from the technical approach and accomplishments presented by the PIs. For example, a strength of the program is that each project demonstrated good relevance to the overall effort. The management plans for all projects contained the pertinent components necessary to carry out the project, with the general exception of adequate risk analysis and mitigation. The program would be strengthened by better inclusion of risk mitigation approaches as part of project management. Future research efforts generally seemed well linked to the results obtained by the PIs.

The panel recognizes that clear communication and alignment between project partners and BETO is essential, but it needs to be as efficient as possible. A potential weakness in program management may exist with regard to the number of meetings, conference calls, reviews, and updates required for the PIs and their teams. A tally of these requirements, especially for PIs involved in multiple projects, would appear to consume a large amount of time. It would be useful for the program to comment on this issue and helpful to technical progress if there was a way to reduce this part of the effort.

IMPACT

Separations

Separations remain a critical barrier to biorefinery development and operation, as the process streams resulting from biomass conversion offer challenges not seen in conventional petrochemical refining. The PIs presented the very interesting statistic that industrial separations account for as much as 15% of total U.S. energy use, while improved separations could reduce fuel costs by 50%. Thus, success in this area would have a significant impact on overall biorefinery operation.

The efforts underway by BETO's BioSep suggest a number of novel approaches to realizing this potential and, as desired, a route to improve the state of technology with regard to the unique issues that face biomass/biorefinery separations. BETO is supporting efforts in separation research and separation process analysis, which is helping to place the various projects in the context of eventual industrial utility. In parallel, the research activities are closely coupled with a well-organized economic analysis capability within the consortium, which is of particular importance and a true program strength, as it provides the economic basis for project evaluation and direction and crosscuts almost all projects in the portfolio. The team is currently focused on getting bioproducts out of fermentation, separating products from biochemical lignin valorization, and isolating products from pyrolysis mixtures, all key areas to BETO's mission. Further, the more efficient the separation, the more profit one can wring from conversion technology (i.e., improved industrial utility). These issues are well integrated within the program and fully relevant to BETO's broader programmatic directions.

The program faces some issues that may reduce the overall impact. First, as will be described in subsequent sections, a wide range of novel separation techniques are being evaluated with respect to other research in BETO's biorefinery effort. However, there is a gap in understanding whether a separation technology would ever be industrially viable. A given approach might work well, but also might be considered too exotic for industrial application at scale. This data gap, which was acknowledged by the PIs, is an important barrier to address, as the impact of the program is significantly diminished if industry fails to adopt a given technology.

Second, the impact from thermochemical approaches remains unclear. The panel saw an excellent presentation on separation of thermochemical process streams, but more broadly, the scientific challenges underlying pyrolysis may be too large to make an impact on the gallons gasoline equivalent (GGE) regardless of separation. There are simply too many examples of pyrolytic processes in the literature that have been unable to show that pyrolysis can lead to an economically viable process. Generating a complex mixture of low molecular weight compounds simply isn't the way to valorize biomass, and it is not obvious that improved separation methods will overcome this challenge. The program would benefit by a clear description of how these approaches may finally crack these historically intractable issues.

Finally, the panel saw a number of projects displaying an end date of September 2019, making it unclear as to what happens next. Separation research, and particularly the analytical component, is a necessary and evergreen type of effort. But it's not clear what BETO has in mind or how they plan to continue the effort. The presentations described that the time required to complete the steps between an initial concept and its inclusion as a funded effort could take as long as a year, which seems unnecessarily long. The panel recognized that the effort will likely continue, but more clarity around the mechanism would be helpful.

Products

The potential impact of this portion of BETO's portfolio is clear. Development of industrially relevant bio-based products is at the core of BETO's efforts to achieve their GGE targets. The coupling of high-volume bio-based fuels with high-value bio-based chemicals will lead to a biorefinery operation that is overall economically viable and able to compete with the petrochemical industry. To achieve these goals, BETO has constructed a promising and innovative program that couples solid scientific research with rigorous economic analysis and computation. By understanding the properties and performance (which are, in reality, the true products sold by the chemical industry) of bio-based chemicals and defining the technology needs to derive these properties from biomass, the program will demonstrate that the biorefinery can be as important to the chemical industry as the petrochemical refinery.

Economic analysis of the chemical product space is central to the program. In the last two years, the program generated an initial white paper describing product opportunities and is now moving to develop a more comprehensive evaluation, which will be useful in providing a context for broader research. This new report is fairly early stage, and thus its overall impact is somewhat more difficult to assess. However, the PIs appear to be using a market-driven approach. This will be useful as it avoids efforts to "pick winners" by focusing on broad-based conversion technology rather than targeting single products.

The program has demonstrated several successes that can be directly linked to eventual industrial utility:

- Of particular importance is the Carbon Fiber Consortium. By building on some initial, elegant science, the team has moved from the lab to larger scales, has assembled industrial partners, and is ready to generate bio-based acrylonitrile (bio-ACN) at a scale necessary for industrial testing and deployment. The project has followed a trajectory fully in line with BETO's definition of success: initial concept ⇨ lab demonstration ⇨ initial scale-up ⇨ transition to industrial use.

- The program includes work at Oak Ridge National Laboratory (ORNL) that has successfully generated several new lignin-based polymers. The final materials are elastomers made from a polyethylene glycol (PEG) derivative and ACN-refined lignin. This approach appears to have considerable breadth as acrylonitrile-butadiene-lignin polymers give shape memory and 3D-printable composites. Further, the lignin could be mixed with nylon and carbon fiber to give new polymers that meet and exceed automotive strength requirements, which is an important potential application market.

- The program also includes an effort targeting materials production rather than discrete chemical entities. This work at ORNL is markedly different from the other projects in the BETO portfolio but nonetheless is interesting. The project does no real conversion of the biomass; instead, biomass is used as a component of a plastic in 3D printing. The PIs have been able to make a wide range of fully bio-based materials, shapes, and structures at the ORNL manufacturing facility from 3D printing of polylactic acid reinforced with bamboo fibers and are targeting the use of other natural fibers in future work. The strengths of this concept include an approach that is straightforward, easily understandable, and gives final products with utility easily perceived by a wide audience. The wider goal is to test the use of natural fibers as a replacement for carbon fibers in certain 3D-printing applications. This is a strength, as it helps define a different range of market segments where the strength of carbon fibers may be overkill. This project is on the "applied" end of the BETO project spectrum but demonstrates a balanced program that will lead to greater impact.

INNOVATION

Separations

Several of the presentations on separations were more overviews than detailed research summaries, making it more difficult to evaluate the program's potential level of innovation. Nonetheless, the panel was presented with a scientifically solid program that employed what appear to be a number of cutting-edge technologies. The presentations further emphasized separation technologies identified as uniquely suited for projects generating bioproducts from fermentation and lignin. The recognition of these opportunities across the whole biorefinery process chain and the effort to tailor separations to these needs is a strength. More broadly, the incorporation of these more fundamental efforts needs to remain at the core of BETO biomass research, as it couples basic scientific knowledge to successful biorefinery development and bridges fundamentals with applications. The willingness of BETO to include such efforts (in contrast to efforts supported by earlier incarnations of BETO) is a real strength of the program. The program's cooperative research and development agreement (CRADA)-lite effort with industry (detailed below) is a nice example of an innovative approach to industrial engagement.

The program's innovation would be strengthened, however, with a clearer discrimination between the potential of the different approaches. That is, all projects seemed to be given approximately equal importance and priority, even for processes that would be considered by industry as exotic. Examples include:

- The program has developed a phosphate oil/aqueous-based two-phase separation process for organic acids. It works, is scientifically interesting, and has led to publications. But is it industrially relevant? Issues around the lifetime of this material, its expense, and the impact of entrained impurities at higher levels remain unaddressed. Moreover, mineral oil + tri-*n*-octylphosphine oxide (TOPO) + undecanone could be expensive. It is not clear that the separation improvement justifies a higher cost than alternative separations.

- Two separation paths are described for two methods of lignin conversion, but neither is shown to be better than the other, nor are they categorized as to their potential for industrial utility.

- All projects are shown to have a positive impact on the GGE goals, show success, and are well organized and managed. But they can't all be equally good, or alternatively, they can't all be incorporated into the biorefinery. Are electro-separation methods currently used within industry at the scale necessary to meet GGE targets? Where? If yes, does this represent an improvement? If no, why would industry adopt them? These questions apply to each of the technologies described in the presentation. Surprisingly, several of these approaches have been under investigation for 2–3 years but have not yet been subjected to a comparative analysis.

As such, it would be helpful if the PIs could cite large-scale examples where such approaches are used for commodity chemicals as targeted in the program. The examples need not be direct, step-by-step analogies, but rather approaches that have a similar level of complexity. Alternatively, examples of ultrasonic separations, or two-phase extractions with chemicals of similar complexity and expense would be useful in generating greater justification for the effort. Presenting examples of how (or whether) a project was working with entities in the commercial separations sector to identify, improve, and innovate technology, such as membranes, materials, and equipment development would lend additional credibility to the technology choices. Further, application of TEA (or even a literature search targeting examples of larger-scale use of these processes) against some kind of industrial baseline will be very important. The panel noted that the relative significance of the projects may be indicated by the funding allocated by BETO.

Products

The level of innovation within the program is high. A particular example is the National Renewable Energy Laboratory (NREL) project carrying out computational evaluation of new biopolymers. The foundation for this project is straightforward and important. Computational analysis will be used to define easily obtained bio-based starting materials that can serve as monomers in polymer production and offer advantages over petrochemical materials. This is a novel concept and a strength of the project. Overall, the project will query a set of polymer properties (e.g., glass transition temperature and stiffness). A hypothetical bio-based monomer, which will exhibit these properties when polymerized, will be predicted computationally. The potential impact of this project is clear and presents a new means of addressing the questions of what makes a good PABP. It incorporates the considerable computational strength of the NREL team and directs it toward developing a powerful means of defining those products that could be made most easily in the biorefinery. This is a terrific new effort that could be significant for the overall BETO program. The project would benefit from incorporating readily available molecular weight data or polydispersity in their database. Molecular weight is likely one of the most important properties in polymer production, and one of the most widely reported properties of a new material. Polydispersity, directly calculated from the molecular weight data, gives an indication of the polymer's homogeneity. The ability to tell a manufacturer that structure X, because of a computational evaluation, would be able to give a new polymer with molecular weight Y would be a real coup. If that information could then be overlaid with a credible prediction of performance properties, a tool of broad applicability would result.

The program's efforts in bio-ACN production within the Carbon Fiber Consortium and at Southern Research are both based on innovative and scientifically interesting approaches. The PIs in both projects did an excellent job of linking their innovation to the potential impact of their technology. If made less expensively, carbon fiber can replace heavier materials in different segments of the U.S. manufacturing sector. For example, increased use of carbon fiber in automobiles will lead to light-weighting of the fleet and a significant improvement in vehicle efficiency without loss of strength. Based on their research, the PIs have identified clear metrics that define success in their upcoming efforts. The Southern Research effort has operated their process at batch scale for several hundred hours and have achieved the ability to make relatively large amounts of bio-ACN. This would appear to be a significant success.

The program is also supporting innovative early-stage projects. Efforts at Los Alamos National Laboratory (LANL) target the production of new polymeric materials from novel and unique bio-based building blocks. The expected outcome is the production of new materials with new properties, which is a good fit with the BETO conceptualization of PABP. A particular strength of this project is the development of degradation paths in parallel to the synthesis paths, where the choice between biodegradability versus recyclability might be determined by the practical ability of the product to be reclaimed versus recycled. Given the current level of concern over plastics in general, incorporating end-of-use ideas into new polymer development is important. The PI has chosen polycarbonates as a target, addressing a large market with multiple applications. Their effort also incorporates specifications from industry in order to determine targets for these new materials.

SYNERGIES

Separations

The development of a multi-lab consortium to address the cross-cutting issue of separations is a strength of BETO's efforts and demonstrates clear synergies within the laboratories. The management structure is appropriate for a multi-institutional effort such as this. The PIs presented a clear impact statement associated with the challenges of running this organization and did a good job of emphasizing the strengths within this cross-cutting support function. The current partners in this effort are terrific (NREL, LANL, Lawrence Berkeley National Laboratory [LBNL], and Argonne National Laboratory [ANL]), well-coordinated, and integrated across multiple labs. This is an excellent means of leveraging DOE facilities to solve a common problem and reduces unnecessary lab competition around a technical challenge that can negatively affect all the scientific effort.

Products

The overall program has a current focus on bio-based polymers, and as a result, there is considerable opportunity for interaction between projects. Longer-term work at NREL based on their biochemical funneling approach has led to the production of a number of new polymeric materials based on compounds such as beta-ketoadipic acid as a starting monomer. In parallel, the NREL team has commissioned a new polymer characterization lab that will offer important capacity for evaluating the performance of new bio-based materials generated by BETO research. The NREL project included some nice examples of how new monomers from biomass can be incorporated into new polymers, leading to some examples of performance advantages, in the sense of being able to modify performance and properties through inclusion of bio-based structural units. The new NREL effort in computational prediction of polymer properties is particularly interesting in this regard. If the team is able to develop a robust *in silico* approach for evaluating bio-based monomers, it will have direct and immediate applicability to multiple projects within the BETO portfolio.

Synergy should also exist between the parallel carbon fiber projects from Southern Research and the Carbon Fiber Consortium in the portfolio, but there did not appear to be a connection between the efforts. When compared, the consortium's approach seemed to have a much better chance of succeeding. A better understanding of the interaction/competition between this project and the one underway at Southern Research would be helpful. Will there be a downselection at some point?

FOCUS

Separations

It is critical to understand the intent of the comments that follow. First and foremost, BETO's willingness to support multiple projects and approaches to biorefinery separation is a real strength and must remain a driver in future work—the technology for biomass conversion still requires a broad-based and flexible effort to define the best approaches, even if it takes longer to reach an answer. If the choice was between supporting multiple, diverse projects and trying to choose a single winner at this point, the undeniable recommendation would be for the former. To this point, the consortium has developed and is investigating eight different base cases requiring separation as a key component. These analyses help identify the most important barriers to overcome for a successful conversion process. This, in turn, helps the researchers focus their efforts where they will do the most good and provide credibility to industrial stakeholders regarding the potential utility of a given separation process.

The separations effort for thermochemical processing offers a nice example of a well-focused investigation. The panel was presented with three well-defined purification methodologies (removal of impurities, capturing carbon from aqueous streams, and intensifying separation processes) designed to make downstream catalytic upgrading of pyrolysis vapor more effective. This project addresses a high-cost component in the generation of bio-based products, and as a result, has the potential of making a large impact on overall economics and GGE goals. Hot gas filtration successfully removes certain interferences and components that lead to coking and is able to use industrially accepted filtration systems to achieve the results. This is a strength, as it will ease the transition to commercial deployment. Further, the PIs were able to show that char, an interfering component in pyrolysis processes, is effectively removed and eliminated from the system using their separation technologies. Finally, their processes can extract acetic acid to give fairly high concentrations in aqueous solution, and at a level that could be economically viable. The project was unique in the separations portfolio, as it included quite a bit of intellectual property that will be helpful in tech transfer efforts. This is a key strength for this technology as it transitions to industrial use.

There are areas where the program focus would benefit by a little tightening. Several examples of different separation technologies under investigation were described, but they all exhibited a similar weakness. The following is illustrative: for an ongoing algae project, ultrasonic filtration was employed and led to the successful achievement of a technical separation goal. But it is less clear when the next step comes in, which is to evaluate the economic feasibility of separation itself, and more importantly, whether industry would ever use it on the scale necessary to achieve GGE targets. Ultrasonics would seem to be exotic and expensive. Thus, while the technology offers a way to meet a technical goal, understanding whether it is affordable at the scale necessary for a biofuel project would be important. The industrial baseline used in biochemical separations is the simulated moving bed. Are there others that would work? The same questions exist for other separations methodologies included in the presentation.

To their credit, the PIs showed a block diagram comparison of how an analysis is set up. One of the strengths of the program is the existence of a well-defined template for analysis. However, the presentation did not include illustrative results. It would be useful to know for each project where analysis is pointing the researchers when there are several separation technologies under consideration, for example in the lignin and pyrolysis projects. Of the multiple separation approaches described in the presentations, none appeared to have been subjected to TEA, despite having been under investigation for some time. Can the PIs point to actual use of such approaches in industry at the scale needed to meet BETO goals? At what point does BETO look at the various comparative analyses and decide to focus on the lowest-cost approach? It was not clear when such prioritization takes place or how such a process would be carried out. In the absence of any prioritization, the overall focus of the program suffers. Drawing on the expertise of the industrial advisory board (IAB) members could also offer some insight into this question. Indeed, it was stated that the IAB may have seen these approaches. What comments and suggestions were received and did they/will they impact future research directions?

Overall, this perceived lack of focus may diminish the program's relevance. The work coming out of the consortium is scientifically great, but it is more basic than typical BETO projects; it looks more like a DOE Office of Science effort—basic science projects with an "applications" wrapper may not meet BETO's goals. Please do not misinterpret these comments; the approaches are scientifically interesting, and the work is being carried out well. The concern is whether they can make the transition to commercialization, which is a key part of the overall philosophy within BETO.

TEA would be an important contributor to improving program focus, but again, it is critical to understand what is meant. TEA needs to be applied with discretion, and its level of detail must be commensurate with the current state of development of a given project. There is a big opportunity to develop a "TEA-light" so that a promising program wouldn't be missed because sufficient data weren't yet available. This type of evaluation would be a "best-case" scenario for low-technology-readiness-level projects where the cost of an effort could be evaluated assuming each step went in the maximum possible yield (i.e., a simple demonstration of broad economic possibility), but more importantly, an initial demonstration of where the greatest impact of research would be on the cost of a process.

Products

Overall, the focus in this part of BETO's program appears quite good. One could argue that research is currently limited to bio-based polymers (several projects), materials (ORNL), and bio-ACN (the Consortium and Southern Research). This is a strength, as these activities address key components of BETO's overall goals: large market opportunities (polymers), bio-based materials (direct use of biomass), and transition from the lab to commercialization (bio-ACN/carbon fibers). As with the Separations program, the inclusion of these multiple efforts is to be applauded. Further, it appears that early-stage projects are being given sufficient funding and time to demonstrate principle without being too heavily burdened with economic evaluation.

Projects are incorporating efforts to understand fundamental molecular-level interactions, which will be critical to process control and operation and tailoring of product properties for performance. As an example, the ORNL effort in developing a printable resin did an excellent job of placing the work in the context of molecular-level interactions within composites.

The focus of the BETO products effort is always challenged by the huge number of product opportunities available. As a result, the crosscutting analytical work at NREL will be an important component of the overall program. As the analysis proceeds, it will be most effective if it maintains a broad technology development focus and does not become an effort driven by identifying specific compounds for study. Further, analysis will benefit by carefully defining how a new report/analysis differs from the many similar analyses now in the literature, and from those that have been done by DOE itself. The presentation on product analysis identified the understanding of performance traits as highly important. In actuality, one could argue that the industry has already defined these traits within their well-defined market segments: coatings, resins, surfactants, etc. Additionally, polymers also have well-defined property and performance specifications. The bigger challenge, which did not seem to be emphasized, is a definition of technology opportunities, and identification of the products that can be most easily made from that technology. This concern is particularly acute with regard to the PABP concept. Identifying key compounds that come from biomass is good, but many of the compounds described in the presentations exhibited higher molecular complexity than is normally generated by the chemical industry. The PIs might consider looking at the literature on quantitative scales for molecular complexity to see if their materials fall within indices representative of what the industry currently makes.

It would be useful if the analysis could also describe the strengths and weaknesses of the current prototype targets in other parts of the program. For example, the panel saw descriptions of butanediol (BDO) and adipic acid in the design cases of the biorefinery and GGE calculations. But what if other products were substituted? Do the assessments change if 2,3-BDO (a biochemical with little or no current market) is substituted with 1,4-BDO, a known material with known markets? These types of evaluations are needed for multiple families of chemicals to assure interface with the chemical industry. Otherwise, the project runs the risk of becoming internally consistent, but having less utility when compared to existing markets.

As with Separations, TEA will help focus the program on the most promising opportunities. For more advanced projects, presentations in several sessions presented a well-organized TEA template developed at NREL. However, this methodology was not employed uniformly. Some projects used these techniques, while others used internally developed analyses or employed TEA carried out by the project PI that was not well supported. Several examples illustrate this issue:

- The ORNL effort in 3D printing targeted a composite cost of $3.00/lb, or 50% of the carbon fiber cost. Can the PIs show that even with a reduction to $3.00/lb, the industry would use such a material? How/where do the PIs see these materials fitting into the market and for what applications? Are these markets of sufficient volume to make a difference? Are there data on these potential uses? In addition, many of the other projects in this portfolio describe the cost impact with regard to its impact on GGE, and thus it would be helpful if the PIs did the same thing here, projecting the reduction in GGE as a result of producing these materials within the current state of technology.

- During a question and answer (Q&A) session on the ORNL effort to develop a printable resin, it was indicated that the TEA was carried out by the PI and not by any of the TEA experts within the BETO organization. Further, it became clear that the assumptions used and conclusions resulting from their analysis were murky and difficult to understand. One was left with the impression that good science had been accomplished but the costs could be too high for the project ever to make the leap to commercialization. The PIs did not include the cost of lignin extraction and isolation, which could be significant. The milestone slide indicates a goal of increasing lignin's "value," but the meaning is not clear. The implication is that the lignin must have a certain minimum value in order to meet GGE goals, which is an odd way to describe how TEA is being used. It would seem that the more appropriate goal would be to minimize the product cost so that it could be economically competitive. If the lignin cost is too high, the new composites will also be expensive and of limited market. Greater clarification of these arguments would be helpful.

- The NREL effort to generate monomers from pyrolysis oil was also not convincing. The relevance (as acknowledged by the PIs) of this project is hampered by the potentially small amounts of material that could be derived from pyrolysis oil. To better assess the approach, the PIs would benefit by completing a rough mass balance diagram that indicates (under optimum conditions): 100 g biomass ⇨ XX g oil ⇨ XX g phenolics ⇨ XX g starting monomer ⇨ XX g of a "performance-advantaged" biopolymer. The numbers will likely be very, very small, thus bringing the viability of this approach into question. Using some of the PI's own numbers, and starting from 100 g of biomass, one might get 25 g of pyrolysis oil. Of that, one might obtain 3.5% of cyclopentenone even before the start of a multistep polymerization. In a 2,000-tonnes-per-day biorefinery, that's a very small amount of polymer. They would further benefit from a clear description of the separation technology needed to get fully purified cyclopentenone (for example) from the pyrolysis oil mixture.

TECHNOLOGY DEVELOPMENT PIPELINE

Separations

The Separations program demonstrates high scientific quality nicely coupled with analytical evaluation. However, the path to commercialization was less clear. This may not be a weakness at this stage—optimal separations for biomass and biorefinery process streams are not yet developed, and the effort to carry out more fundamental research is worthwhile. Such research should be given sufficient time to reach fruition without being fully driven by efforts to reach commercialization. Nonetheless, the PIs described a clear interest in presenting capabilities within the consortium to potential industrial partners. That shows a balance between internal separations development and access to facilities for external partners, which is a strength.

The listening day (and the industrial outreach, more generally) is interesting and potentially useful. A particular strength is that in this outreach it appears that these activities are coordinated more at the management/program level, rather than making it the responsibility of the individual PIs, as seen in other programs. A further strength of the program, and useful for engaging stakeholders, is the consortium's website describing the capabilities of the consortium.

The panel was impressed with the innovative "CRADA-lite" effort funding short-term screening efforts in separations with industrial partners. This is an interesting approach for engaging industry and offers an opportunity to examine a focused concept for a short period of time to see if it has promise and could contribute to BETO's goals. The concept of seed grants to increase industrial participation in BETO projects is useful and could serve as a model for other portions of the program. The panel felt that the total number of interested applicants could have been larger, and that future rounds of CRADAs should be planned sufficiently in advance to provide continuity of effort and use of resources. Such modifications to the program could serve as positive advertisements for future CRADAs. Overall, the presentation demonstrated that the PI's approaches are reasonable and are addressing one of the larger goals of the subset of the BioSep presentation—industrial participation and outreach.

Technology development could be strengthened in some areas. For example, the CRADA-lite funding levels seem low, and BETO would benefit from limiting the number of partners that could be involved on any single grant. For example, the Kalion and HelioBioSys CRADAs have $200,000 with three national lab partners spread over two years. It is not clear that this is an effective use of funds given the costs at the labs. A better description of how the industrial partnerships "speed-dating" process operated would be helpful in understanding how the partners were chosen and invited to participate in the program. The review panel expressed mixed views on partnering choices. Some thought it a clear benefit to partner with smaller entities to provide missing expertise, equipment, and bandwidth, while others on the panel felt that the lack of chemical companies like DuPont or BASF, for example, could be perceived as a weakness, as they would bring greater industrial credibility than a small startup. The Q&A revealed that some larger industries were in the proposal mix but did not make the cut.

A stronger description of how the listening day differs from standard BETO road-mapping workshops would be helpful, as would a description of whether this approach is any more successful than others. There are many historical examples of putting the lab researchers and industrial representatives into a room for a day in order to "find out what industry wants." They're often quite valuable for industry, as they get a sense of what's going on in the labs, but much less useful in the other direction, as industry is slow to reveal what they're working on and what problems they need to solve.

Products

The Renewable Carbon Fiber Consortium is a great example of science being translated to commercial use. It appears that the team has moved to precommercial scale and testing, and presumably has the economics to make it work. What is presented is an excellent example of good science and good application following a well-laid-out path to a potentially important product. The weaknesses are minimal, in that the route to bio-ACN has been demonstrated, and initial work in scale-up is also showing success. The project has a clearly defined goal and is therefore directly understandable to a wide audience (i.e., "we will make cheap carbon fiber"). A real strength of the project is its identification of the key members of the team needed to carry out each of the steps in production and evaluation. Overall, all the steps, partners, and planned work is exactly what is needed to move this program to the next phase. All important questions are being answered and all challenges have appropriate plans in place to make it work. The handoff from one partner to another is really well laid out. They have experts on each step in place. Bigger picture, this is a really nice organization addressing exactly the needs necessary to prove out the overall approach. Good science has led to good applications that attract industry and offer opportunities for commercial deployment.

As the effort proceeds, the program will need to continue their close organization of a number of partners to make sure that problems with one do not impact the overall plan and schedule. It would be helpful to have more detail on how the partners were vetted. For example, it is interesting (and surprising) that the PIs are using an external producer of their carbon fiber, given the availability of the carbon fiber manufacturing facility at ORNL. Finally, catalyst deactivation seems important, and the team has identified it as a key issue. Getting a sense of whether there might be multiple solutions to the issue would also be useful to know. This could be a showstopper, so some insight as to what's going on would be helpful.

A primary opportunity for improving the potential for technology transfer would be a deeper analysis of whether a given project has a chance of being industrially relevant. The panel saw several projects where this question was of concern:

- The LANL effort to generate new polymers begs the question of whether the industry would adopt compounds of this complexity, especially when they require multiple steps for their synthesis. The answer may eventually be yes, but the project would benefit from industrial examples that might have an equivalent number of steps from raw material, to monomer, to polymer, and which exhibit similar structural complexity.

- The Southern Research effort in bio-ACN would benefit from a better understanding of the dependence of ACN cost on propylene glycol sales and a clearer delineation of TEA assumptions. Industry tends to avoid coproduct schemes, and thus understanding how the PIs will avoid this problem would be helpful.

- The industrial utility of the ORNL effort to make printable resins would be strengthened with a better understanding of the true target cost of these composites, and whether it will be low enough to compete would be useful. For example, the presentation suggested competition with resins at $1.12/lb. But the complexity of the process suggests that the cost may be significantly higher for this process. Thus, a clear, simple presentation of targets and economic assumptions is needed. The process requires lignin preprocessing (for example, extraction of the initial lignin with acetonitrile) to get a refined lignin for the 3D and composite applications. The lignin is then mixed with a polymer under high-shear melt mixing to give the final product. As the presentation proceeded, the number of steps and actual yields became a concern with regard to final lignin cost and process complexity. The PIs did not indicate the amount of material derived from their extraction process. Is it 10% of the starting input? 50%? Further, the use of acetonitrile for extraction would seem to be an overly complex process for an industrial plastic. In the BETO context, do the costs establish a credible case for industrial adoption?

- More broadly, the program's interest in bio-based polymers needs to face the reality of the polymer industry: introducing new polymers into the market is a real challenge. The current polymer industry has a huge amount of experience in formulation and process modification to introduce properties of interest. In fact, the last polymer to be introduced at a large scale was probably DuPont's 1,3-propanediol polyester. And before that, it would have been years and years between introductions. The polymer market is particularly tough to crack, and thus simply because something is polymerizable doesn't mean that it can be commercialized. To that end, the PIs need to describe how a new material might make it to market, and answer questions regarding comparisons between the candidates and the existing market (e.g., "bio-based polymer X is most like polystyrene, or polypropylene…"). It is not clear that improved properties alone are sufficient to make a difference and generate the revenue needed to meet GGE targets. Can the program make a credible argument that a new structure would have a reasonable chance of becoming commercial?

- NREL is carrying out efforts to isolate specific compounds from pyrolysis oil for the purposes of generating new polymers. The general concept of extracting greater value from pyrolysis oil is laudable, and the PIs describe some approaches that are reasonable on paper. However, this program faces the considerable challenges of trying to extract a very small amount of their starting chemicals in purity sufficient to drive downstream conversion. The further complexity in their process may make it difficult to get the project transitioned to industry. The PIs acknowledge the most critical challenge of this project: pyrolysis oil contains dozens of identified products, and maybe hundreds unidentified. It is not at all clear how this complex mixture can be a reasonable source of polymer starting materials. Further, the proposed synthetic sequence to monomers from cyclopentenone is not convincing if considered in an industrial context. The approach is scientifically interesting, but hard to accept as a reasonable way to make barrier materials. In the BETO context, it is not clear that such an approach could ever be commercial. If the PIs are using this simply as a demonstration of principle, they also need to present some idea of how it could be improved. Unfortunately, the yields do not seem to be sufficient even at a lab scale. These weaknesses are all considerable barriers to technology transfer.

RECOMMENDATIONS

- Continuing the multifaceted approach by supporting multiple separation and product development efforts will be critical in understanding the technology space needed for optimal biorefinery separation processes

- The integration of science and molecular-level understanding with industrial applications should continue, as this will form the best foundation for process development and control

- There are opportunities to improve the focus of the program, but they must not be done at the expense of promising but unproven separation or product development approaches.

PABP/SEPS PROGRAMMATIC RESPONSE

INTRODUCTION/OVERVIEW

BETO would like to take the opportunity to thank the reviewers for their time and careful review of the portfolio. The program recognizes that this was a difficult review process because additional projects relevant to this area presented in other sessions due to time constraints. BETO agrees with the review panel that these two areas have strong potential for helping their office meet future GGE targets and appreciates the detailed feedback across both areas. The recommendations from the review panel will be discussed and taken into consideration when working on future project selection and program design, as future appropriations allow.

For each recommendation, BETO provided a general response followed by some specific examples of how they will be integrated into the two technology areas covered in the session.

Recommendation 1: Continue multifaceted approach.

BETO is committed to continuing support for a diverse slate of separations and PABP as appropriations allow. The program agrees that a strength of their approach to both of these areas is the ability to fund a number of different technology types across a broad range of funding recipients. BETO also recognizes that part of funding such a large number of technologies is the ability to identify those that are not likely to be successful or those that no longer are at a stage requiring government funding, and either downselect or graduate those technologies. Moving forward, BETO will work on communicating how different projects, as well as their office as a whole, goes about those processes. Further, we agree with the review panel comment that researchers can be overburdened by coordination efforts, and BETO staff will be cognizant of this moving forward.

Separations: After the review completed, BioSep conducted an internal review of the existing projects and reprioritized some of their work in response to feedback from the panel, as well as selected work in new areas. BETO is committed to this kind of exercise, which will allow the consortium to integrate new separations technologies and move on from those that are either ready to transfer to a higher technology-readiness level or that do not appear likely to be economically viable in a commercial biorefinery setting.

Products: The PABP Technology Area is relatively new to BETO, and several of the projects that presented were only selected in the last review cycle. BETO is committed to investigating a wide range of options for PABPs, and the projects that presented in this session will be joined by additional national labs and competitively selected projects over the coming fiscal years. Several projects selected in FY 2018 competitive solicitations had not completed enough work to participate in the full review but did present in the poster session. The two Renewable Carbon Fiber Consortium efforts were specifically cited by reviewers as an example of projects that could use either additional collaboration with each other or consideration from BETO for a future downselect. Both of these projects were selected from the same FY 2014 funding opportunity, and due to the structure of competitive awards would not specifically be considered for collaboration with one another. BETO will, however, consider how to best integrate their results into new work in this area moving forward, as appropriations allow.

Recommendation 2: Continue to integrate science with industrial applications.

BETO agrees with the reviewers that a crucial piece of both of these areas is the commitment to interacting with industrial entities and will continue to focus on linking research to industrially relevant goals. To help facilitate this process, BETO is committed to the continuation of soliciting feedback from external stakeholders on the portfolio through listening days, workshops, and requests for information. Generally, road-mapping workshops are specifically designed to answer a set of questions about how BETO can provide value in an area of research over a set timeframe, whereas listening days are used to gather more general feedback on a broader number of topics. BETO has found both are useful depending on the final desired outcome. Feedback from a public workshop in the summer of 2017 led directly to the creation of the national lab PABP Consortium, and feedback at other similar events has resulted in BETO moving into new work on different types of potential PABPs, including novel plastics.

Separations: The CRADA-lite projects that BioSep presented on were launched in FY 2019, and BETO appreciates that the reviewers found these projects promising. BETO will track the progress of these projects and the other similar efforts funded throughout other parts of the portfolio and hopes to fund additional projects in this space as appropriations allow. Additionally, BioSep will continue their work with their IAB.

Products: The national lab consortium PABP projects appreciated the reviewers' suggestions to consolidate under a single IAB and have started efforts to combine their industry contacts. This work should continue throughout FY 2020.

Recommendation 3: Improve focus while still investigating novel approaches.

As with Recommendation 1, BETO agrees that a strength of both of these areas is the ability for researchers to investigate a number of different approaches, some of which are often too novel and/or risky to likely be funded through other means. BETO also understands that a result of funding work like this is that these projects are often less likely to be economically viable in an industrial setting, and that once this becomes clear, it is not an impactful use of funding to continue work. To help identify points where certain pieces of these larger consortia projects may no longer be successful, BETO is committed to continue to require all projects to use feedback from external reviewers and TEA results to help adjust research priorities and keep them relevant. BETO is also committed to finding an appropriate level of TEA for more novel technologies, as recommended by the reviewers, and will continue efforts to make sure TEA is applied appropriately going forward.

Separations: As the BioSep moves into a new three-year funding cycle, they have developed milestones and decision points focused on using property-based differences to provide insight into relative advantages and disadvantages of bioprocessing separations approaches. The consortium is committed to developing a standardized and transparent process for making decisions about R&D priorities. They will also continue to incorporate TEA into each technology area that they work on.

Products: As the national lab PABP work matures, BETO is committed to integrating more TEA and LCA with the existing work, as appropriations allow. Due to time and availability constraints, the same teams cannot always perform the TEA for each project, especially across different national labs, which has led to some of the discrepancies identified by reviewers. BETO will continue to make an effort to standardize TEA and make sure different project teams share their assumptions. BETO will also continue to work with competitively selected projects to monitor results based on TEA approaches. BETO recognizes that most current work in this area is focused on polymers and agrees with some of the limitations identified by the review panel in focusing on this product type. As BETO generates more data in the area of PABPs, their office expects to expand focus into other promising products, as well as be able to better identify what will give a polymer or any other product a better chance of industrial uptake.

ANALYSIS IN SUPPORT OF NOVEL BIO-BASED PRODUCTS AND FUNCTIONAL REPLACEMENTS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

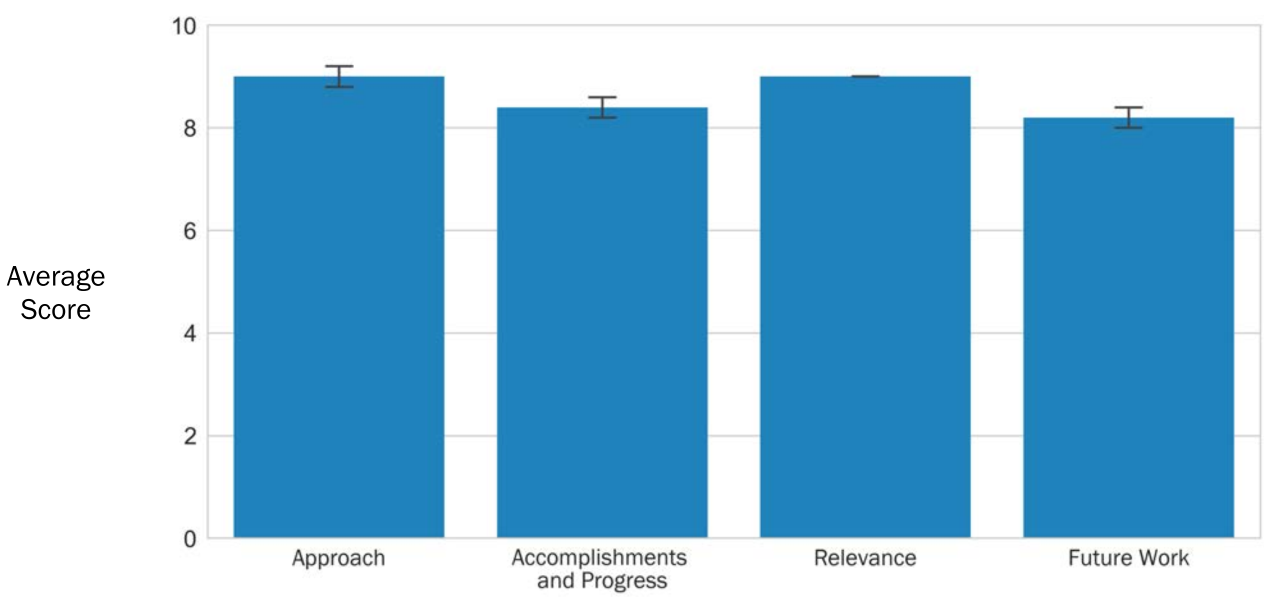
WBS:	2.1.0.500
CID:	NL0033392
Principal Investigator:	Dr. Mary Biddy
Period of Performance:	10/1/2017–9/30/2020
Total DOE Funding:	$500,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$250,000
DOE Funding FY19:	$250,000
Project Status:	Ongoing

The production of chemicals is a major driver of the U.S. economy, as it has accounted for roughly 2% of the U.S. gross domestic product over the past several decades and has a growth rate projected by the industry to produce well over one million new jobs. Therefore, producing chemicals from biomass has the opportunity to significantly impact the future growth of the chemicals industry and the U.S. economy overall. In fact, recent reports by the U.S. Department of Agriculture have concluded that there are roughly 1.5 million jobs in the United States directly associated with the production of bioproducts.

Two primary approaches have been adopted to produce chemicals from biomass. One option is to produce chemicals that are identical to those currently derived from fossil feedstocks and are often referred to as direct or drop-in replacements. Such bio-based chemicals are indistinguishable from their fossil-derived counterparts in terms of their chemistries, compositions, purities, and properties. The other option is to produce chemicals that are different from fossil counterparts, but that have unique properties or improved performance. These bio-based chemicals are thus referred to as PABPs. While a number of examples of performance-advantaged bioproducts are produced commercially, one of the

Weighted Project Score: 8.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

biggest challenges facing growth in manufacturing and research and development activities in this area has been understanding what specific characteristics and performance traits are desirable for these chemicals.

The NREL project on analysis in support of novel bio-based products and functional replacements aims to fill this information gap. The objective of this project is to understand and outline the value propositions and potential drivers for producing PABPs. Within this analysis effort, the team is working to outline specific properties needed for a wide range of end-use applications. The result of this three-year analysis effort will be a guiding document that can be used by industrial and academic researchers to focus their R&D on PABPs with the biggest potential to impact and grow the U.S. bioeconomy.

OVERALL IMPRESSIONS

- The project must filter down choices quickly to focus on few chemicals to move forward. Two years seems long to filter down. Suggest that they should group materials together in terms of similar functionality to target mixtures that could replace things like chelants, aqueous viscosity modifiers for consumer products, or even lower molecular weight, water-soluble-type oligomers may be easier targets for functional materials in the 20,000 molecular weight average range or lower. This could avoid costly separation of single materials in some cases while providing a bigger cost reduction to fuel cost/GGE and a bigger chance to be successful overall.

- This has potential to be a very valuable publication when completed. Would be good if it could somehow identify pointers to next-generation molecules.

- The project is addressing a core goal in biorefinery development—understanding the properties and performance that are the true products of the chemical industry. Incorporating this understanding with a definition of the technology needs to derive these properties from bio-based building blocks will need to be a key component of any report or white paper resulting from this work.

- The project aims to generate a list of desirable bio-based targets, differing from prior work by including more performance and characteristics criteria to prioritize performance-advantaged bioproducts. With the pressing need to improve biorefinery economics via better valorization of streams, this effort is of strategic importance and, if successful, can be a guiding decision tool to focus valuable R&D time on better target choices.

- Great integrated approach to share information, results, and resources. Very well presented and the explanation of the framework for analysis of evaluating performance-advantaged bioproducts was clear. External advisory panel with eleven advisors provides a wide variety of industry perspectives. This is very thorough research and analysis to outline the value proposition and market pull.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their helpful feedback and comments. We will work to incorporate these suggestions in the project going forward.

ANALYSIS IN SUPPORT OF PERFORMANCE-ADVANTAGED BIOPRODUCTS FROM CATALYTIC FAST PYROLYSIS

National Renewable Energy Laboratory

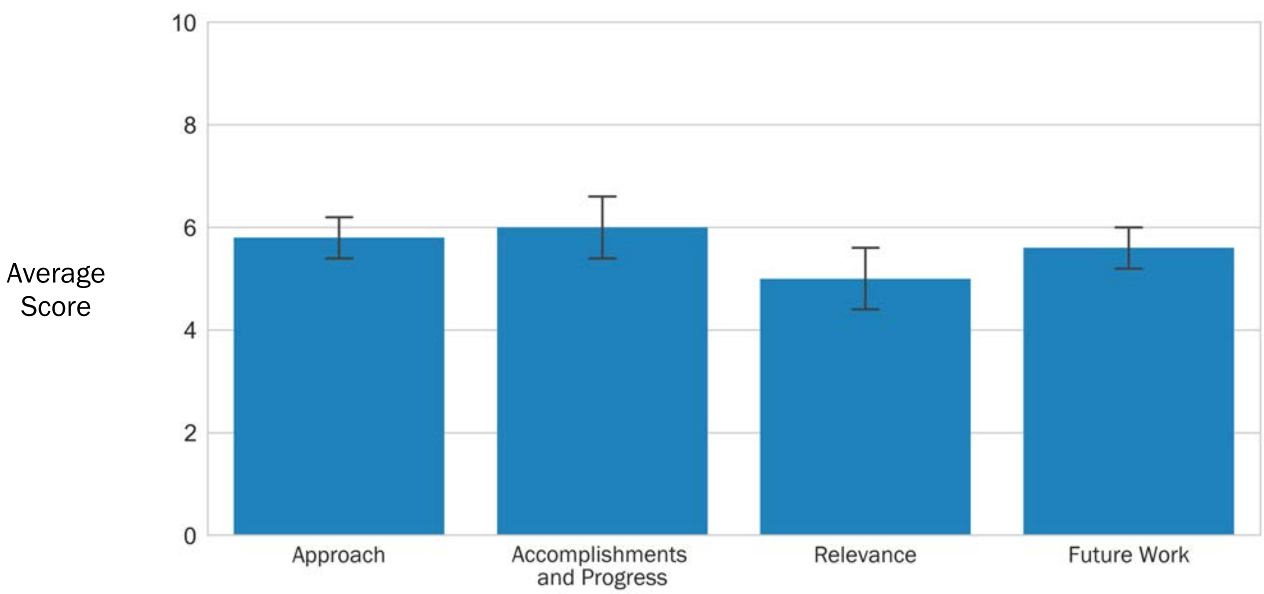
PROJECT DESCRIPTION

WBS:	2.1.0.501
CID:	NL0034074
Principal Investigator:	Dr. Mark Nimlos
Period of Performance:	3/31/2018–9/30/2020
Total DOE Funding:	$400,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$200,000
DOE Funding FY19:	$200,000
Project Status:	Ongoing

The high oxygen content in biomass (40%–50%) enables the production of oxygenated molecules that can be used to produce novel polymers that often have superior properties over existing materials. Synthesis of these same molecules from nonoxygenated fossil fuels is often expensive and requires hazardous and environmentally damaging transformations. Thus, there are clear potential advantages for biomass-based polymers in terms of performance, cost, energy use, and environmental impact. Catalytic fast pyrolysis (CFP) of biomass offers an inexpensive, high-throughput route to deconstructing the biopolymers found in plant cell walls, but there is a knowledge gap concerning how to use this technology to produce novel and performance-advantaged polymers that preserve the unique chemical structure and composition of biomass. In this project, we bridge that gap by providing experimental work that shows pathways to performance-advantaged polymers from CFP-derived monomers. Novel polymers are synthesized using the oxygenated molecules found in CFP biocrude, and their properties (glass transition temperature, permeability, Young's Modulus, etc.) are measured to identify performance enhancement needed to meet industrial specifications.

Weighted Project Score: 5.6

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

The results of this work will help advance the bioeconomy by providing pathways to high-value coproducts that can increase the commercial viability of biorefineries.

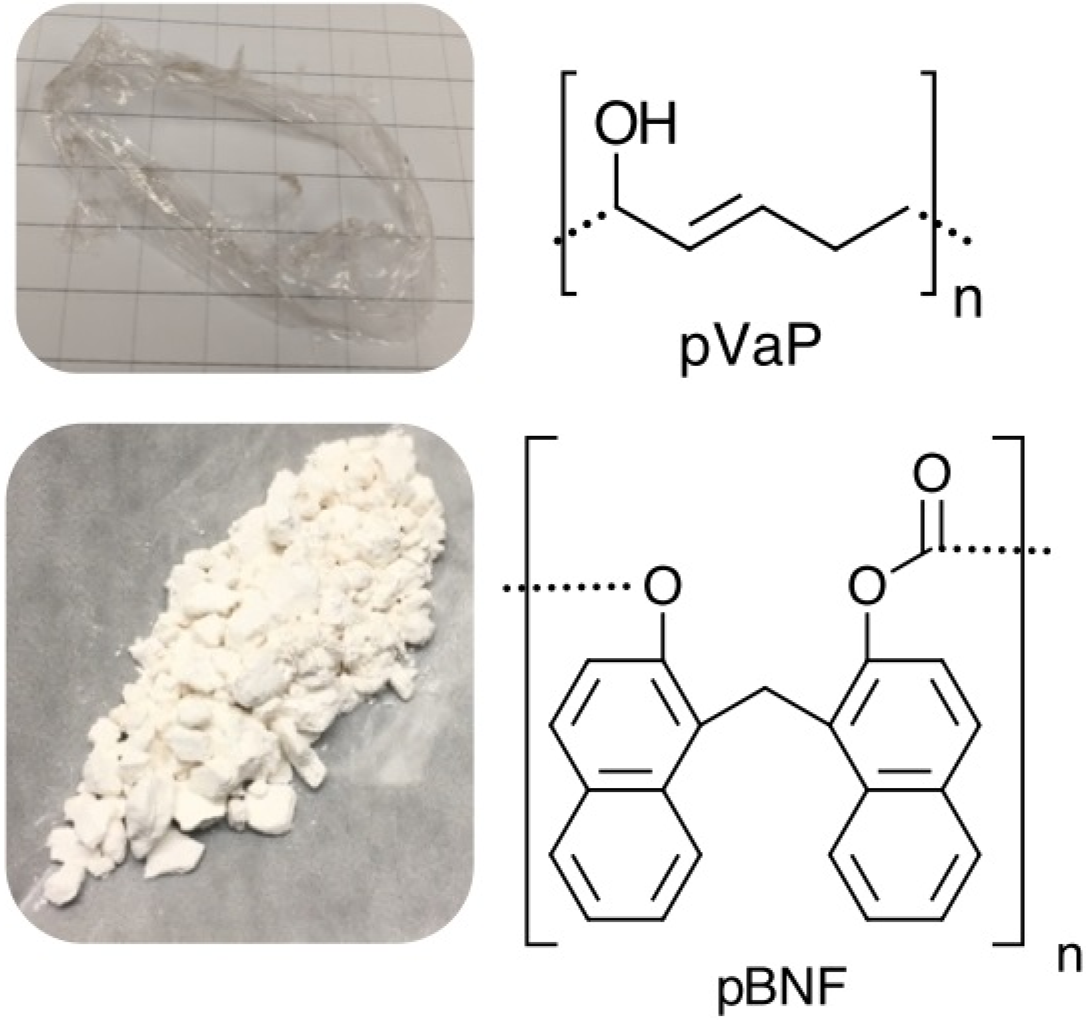


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Great work to produce a variety of polymers for potential evaluation using various identified CFP lignin products. This work result could be valuable in general outside of the BETO projects by identifying new classes of polymers for commercialization in the near term. However, there is concern over the level of these monomers in the CFP process and isolation of these individual compounds appears to be of low probability for use. My main feedback would be to group together a number of distillation products in similar boiling ranges to see if the total weight percent in lignin products could reach a reasonable amount of, say, 10%–15% total. Next, see what chemistry can be done similarly to that group to form monomers of use, which perhaps could also be copolymerized to make new polymers or isolated at this stage to feed to different processes. Simplification is key to this project success. The more consolidation that can be done to simplify the isolation and number of process steps and volume of material converted, the better the economics and viability could be.

- It was not clear what the number of processing steps is for a TEA to be attractive. The fraction of the biomass to products seems extremely low to capture a meaningful market share. It would have been good to understand the value proposition here from industry.
- The general concept of extracting greater value from pyrolysis oil is laudable, and the PIs describe some approaches that are reasonable on paper. However, this program faces the considerable challenges of trying to extract a very small amount of their starting chemicals in purity sufficient enough to drive downstream conversion. The further complexity in their process may make it difficult to get the project transitioned to industry.
- Potentially useful. Products look challenging.
- The overall approach of deriving value by synthesis of PABPs from CFP seems very challenging due to the complex mixture of chemicals (and hence product streams) that are likely to result.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate this valuable feedback.
- As we acknowledged in our presentation material, the selectivity of individual molecules from CFP is low where this conversion is currently being studied. These studies (at NREL, RTI International, Chemical Process Engineering Research Institute [CPERI]/Centre for Research and Technology-Hellas [CERTH] in Greece, and VTT Technical Research Centre of Finland) have focused exclusively on producing biofuels, where organic yields, not selectivity, are important. However, there are examples in the literature and industry where selectivities of individual molecules are much higher. For instance, levoglucosan, levoglucosenone, furans, some phenols, and aromatic molecules have been produced at concentrations ranging from 5%–30%. Aromatic molecule production for chemicals is being commercialized by Anellotech, Inc. and BioBTX.
- Given that there is literature and industrial precedent for higher selectivity of molecules from CFP, the goal of this project was to identify novel, performance-advantaged polymers that could be produced from CFP biocrude. We have started with molecules identified in CFP biocrude from a biofuels processes and used these to synthesize and test novel polymers. Once we have identified performance-advantaged polymers and their molecular precursors based upon their properties and industrial need, that is the point where increasing selectivity should be improved. There are other projects in the BETO portfolio that are working on ways to improve selectivity and separations and they have the capability and means to address this.
- This is exactly the approach that was used for many polymers such as polycarbonates. They were discovered in spite of the fact that phenols were found in low concentrations from coal tars, etc. It wasn't until the commercial importance of polycarbonates were established that the Cumene process was discovered for making phenol. We propose to establish the importance of new materials and then find a way to improve the production.
- The idea of attempting to use 10%–15% of the CFP biocrude as a class of compounds is an excellent one, and there is work in other projects to do just that.
- TEA efforts for coproducts is an ongoing effort in parallel projects, and we agree with the challenge of economic coproduct production.
- The polymers that we are investigating use biomass-sourced molecules and thus, due to their elemental composition, have a shorter pathway to products. For instance, commercial polyvinyl alcohol (PVA) is synthesized from ethylene, which comes from the cracking of petroleum and vinyl alcohol, which is made from acetic acid and ethylene. Acetic acid is made by the carbonylation of methanol, which is

produced by the gasification of natural gas and catalytic synthesis. There are five steps from the raw materials and a number of separations processes required:

  - Natural gas ⇨ syngas ⇨ methanol ⇨ acetic acid [+ ethylene] ⇨ vinyl acetate
  - petroleum ⇨ ethylene ⇨ ethanol
  - ethanol + vinyl acetate ⇨ PVA

- Our process to make a novel polyvinyl alcohol propene (PVAP) is when biomass is converted with CFP, the cyclopentenone is reduced, and the product is polymerized. There are three steps fewer in the separations processes:
  - Biomass ⇨ cyclopentenone ⇨ cyclopentenol ⇨ PVAP
- Market share alignment is part of current TEA efforts. The value proposition is creating value from materials that cannot be achieved through conventional petrochemicals.
- As discussed above, we recognize the problems associated with low selectivity, but other projects are addressing these issues. Our goal is to prepare and test PABPs.

BIOMASS CONVERSION TO ACRYLONITRILE MONOMER-PRECURSOR FOR PRODUCTION OF CARBON FIBERS

Southern Research

PROJECT DESCRIPTION

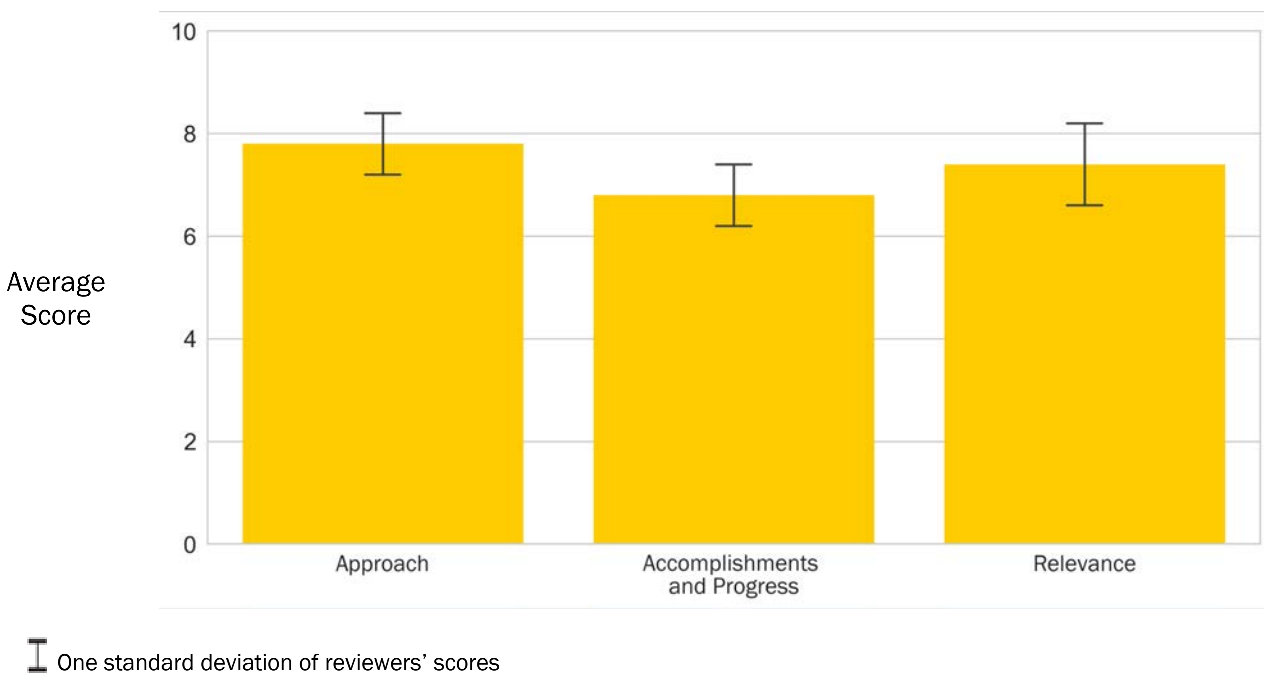
WBS:	2.3.1.200
CID:	EE0006781
Principal Investigator:	Dr. Amit Goyal
Period of Performance:	2/1/2015–2/28/2019
Total DOE Funding:	$5,981,713
Project Status:	Sunsetting

Polyacrylonitrile (PAN)-based, lightweight, high-strength carbon fibers are receiving great interest from the automotive industry, particularly in their bid to improve fuel efficiency of vehicles. However, widespread application of carbon fibers is presently deterred by high manufacturing cost (greater than $10.00/lb). Ninety percent of the world's carbon fibers are PAN based, derived from an ACN monomer and commercially produced from petroleum-based feedstock (e.g., propylene). Propylene prices are volatile, and its production is decreasing in the United States. In order to effectively reduce the cost of ACN (to less than $1.00/lb), an alternative feedstock available at scale, commercially viable with a sustainable conversion process and a high-purity product are desired.

Southern Research has developed a multistep catalytic biomass-derived non-food sugar-to-ACN process under a cooperative agreement with DOE. The catalytic steps are the hydrocracking of sugar to glycerol (R1), dehydration of glycerol to acrolein (R2), and ammoxidation of acrolein to ACN (R3). Southern Research has successfully completed the phase one part of the study where novel high-performance catalysts have been developed and tested at laboratory scale. Based on the Phase I results, significant reductions in ACN production cost ($0.70–$0.80/lb) and greenhouse gases were predicted from preliminary TEA and LCA. The

Weighted Project Score: 7.2

Weighting for Sunsetting Projects: Approach - 25%; Accomplishments and Progress - 50%; Relevance - 25%



produced bio-ACN from Phase one was validated by a commercial carbon fiber manufacturing partner (Solvay) for drop-in quality and was subsequently polymerized.

Following the Phase I study, the Phase II scale-up study has been initiated. For this part, three bench-scale skids for the three catalytic steps (R1, R2, R3) have been fabricated for decoupled operation. Design and fabrication of these skids include critical safety and operational controls. From lab scale (Phase I) to bench scale (Phase II), up to 1,000 times scale-up has been targeted. A continuous run on the first skid (R1) using commercial sugar hydrolyzates has been completed for more than 500 hours. The scaled-up catalyst did not show any sign of deactivation in the testing duration. Parallel to this study, impacts of various process-derived impurities on polymerized ACN (PAN) properties have been studied in a small-scale one-liter reactor. From this study, the allowable limit of these impurities has been determined, which will guide the purification steps of produced bio-ACN.

In the next few months, continuous runs on the remaining two skids (R2, R3) are planned. Southern Research will produce 200–250 kg of bio-can, which will be used by Solvay for polymerization and spinning. The TEA and LCA will also be updated with Phase II results.

OVERALL IMPRESSIONS

- Outstanding program and progress towards the BETO goals contributing to overall reduction in renewable fuel cost. I could find no major weaknesses in the program, which was well managed with clear milestones and achievements throughout the program. I expect the last phase of the project to achieve the goals with no major issues.
- The PIs have made progress on a challenging project to lower ACN costs for the production of carbon fiber and are trying to transition to larger scale. A better understanding of the dependence of ACN cost on propylene glycol sales and a clearer delineation of TEA assumptions would improve the presentation. Industry tends to avoid coproduct schemes, and thus a clearer description of how the PIs will avoid this problem would be helpful.
- Potentially promising technology. I am concerned about waste streams and economics.
- This project has made significant progress on each of the process steps to produce bio-ACN from non-food sugars. It would be interesting to see how the process scales, and how it performs on different substrates. It was refreshing to see a project that laid out incumbent product specifications as criteria for success. Some attention should be given to side products and the number of steps where yield losses can stack up and disadvantage the route.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The recipients choose not to respond to the reviewers' overall impressions of their project.

RENEWABLE CARBON FIBERS CONSORTIUM

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.4.102
CID:	NL0033912
Principal Investigator:	Dr. Mary Biddy
Period of Performance:	1/1/2018–9/30/2020
Total DOE Funding:	$2,864,600
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$2,300,000
DOE Funding FY19:	$564,600
Project Status:	New

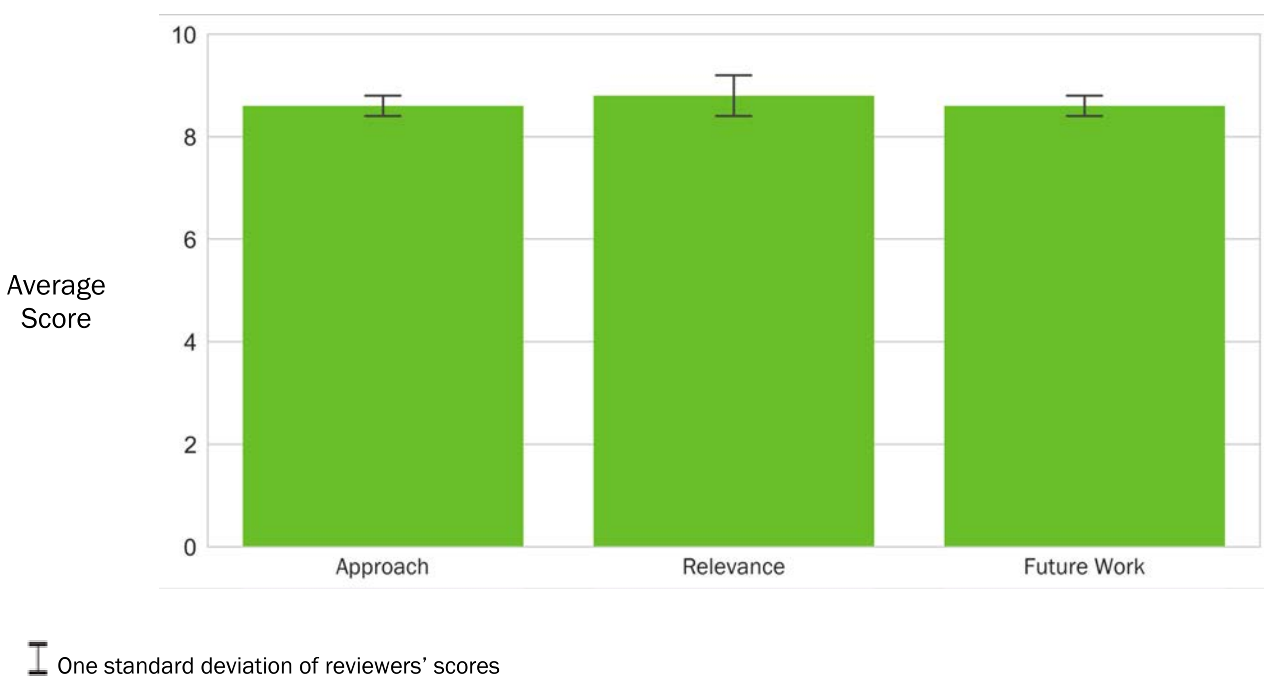
The Renewable Carbon Fibers Consortium project goal is to demonstrate cost-effective production of renewable carbon fibers through bio-ACN. The final product will be 50 kg of ACN converted into a carbon fiber component for performance testing, with a modeled cost of less than $1.00/lb. This work will identify bioenergy product and coproduct opportunities for industry evaluation with associated TEA and LCA, as well as industrially relevant improvements for bio-ACN and carbon fiber production via 3-hydroxypropionic acid (3-HP) pathway. The project leverages knowledge from a previous funding opportunity announcement, building on existing work.

Carbon fiber produced from renewable sources has many advantages. In addition to environmental benefits from renewable sugars as a feedstock source, the use of bio-based sources can potentially level out historically volatile acrylonitrile prices. The final report for the project will detail the process design to meet economic and sustainability metrics, document assumptions, and present R&D for further improvements via the bio-based route.

The bench-scale portion of the work focuses on improvements to the catalyst performance during the conversion of 3-HP to acrylonitrile. Catalyst deactivation during this stage is undesirable and adds to the cost of production. The goal will be to understand how critical process variables (reactant feed concentrations,

Weighted Project Score: 8.7

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



temperature, etc.) affect catalyst deactivation and ACN production. We will perform design of experiment studies to determine optimal reaction conditions to mitigate deactivation rate, as well as investigate the addition of chemical dopants to alleviate deactivation.

The scale-up component of the project is the largest portion and involves several external partners. The production route is 3-HP production ⇨ bio-ACN production ⇨ carbon fiber production ⇨ carbon fiber product manufacture. Partner involvement is as follows:

- Cargill, with extensive experience in strain engineering and fermentation optimization around 3-HP, will generate 3-HP from first-generation sugars (i.e., sucrose) via fermentation.
- The 3-HP will undergo esterification and nitrilation, converting it into bio-ACN at the Mid-Atlantic Technology, Research, and Innovation Center (MATRIC), which has extensive experience in development, testing, and scale-up of catalytic processes and handling reactive monomers. Johnson Matthey will provide the nitrilation catalyst to MATRIC.
- The bio-ACN will be converted into polyacrylonitrile and carbon fiber at Fisipe. Fisipe has experience in polymerization, polymer solution preparation, acrylic fiber extrusion, and carbon fiber production. Finally, the carbon fiber will be manufactured into a carbon fiber component by Ford Motor Company, where it will be performance tested. Ford has wide experience in this area.

This project directly supports BETO's mission to "develop industrially relevant bioenergy technologies to enable sustainable, domestically produced bioproducts." It will provide a renewable route to ACN, as well as project metrics and technical targets driven by TEA. By leveraging previous work, the goals of (1) a complete single carbohydrate to carbon fiber product demonstration run with industrial partners and (2) continued bench-scale work are both possible to meet the goal of cost-effective production of renewable carbon fibers through bio-based ACN.

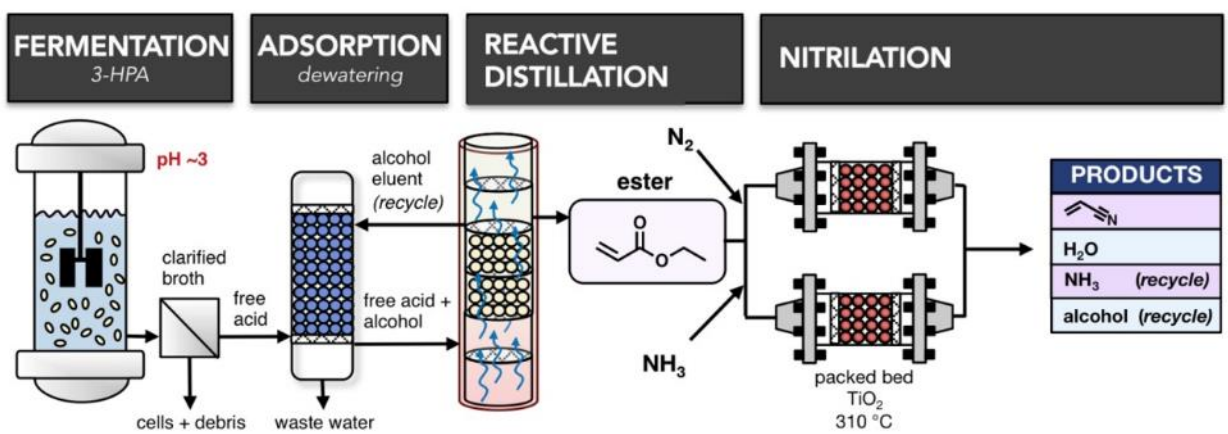


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Outstanding achievement on conversion from 3-HP by the team with existing catalyst on all processing steps. However, concern over commercial-scale activity time frame before regeneration could be a project killer. An additional concern is whether even reaching $1.00/lb (~$2,200/ton) can be sufficient to compete with the propylene process to ACN. Market dynamics have been lower as of late and only a few years ago the ACN price was in the $2,400.00/ton range. Some think the price will go down further. Thus, to have market pull, I believe the price target must be much lower than $1.00/lb, which their current economics indicates as $0.78/lb. If they can truly meet this price at scale, they can have a robust competitive price for bio even without a bio premium, which may be add on. Also, I am surprised that they did not include information on previous commercial-scale plants using sugar to glycerin glycols production. The company in China, Global Bio-Chem Technology Group, was making its corn-based propylene glycol since 2007 at its 200,000-tonne-per-year plant (total production of this and other chemicals) in Jilin Province and was big news in 2013 around the collaboration on a catalyst with Archer Daniels Midland Company. I believe they are no longer producing and believe it was due to the price of sugar increase around 2014 or so. This information would have to be confirmed, but perhaps a discussion with them could help the team understand real challenges commercially.

- This project is an excellent example of what BETO wants to do with the science and lab-scale investigations being carried out by their labs. Good science has led to good applications that attract industry and offer opportunities for commercial deployment.
- Looks very promising. Industry partners are a plus.
- The techno-economic advantage of this project is in a minimal unit operation, the chemocatalytic conversion process from 3-HP to bio-ACN, which should help mitigate yield losses. Very high yield has been demonstrated previously, although catalyst deactivation was an issue. This, along with scale-up, and subsequent carbon fiber and composite production and testing are areas for future work. Although apparently out of scope for this project, codevelopment of a highly efficient fermentation organism and process to 3-HP is going to be a prerequisite for a non-food sugar process to achieve success, so cross-talk with projects that may be working on this component is critical. Assuming success, this has the potential to be a highly advantageous process route.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the panel for their helpful review and suggestions. Going forward, we will work to incorporate these suggestions into the project.

PERFORMANCE-ADVANTAGED BIOPRODUCTS VIA SELECTIVE BIOLOGICAL AND CATALYTIC CONVERSIONS

National Renewable Energy Laboratory

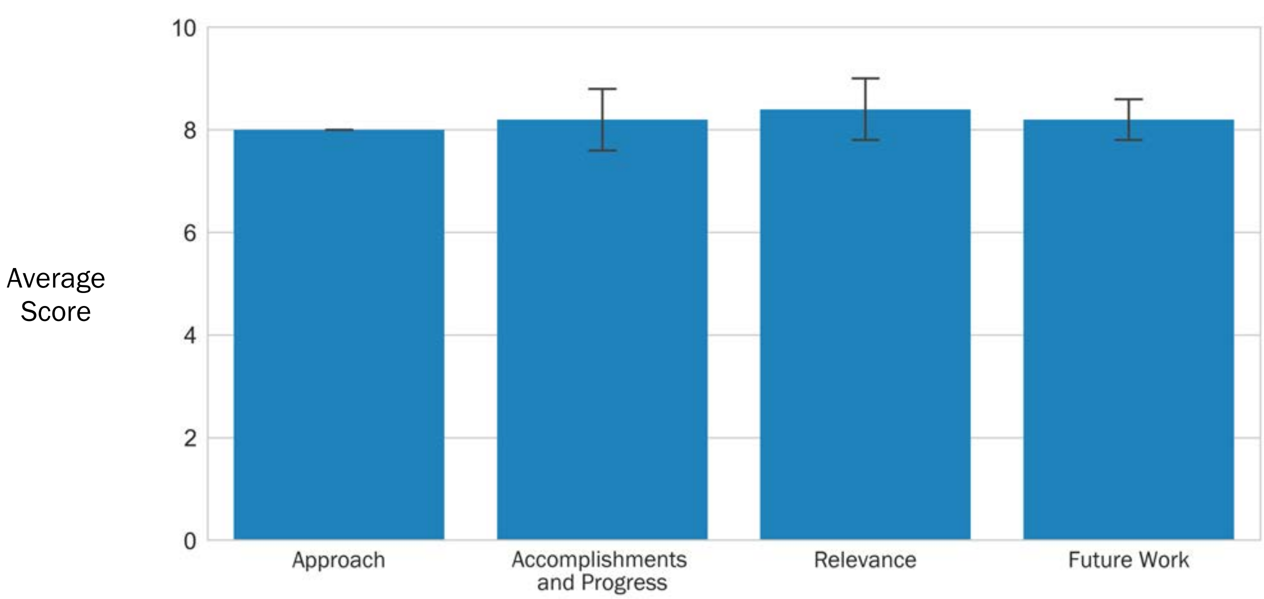
PROJECT DESCRIPTION

WBS:	2.3.4.501
CID:	NL0033411
Principal Investigator:	Dr. Gregg Beckham
Period of Performance:	10/1/2017–9/30/2020
Total DOE Funding:	$1,000,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$600,000
DOE Funding FY19:	$400,000
Project Status:	Ongoing

This project began in FY 2018 as one of four projects in the PABP mini-consortium. The goal of this project is to develop PABPs that employ intermediates derived from atom-efficient and selective biological and catalytic conversion of biomass and other waste oxygenated feedstocks. Given the slate of monomers that can be derived from sugars or lignin-derived aromatic compounds through selective biological and catalytic conversions, in combination with the vast chemical space available for polymer synthesis and formulation, the possibilities to derive new bio-based polymers are immense. This project (1) leverages a portfolio of selective biological and catalytic processes in the BETO portfolio to produce novel bio-based monomers, (2) synthesizes new polymers from combinations of bio-based monomers targeted to specific materials classes across a broad suite of polymeric materials, and (3) measures critical material properties to ascertain if these bio-based materials are performance advantaged over their petroleum counterparts. “Performance advantage” is measured relative to a petroleum-derived counterpart synthesized in the laboratory in the same manner as the bio-based product. The goal of the project in the three-year project cycle is to produce 50 new bioderived polymer formulations for multiple applications at the gram scale and to

Weighted Project Score: 8.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers’ scores develop ≥10 materials that are considered performance advantaged relative to petroleum-derived materials. This work is done in close collaboration with multiple projects, including the Inverse Biopolymer Design through Machine Learning and Molecular Simulation, Performance-Advantaged Bioproducts from Catalytic Fast Pyrolysis, and Tailored Polymers through Rational Monomer Development.

The first major accomplishment in this project was the establishment of a small-scale polymer synthesis and characterization laboratory at NREL that is used by all three experimental projects in the PABP mini-consortium. Up to 30 polymerization reactions can be conducted in parallel, and thermal, mechanical, and barrier properties can be measured for polymer formulations at the gram scale. Additionally, industry engagement is an important part of this project, and to date, over 50 companies have been contacted, with multiple in-depth customer discovery interviews conducted. This activity has directly informed what industry considers performance-advantaged across a wide range of materials and will be conducted continuously throughout the project. In terms of new polymer formulations, new nylon formulations have been produced through the use of ß–ketoadipic acid, which has been used in place of adipic acid in nylon-6,6. The resulting material exhibits significantly lower water uptake properties and dramatically improved thermal properties, both of which are considered performance advantaged. Additional results include the use of other aromatic-catabolic intermediates, such as pyrone-dicarboxylic acid (PDC) in place of isophthalate in multiple formulations; PDC exhibits a lactone functionality, which in turn imparts ease of chemical recyclability at the end of the material lifetime. Multiple lignin-derived compounds have also been tested in place of bisphenol A in polycarbonates and epoxy resins, which exhibit similar or improved mechanical and thermal properties. Endocrine disruption tests relative to bisphenol A demonstrate essentially zero toxicity. Multiple additional examples are under active development.

Future work includes the use of new monomers that encompass heteroatoms (e.g., nitrogen and sulfur), monomers from other bioderived sources (e.g., fatty acids), and new material formulations that enable expansion into other materials markets (e.g., rubber, coatings, nitriles, thermosets, and applications beyond polymers such as lubricants and surfactants).

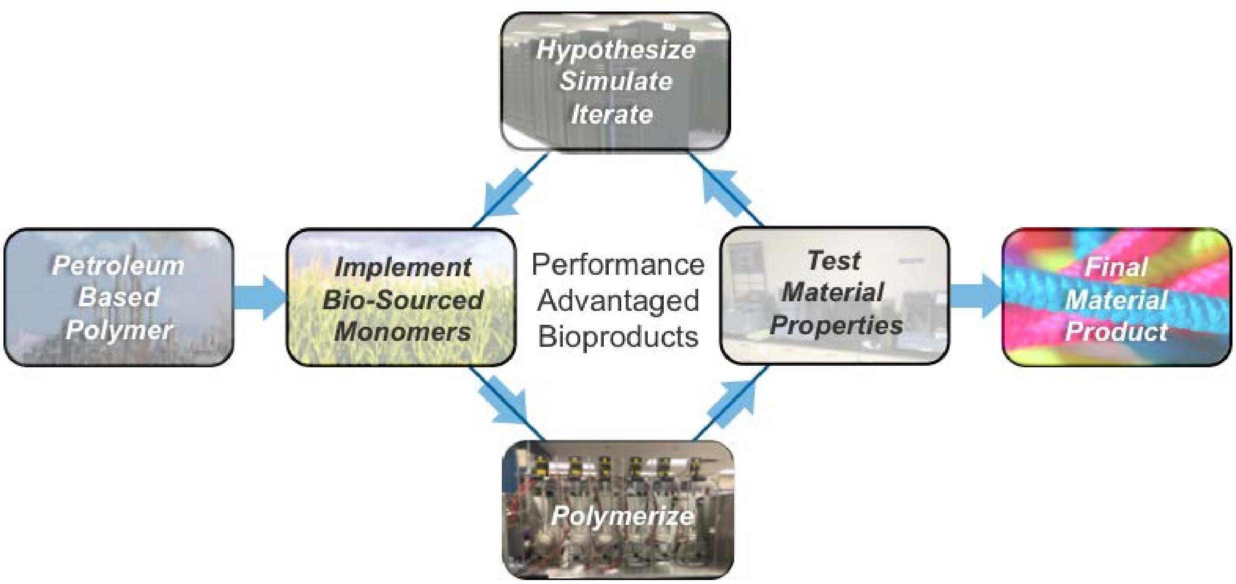


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Excellent work results and progress on polymers. I would have liked to see some end uses that are water-soluble oligomers potentially useful in many consumer goods products and industrial applications; however, I'm glad to see future work on other applications. ß–ketoadipic acid work is exceptional and I'm glad to see results here as I feel this may be a first work moving forward in industry. Don't rely on weak links and biodegradability of polymers. Better to focus on recyclability because the European Union may in the future ban weak-link polymers and U.S. policy usually takes time to adjust, but often follows stiffer guidelines in the future.

- It seems like bioproducts do have great potential to deliver better properties. The question becomes how does this reach an innovation level great enough to bring sufficient investment to make a commercialized product.

- This is an interesting project to build and test new polymers from bio-based monomers and measure their properties. Very good progress on synthesis of new formulations have been reported, some of which exhibit enhanced properties. This program has received extensive input from industry on worthwhile performance characteristics and is nicely synergistic to the inverse learning program, as it will generate novel information to augment databases and improve predictive tools for new polymers.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the positive comments from the reviewers. We agree that it would be ideal to expand beyond the current applications to include others, which additional funding would enable to increase bandwidth. The comment regarding biodegradability is excellent and we fully agree. We are attempting to make polymers that can be more easily chemically recycled.

- We agree that the bio-based materials need to reach a level of innovation to catalyze industrial investment. To that end, we are in close coordination with industry regarding the innovations coming from this project to offboard them as we reach a sufficient technical readiness level.

TAILORED POLYMERS THROUGH RATIONAL MONOMER DEVELOPMENT

Los Alamos National Laboratory

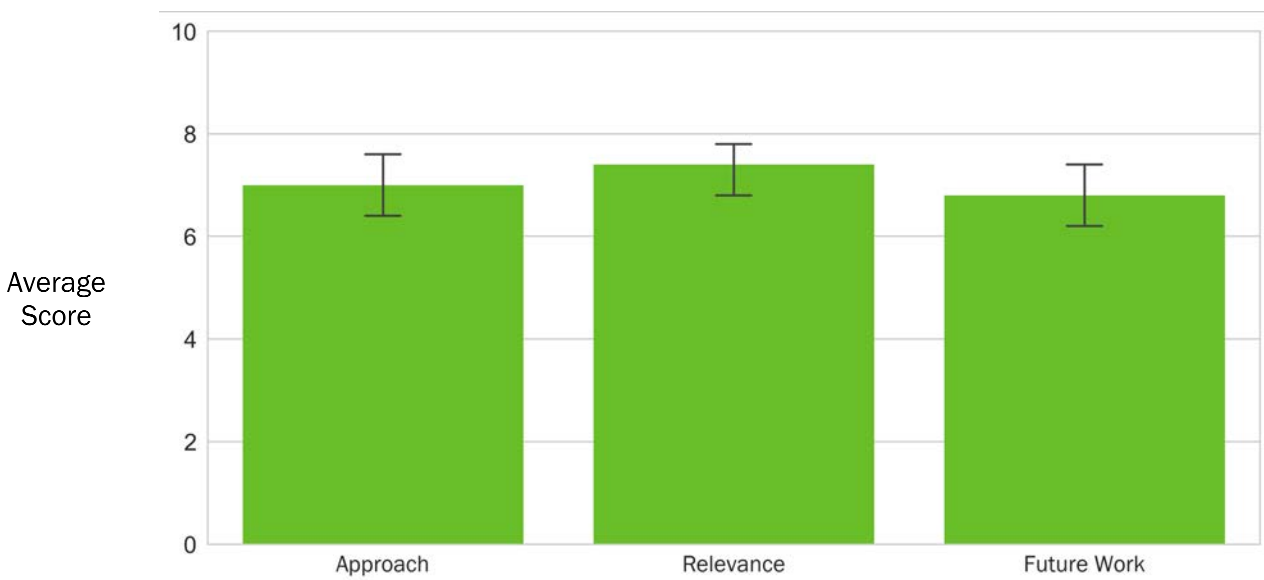
PROJECT DESCRIPTION

WBS:	2.3.4.502
CID:	NL0034401
Principal Investigator:	Dr. Andy Sutton
Period of Performance:	10/1/2018–10/1/2020
Total DOE Funding:	$225,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$225,000
Project Status:	New

Plastics are synthetic polymers that are constructed of repeating subunits of a variety of petroleum-based monomers. The judicious choice of the monomer and its polymerization method enables the fine tuning of strength, stiffness, density, heat resistance, and biodegradability of the resultant polymer. While there has not been widespread market penetration of bioplastics, one example of a biodegradable thermoplastic found in single-use packaging products is polylactic acid. However, the low strength, durability, and heat resistance of polylactic acid currently limit its widespread utility. Our approach to developing a new bioplastic will apply a retrosynthetic analysis; monomers will be synthesized from bioderived building blocks with inherent chemical and environmental safety. Thus, the materials engineered herein will not degrade to toxic or harmful molecules (such as bisphenol A [BPA]). By incorporating the ability to degrade into these benign intermediates, the long-term accumulation of plastics in the environment and the elaborate recycling pathways used for traditional plastics and polylactic acid, which often require a specialized reprocessing facility, can be avoided. A durable and fully recyclable bioplastic would reduce our dependence on a nonrenewable carbon source, eliminate hazardous processes that use toxic materials (such as phosgene), and produce a plastic that has no long-term environmental impact. The utilization of biomass to generate new

Weighted Project Score: 7.0

Weighting for New Projects: Approach - 25%; Relevance - 25%; Future Work - 50%



One standard deviation of reviewers' scores

polymers provides us the unique opportunity to produce materials with improved performance over current technology by taking advantage of the variety of functional groups in bioderived molecules as structural and electronic handles to tune the properties of the monomers and their resultant polymers. This project will synthesize bio-based monomers and the corresponding polymers with a focus on engineering a rational decomposition pathway to yield environmentally benign decomposition products. If successful, this work will help significantly reduce the amount of plastic that is discarded or incinerated and help pave the way for a circular carbon economy.

OVERALL IMPRESSIONS

- Good initial progress towards program goals. No major inputs or questions except for perhaps some nearer-term goals versus the broader quarterly goals would have been nice to have but not significant enough for a new program.
- The project performers clearly described how their project contributes to meeting PABP/BETO's goals and objectives. The project performers considered applications of their expected outputs. The project performers have presented the relevancy of this project and how successful completion of this project will advance the state of technology and impact the viability of commercial biorefinery concepts.
- The PIs present a scientifically interesting route to new polymeric materials that addresses the BETO PABP concept. The primary issue is whether industry will accept and commercialize materials of this complexity, which require multiple steps for their synthesis. The project would benefit from industrial examples that might have an equivalent number of steps from raw material to monomer to polymer, and which exhibit similar structural complexity.
- Early-stage seed project at this time.
- Creating polymers that can be reversibly degraded into nontoxic components is an intriguing idea. It will be interesting to determine how the balance between product performance versus degradation plays out and directs these polymers into various application areas.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the constructive and thoughtful feedback, which is especially useful to this project as it is a new start and receiving this guidance at such an early stage will help focus our efforts for the remainder of the project. The main concerns raised by the reviewers include the current multistep synthetic pathways to our current monomers, the complexity of the monomers, and the potential position of our polymers in a very competitive and cost-driven marketplace. The current synthesis was performed to provide an initial proof of concept for the project to demonstrate that at the three-month mark of the project we could use our approach to construct polymers from our proposed building blocks and subsequently deconstruct them. With this achieved, we can further refine and optimize the synthesis in collaboration with TEA. This will identify costly unit operations and allow us to determine the economic feasibility and potential price point we could achieve via this strategy. In collaboration with the machine-learning project, we will iterate through molecular structure variations that have the potential to both simplify the monomer structure and enhance performance of the materials we can prepare. We are very aware that a simple approach would be more amenable to scaling and we thank the reviewers for reminding us of this. The polycarbonate market will be challenging to compete in, and we are currently performing customer discovery interviews to identify niche applications or other market opportunities that would be more amenable for this kind of approach.

INVERSE BIOPOLYMER DESIGN THROUGH MACHINE LEARNING AND MOLECULAR SIMULATION

National Renewable Energy Laboratory

PROJECT DESCRIPTION

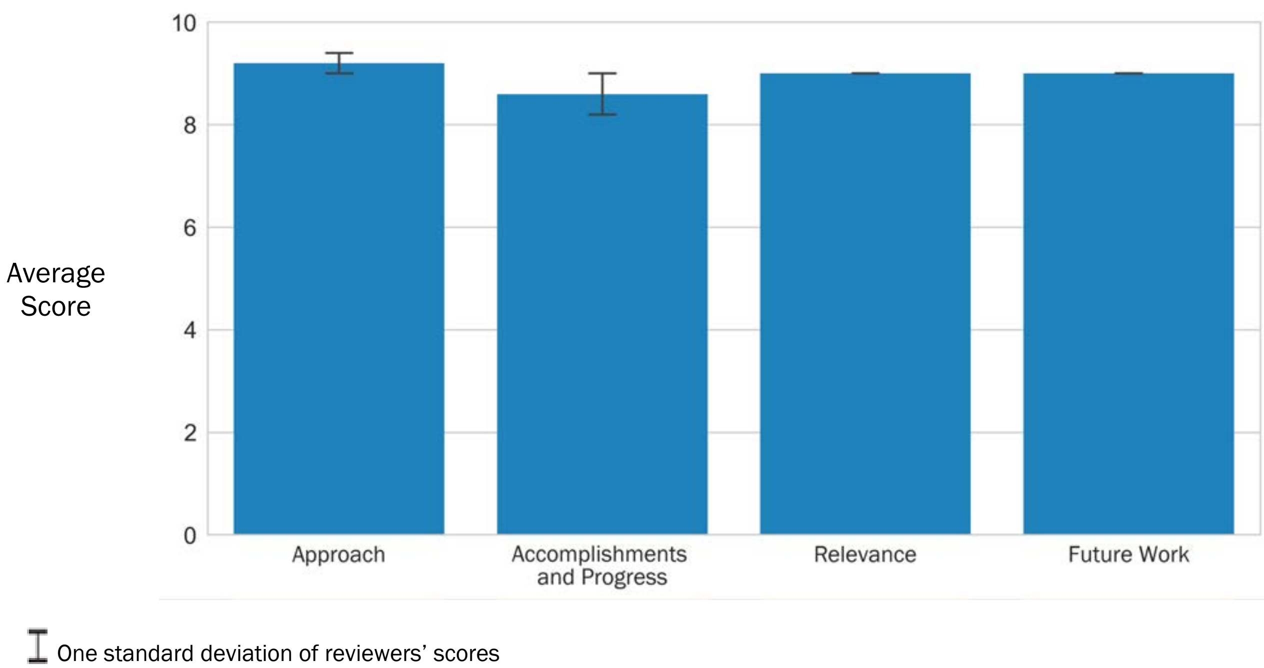
WBS:	2.5.1.500
CID:	NL0033412
Principal Investigator:	Dr. Mike Crowley
Period of Performance:	10/1/2017–9/30/2020
Total DOE Funding:	$850,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$400,000
DOE Funding FY19:	$450,000
Project Status:	Ongoing

An economically feasible bioeconomy will require producing value-added coproducts alongside fuel replacements. Deconstructed biomass offers a wide range of chemical functionality that can likely be harnessed to create inexpensive and high-performance biomass-sourced polymers. A key challenge in commercialization of biomass-derived compounds is deciding *a priori* which functional replacements have the highest potential for displacing incumbent materials. In this project, we develop an integrated approach to reverse-design materials from biomass-derived compounds. This ultimately increases research efficiency, reduces time to market, and creates new opportunities for advanced biomaterials.

In contrast to the traditional approach where applications for a polymer are researched post synthesis, inverse material design starts with desired properties and works backwards to a suitable starting monomer. This field of computer-assisted material design exploits the tendency for many polymer properties to be correlated with molecular structure. The vast majority of methods for inverse design are focused on homopolymers with a high degree of polymerization and low macromolecular complexity. Existing databases and literature will serve as a

Weighted Project Score: 8.9

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



basis for the proposed work; however extending the information in these databases through guided atomistic modeling and experimentation can bridge the information deficiency associated with biomass-derived polymers. Additionally, advanced synthesis methods for performance-advantaged bioproducts aim to control macromolecular complexity to optimize properties through structure. The resulting polymers often feature complex chain branching, block copolymer structures, or controlled tacticity1-2 complications omitted from simple monomer-based group-contribution design algorithms. Models necessarily need to extend beyond basic considerations of monomer chemistry for quantitative structure-property relationship to be effective for biomass-derived polymers. This project leverages atomistic simulation to magnify experimental effort and use *in silico* experiments to help determine optimal approaches for polymer learning.

Molecular modeling and simulation have the ability to approximate physical characteristics of molecular systems *in silico* and provide two valuable functions to this study: (1) avoid the time-intensive process of synthesizing and characterizing polymers and (2) provide deep insight into the molecular and mesoscale causes of polymer behavior. The ability of polymer simulations to produce experimentally measurable properties, such as glass transition temperature, has been established for some polymer systems and is the basis for the work in this project. The modeling data have the potential to produce a fast turnaround in the development of the machine-learning cycle, where predictions can be made and tested *in silico*. Our direction is to develop systematic approaches to attaining accurate polymer properties from all available methods and inferring molecular understanding of the source of the polymer behavior as a function of monomer composition, polymer composition, branching characteristics, polymer length, and dispersity of polymer length. These methods are a key part of developing a machine-learning algorithm and tool, a deeper understanding of how polymers get their properties, and how we can more efficiently tune polymers for desired properties. The breadth, accuracy, and precision of properties from simulation will be less than what is possible from actual synthesis and characterization but will be a huge advantage due to the fast turnaround of learning, prediction, and testing when it replaces synthesis in that process. The algorithmic tuning is independent of the accuracy or precision of the data and can be refined very quickly as simulation data are replaced by experimental data over time.

OVERALL IMPRESSIONS

- Great modeling plan and work results, from my own experience working with modeling teams using state-of-art modeling on much simpler systems than this team. I'm curious why the focus is on high molecular weight polymers first, when it might have been easier to start with lower challenges like small molecule properties such as stated before in future work (i.e., viscosity modifiers/additives to lower plastic melt properties for mold blowing bottles). The current market uses widely fluctuating chemicals that are renewable, like ricinoleic oils, but have limited volume supply and even shrinking volume supply from India as the focus on food crops such as soybeans are causing market issues as growers have stopped growing the plant for ricinoleic oils. Unique, high-performance, water-soluble polymers—like the kind companies like BASF, Dow/DuPont, and others make for consumer goods—which are water soluble and a lower molecular weight, might be another focus area not currently being covered in these programs. Examples might be bio, hydrophobically modified polyacrylates, sulfonated variants used in industry today, or polyethylene glycol-grafted polymers and potential chelant replacements for today's petrol amine-containing chelants, which could be another set of targets to model and develop and perhaps easier to model. Commercialized bio-based chelants from the likes of Dow/Dupont are developed from other processes but not from aromatics like lignin monomers. Another area is solvent modeling for potential replacements for petrol derived.

- Very innovative. I have high hopes for a promising outcome.

- This is a terrific new start for the BETO program that has the potential of answering many questions around PABPs and defining the types of materials that a biorefinery might consider. It could also provide the basis for new, broad-based technology development within the labs. The project will be strengthened by inclusion of molecular weight data and providing information supporting the possibility that the predicted polymers are able to make the leap to industrial use.

- This is a valuable approach to optimize the search for new PABPs by creating *in silico* high-throughput screening and prediction tools. If successful, its value will be crosscutting and substantial in terms of research efficiency and hit rate.
- This project is doing great and groundbreaking work to enable inverse design of new bioproducts and using a high-throughput method for predicting polymers with advantageous properties. They are developing databases for large classes of products and targeting ten new polymer materials.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their suggestions and insights. We appreciate the time and effort of the reviewers to understand our project and to provide valuable constructive comments, insights, and suggestions. We will be looking into moving into these new directions the reviewers suggest as we successfully complete the initial stages of this work. Our machine-learning prediction tool and consolidated polymer databases will be made available when they are sufficiently reliable and usable. We welcome and seek out collaborations with any industrial and research groups with an interest in these research directions.

BIOPROCESSING SEPARATIONS CONSORTIUM – OVERVIEW

Bioprocessing Separations Consortium

PROJECT DESCRIPTION

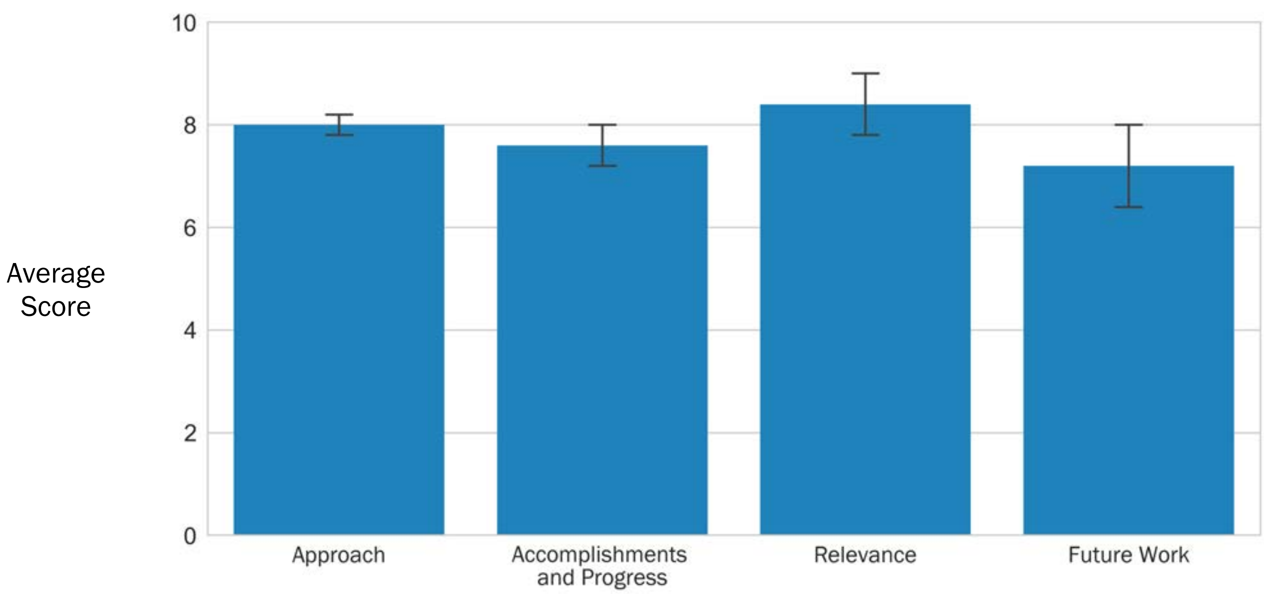
WBS:	2.5.5.501a
CID:	NL0031310a
Principal Investigator:	Dr. Jennifer Dunn
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$11,085,000*
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$0
Project Status:	Ongoing
*This total reflects the summation of funding for all projects contributing to the Bioprocessing Separations Consortium.	

The Bioprocessing Separations Consortium (BioSep) develops cost-effective, high-performing separations technologies through coordinated separations research that targets industry-relevant bioprocessing separations challenges. As a result, biofuels and bioproducts industries will have new, high-performing, low-cost separations technologies available to them. This consortium was formed because BETO industrial stakeholders have long raised separations challenges as a major barrier to cost-competitive biofuels and bioproducts. BETO analyses indicate that separations steps can constitute up to 50% of processing costs. The consortium approach coordinates and brings to bear breadth and depth of national laboratory expertise, capabilities, and resources on this foundational challenge.

The consortium consists of a steering committee, a crosscutting analysis team, and biochemical and thermochemical separations teams. The consortium also has an IAB with eight members that include companies that focus on biochemical and thermochemical processing, as well as separation technology providers. The board helps the consortium maintain an industry-relevant focus and knowledge of recent technology advances and challenges. It also provides advice, reviews results and progress in comparison with

Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

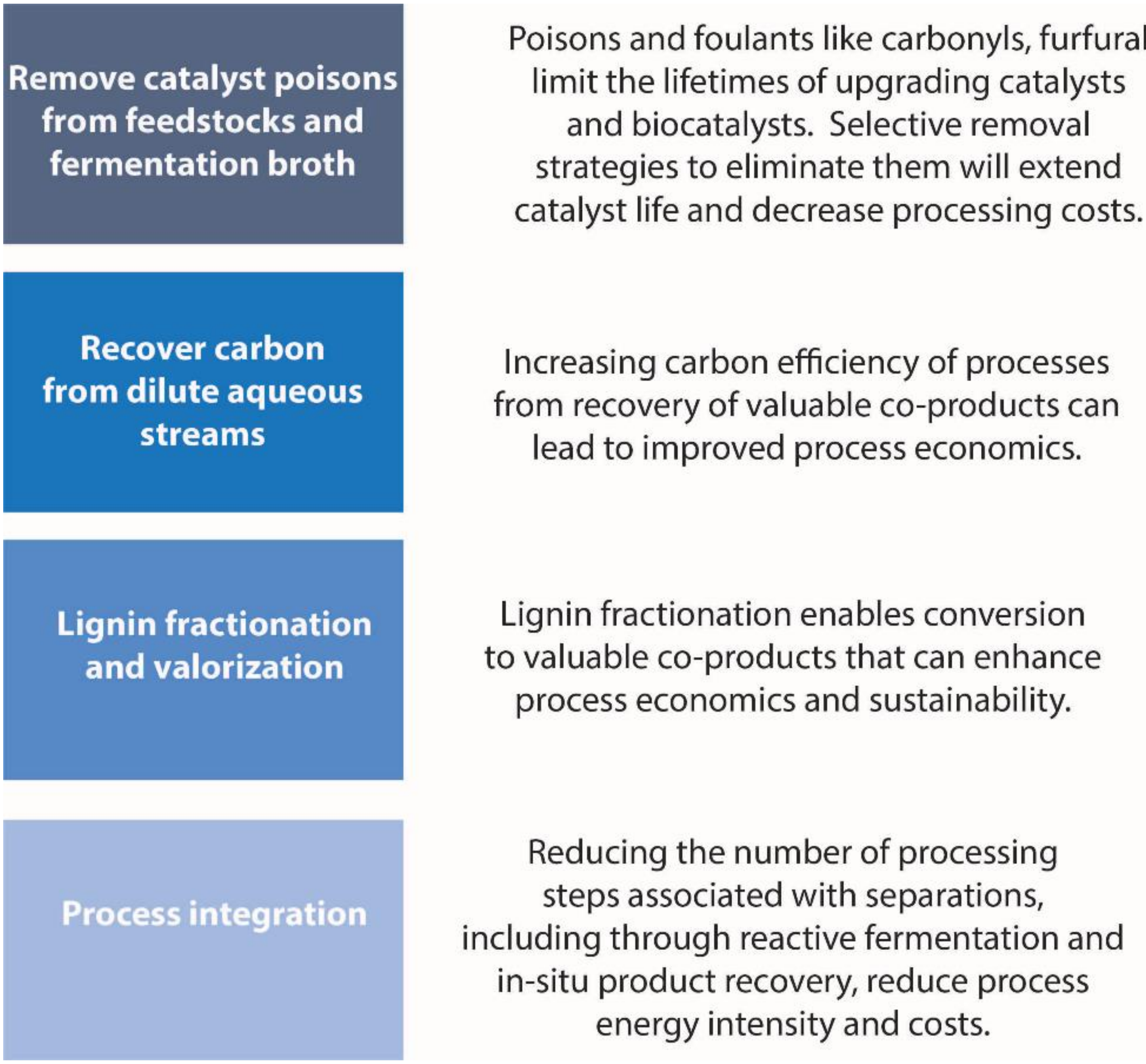


One standard deviation of reviewers' scores

work plans, provides feedback regarding prioritization of research projects (experimental and analytical), and informs development of the consortium's strategy for out years.

In the first two years of BioSep, the steering committee has had the objectives of guiding the consortium, coordinating external communications, and managing consortium business. Particular achievements in this timeframe include establishing the IAB and coordinating meetings with them twice annually; holding an industrial listening day (May 2017); creating and expanding the website to inform stakeholders of consortium capabilities, managing consortium reporting, and organizing; participating in bioprocessing separations sessions at targeted conferences; planning and monthly communications; and coordinating a directed funding opportunity, which is the subject of another presentation in this session. As a result of this interaction with external stakeholders, BioSep has developed a more complete understanding of bioprocessing separations challenges that will inform its plans for future work.

The consortium is in its third year and has an end-of-project goal to demonstrate the consortium's value to BETO and the biofuel and bioproduct communities through documentation of technical advances, influence on process economics, and potential industrial applications of consortium technologies.



Photos courtesy of Bioprocessing Separations Consortium

OVERALL IMPRESSIONS

- Great technical approach. Provided a thorough background of how they ended up where they are, informed by very robust IABs. The project management plans included are well defined and similar across all projects. It was unclear what the technical targets and cost targets are for the highest-impact separations technologies. There is potential for the number of coordination meetings and conference calls to be onerous. It was mentioned several times that separations can be upwards of 50% of the manufacturing costs, but the underlying analysis for this was not presented and it was not clear how much that was for each of the areas/pathways they chose to focus on for separations. It was unclear what technical targets would be needed to achieve the reductions in the areas/pathways they chose to focus on for separations.

- Team has done great job organizing the work and progressing program. One suggestion: the list of engagement parties excludes fuel companies such as Valero, Royal Dutch Shell, BP, Chevron, etc. This would go a long way to provide sound input and evaluation of the technologies, as many are engaged in their own bio-renewable programs and may even provide some insights from their petrol experience. Other suggestion for an IAB member would be a firm such as LyondellBasell.
- Economic evaluation of the different separations' projects going on at the labs and with industrial partners is a crucial part of the overall program and should be continued. It provides needed credibility to potential stakeholders that the lab research effort also understands the needs of their partners. More clarity about BETO’s plans for continuing the project after September would be helpful.
- Enabling technology always has the potential to be impactful. Separations companies need to get involved.
- BioSep is a worthy approach to developing a heretofore underserved focus on separations technology and effectively engaging across national laboratories. Working together with separations technology and equipment providers is advisable so that each can learn from the other regarding emerging needs.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The recipients choose not to respond to the reviewers' overall impressions of their project.

BIOPROCESSING SEPARATIONS CONSORTIUM – SEPARATIONS FOR BIOCHEMICAL PROCESSES

Bioprocessing Separations Consortium

PROJECT DESCRIPTION

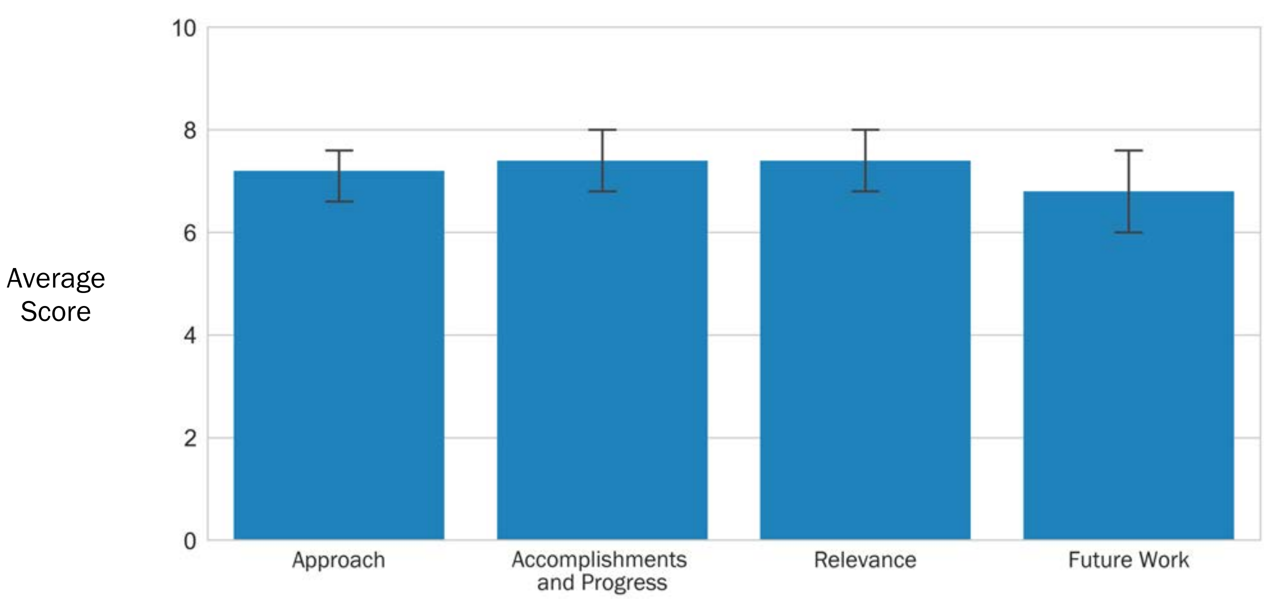
WBS:	2.5.5.501b
CID:	NL0031310b
Principal Investigator:	Dr. Gregg Beckham
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$4,765,000
DOE Funding FY16:	$0
DOE Funding FY17:	$1,605,000
DOE Funding FY18:	$1,575,000
DOE Funding FY19:	$1,585,000
Project Status:	Ongoing

In support of BETO's minimum fuel selling price target of \$2–\$3/GGE for biofuels, the team at BioSep aims to enable cost-effective integrated separation solutions to meet these targets in biological conversion processes. We are tackling two of the cost-driving separations challenges in bioprocesses: (1) recovery of products from fermentation and (2) separations relevant to lignin valorization.

The recovery of bioproducts from fermentation is a well-known cost driver in biorefining that can account for greater than 50% of the minimum fuel selling price. Several challenges exist in fermentation product recovery, including dewatering (products are approximately 5–10 wt % in water), removal of trace impurities, and handling of large volumes of fermentation broth at scale. To address these challenges, four projects are ongoing wherein new separation technologies are being developed that reduce the energy and cost associated with classical post-fermentation recovery methods. First, an *in situ* product recovery (ISPR) system is being developed based on continuous liquid-liquid extraction (LLE) of bio-carboxylic acids. Key results of this project include demonstrated ability to increase fermentation titers tenfold over fed-batch titers, direct recovery

Weighted Project Score: 7.2

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

of carboxylic acids as neat products via distillation of the organic phase, and an energy consumption less than 20% of the heating value of the product. Second, wafer-based electrodeionization technology is being developed for the *in situ* recovery of bio-based carboxylic acids. Key results of this work include >90% acid capture into a tenfold concentrated permeate using <1 kWh/lb of acid recovered. Both of these ISPR systems represent an advance from traditional post-fermentation recovery schemes in their nonthermal dewatering capabilities that lower energy requirements and ability to reduce fermenter size by approximately tenfold. A third project involves the design of advanced materials for selective adsorption of fermentation products. New nanomaterials with tunable surfaces are being developed to bind target products. The materials are unique in their ability to be regenerated mechanically, allowing for novel process-intensified separations systems with nonthermal dewatering abilities. Finally, a recent project focuses on the recovery of alcohols, namely 1,4-BDO, from fermentation. This project utilizes a hybrid extraction-distillation system driven by membrane pervaporation.

The valorization of lignin in a biorefinery is an important step towards meeting BETO's $2–$3/GGE biofuel target. However, lignin-rich process streams are often difficult to handle and present several separation challenges given the broad range of molecular weight components, fines, and debris present. Four projects are aimed at developing technologies to address these challenges. First, ultrasonic separations are being applied to lignin depolymerized streams to remove fines and debris present that make the solution difficult to filter. This project has shown success in removal of fines and debris in a continuous manner, which is promising given that membranes often foul rapidly when applied to lignin-rich streams. With fines and debris removed, molecular weight fractionation of the lignin material is being investigated. Polymeric membranes in tangential flow filtration (TFF) cells are being developed to recover low molecular weight (LMW) lignin monomers, and in another effort, ceramic membranes in TFF cells are being investigated. Both membranes are effective at recovering LMW monomers from the complex solutions and can be regenerated. Finally, we are applying electrochemical separations to simultaneously recover sodium hydroxide from a black liquor while separating LMW acids. This technology has shown 99% sodium hydroxide recovery and 95% carboxylic acid recovery, representing an important advance in recycling caustic deconstruction catalyst.

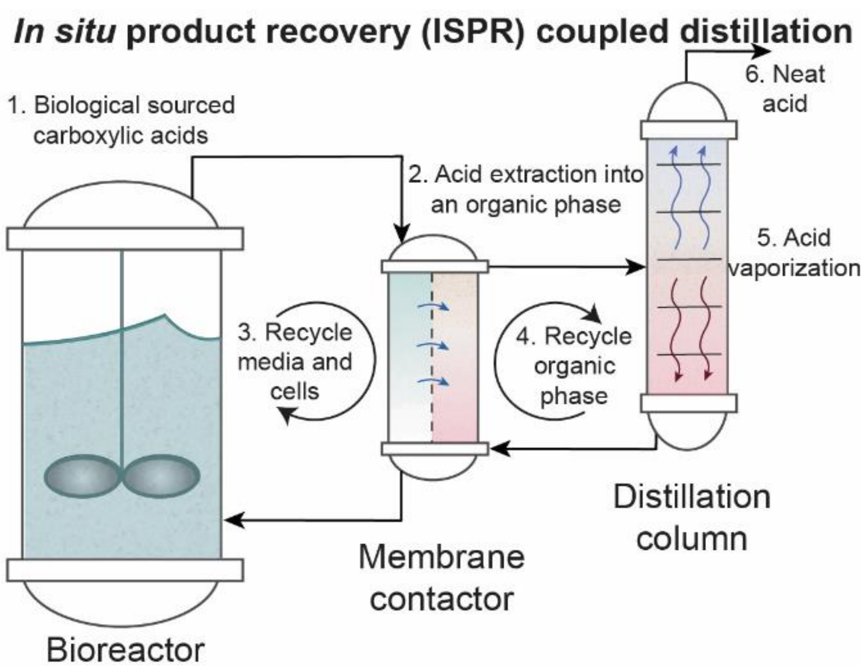


Photo courtesy of Bioprocessing Separations Consortium

OVERALL IMPRESSIONS

- Did the team exploring fines filtration explore filter technology that is used for removal of fines from Raney nickel in processing glucose to sorbitol? These filters have a unique design of multiple layers to retain larger particles, and at a later stage the fines can be removed to avoid pressure buildup and clogging. This could be useful for the issue with fouling of lignin fines. Also, due to the physical properties of 2,3-BDO, did the team explore freeze fractionation since it was mentioned as an alternative? The melting point of the material is 66.2°F, and as such may lend itself particularly with salt also present. I am curious as to why the team did not attempt this well-known approach to chemical purification prior to the others. Indeed, chilling adds energy input to the process, but this may be one way to simplify the recovery. Ultrasonic separation has always been challenging to do in any field of recovery. I also have concern over the scalability of this approach.

- BioSep has the potential to be a vital, crosscutting component of the overall BETO effort in biorefinery development. Separations will always play a key role in the efficiency of a process and will help determine whether it can make the leap to commercialization. The program would benefit by greater focus and differentiation of its stable of approaches so that the observer has an idea of which methods hold the greatest promise.

- This is a potentially important project that is progressing well. Needs connecting to valuable applications.

- The project has made good early-stage progress on innovative and scientifically interesting separation approaches, focusing on high-value impact areas for fermentation recovery and lignin valorization. The scalability of these approaches needs to be critically evaluated.

- There is a significant amount of interesting science and research being performed in a highly relevant area (separations). Project performers have identified a project management plan that includes well-defined milestones and adequate methods for addressing risks. Critical success factors were well defined. It was not clear why these technologies were chosen versus other options. It was not clear what their potential performance is relative to the current state of technology. It was not clear how and if the program would downselect from the technologies being investigated.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We did not investigate the filter technology used for fines removal from Raney nickel in the glucose-to-sorbitol process as a technology for fines removal from an alkaline pretreated liquor stream. Prior to discussion with this reviewer at the peer review we were unaware of this technology. We will follow up with this and explore potentially repurposing this technology for removing fines from lignin-rich process streams.

- Regarding 2,3-BDO, we have internally discussed examining a crystallization/remelt-type strategy for isolating this product but have not pursued it in this three-year cycle. This is a possible approach we have proposed within our next planning cycle.

- Regarding the challenges of ultrasonic separation and its scalability: the challenges posed in general by ultrasonic separation of particles originate in the particle response to ultrasound and the ability to trap particles in the acoustic field, the creation of particle-free channels whereby liquid can pass through the field while particles are held in place, the creation of large aggregates in the acoustic field and their ability to remain intact while settling or floating from the field, and the ability to reach a steady operation, which demands the removal of particles at the same rate as they are entering the acoustic field. These elements depend on the particle properties, the solids content in the feed material, and operating conditions such as the flow rates of input and output streams and power input to the acoustic field. These are the primary factors being investigated in this study. The approach taken to meet any industrial operating scale requires a practical length for the standing wave to be set based on needed power delivery, and then scaling out the technology to meet the requisite flow rate. In this way, ultrasonic separation can be manufactured to fit a broad range of operating scales. Given the simplicity of ultrasonic hardware, there is no intrinsic feature that would preclude the technology from operating competitively at a large scale.

- As detailed in the subsequent analysis presentation, rigorous TEA was performed to inform decision making on the technology selection.
- The technologies developed in this consortium are aimed at reducing separations costs within the biochemical conversion process to meet the $3/GGE minimum fuel selling price target. For example, valorizing lignin is predicted to contribute a $2–$3/GGE cost reduction. However, in the case of lignin, there is no state of technology and thus these projects are aimed at developing that separation process to recover valuable chemicals from those lignin-rich streams from the ground up. For fermentation intermediate recovery (carboxylic acids), separations are known to account for >50% of the processing costs and thus these new *in situ* product recovery technologies are aimed at reducing that cost by avoiding the expensive post-fermentation separations that are typically employed.
- Many of these technologies were developed within this consortium and as they develop are moved into other projects for scaling and demonstration. For example, the LLE-ISPR system is now being moved into a waste-to-energy task wherein it is undergoing scaling to generate pilot-level data for more detailed TEA.
- Regarding why these technologies were chosen versus other options, we are working internally to develop a presentation format that more effectively communicates metrics of both our technology targets and conventional technology performance and will include this information on the BioSep website. The subsequent analysis presentation included rigorous TEA that detailed performance of the technologies compared to the current state of technology, where available (lignin separations do not have a state of technology), and provide context to how the downselect process occurs.

BIOPROCESSING SEPARATIONS CONSORTIUM – SEPARATIONS FOR THERMOCHEMICAL PROCESSES

Bioprocessing Separations Consortium

PROJECT DESCRIPTION

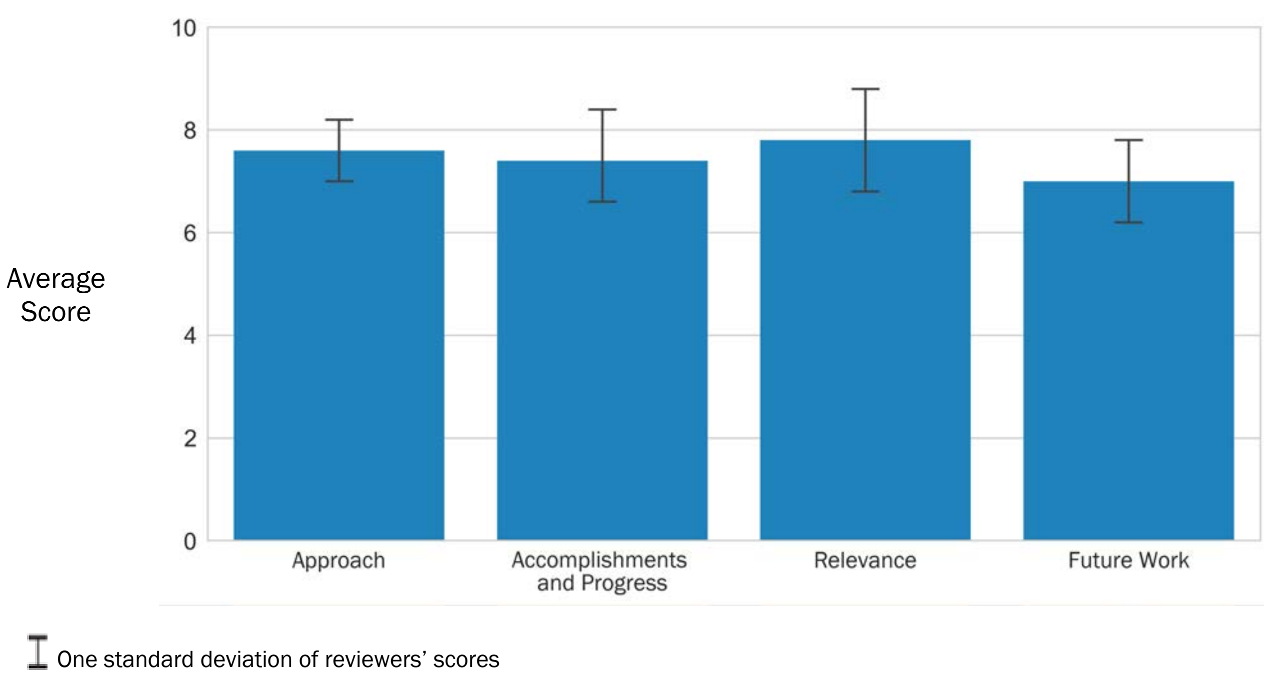
WBS:	2.5.5.501c
CID:	NL0031310c
Principal Investigator:	Dr. Kim Magrini
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$4,130,000
DOE Funding FY16:	$0
DOE Funding FY17:	$800,000
DOE Funding FY18:	$1,645,000
DOE Funding FY19:	$1,685,000
Project Status:	Ongoing

BETO’s stakeholders identified energy-intensive, challenging separations as a hurdle to cost-competitive biofuels and bioproducts. A critical technical barrier is impurities in intermediates impeding downstream biological and chemical catalysts and the need for low-cost purification technologies. Additionally, recovery and conversion of dilute carbon can cut the cost per GGE of renewable fuels. Other opportunities to increase use of renewable carbon to maximize carbon conversion and efficiency in BETO pathways include capturing and converting carbon in the aqueous phase after pyrolysis and tapping lignin produced in biochemical pathways as a feedstock for fuels or chemicals.

Within BioSep, the thermochemical team’s three tasks are Molecular Removal Technology for Preprocessing of Liquid Bio-Oils and Biocrudes (Task C.1), Integrated Membrane Separations Technology for Hydrothermal Liquefaction Aqueous Streams (Task C.2), and Catalytic Hot Gas Filtration for Vapor Chemistry Tailoring (Task C.3). These tasks target significant capital expenditure and operational expenditure cost savings, as estimated by TEA, through catalyst preservation and process-intensification strategies. Technical performance

Weighted Project Score: 7.5

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



is measured by removal effectiveness (wt %) of target foulant molecules from bio-oil biocrude, biogenic carbon recovery efficiency from the hydrothermal liquefaction (HTL) aqueous fractions, and catalyst lifetime and/or reaction yield enhancement.

Task C.1 develops molecular removal technology using adsorbents (functional polymers, inorganic materials), to address a major technical and economic challenge in HTL biocrude upgrading: high nitrogen content. The ORNL-Pacific Northwest National Laboratory (PNNL) teams are developing sorbent separation technology for the removal of light heterocyclic nitrogen-containing species (such as indoles, pyridines, piperidines, pyrazines, pyrroles, and pyrrolidines) from wastewater sludge HTL biocrude, and, potentially, amines ammonia from fatty acid amides in the biocrude. It will enable downstream hydrotreating with reduced hydrogen consumption and improved throughput and has the potential for recovery of nitrogen-containing species as higher-value products.

Task C.2 addresses recovery of organic acids and ammonia from HTL aqueous streams that impact process economics. Organic acids are recovered by integrating: (1) ANL's ion-exchange polymer wafer and membrane to extract carboxylic acids from an HTL aqueous stream to greater than 30 wt % (with simultaneous ammonia separation), followed by (2) ORNL's dehydration dewatering membranes to achieve an overall greater than 90% removal of the water with improvement of membrane material stability at higher acid concentration. Another effort seeks to extract individual organic acids from mixed acids in the HTL waste without additional separations steps. The combined ANL-ORNL process could produce higher concentration of target carbon components, beyond what any single separation process could achieve.

Task C.3 couples NREL expertise in hot gas filtration and pyrolysis vapor upgrading with NREL's and ORNL's catalyst capabilities to develop catalytic hot gas filtration (CHGF) for tailoring vapor chemistry for downstream catalytic upgrading to produce upgraded bio-oils that can be used for fuel and chemical production. This task develops and assesses the use of hot gas filtration to remove reactive alkali and char particles from biomass pyrolysis vapors to improve vapor composition and protect downstream upgrading and hydrotreatment catalysts from fouling. Adding a catalyst to the filter (CHGF) provides chemical tailoring (such as deoxygenation) of the feed vapors before they are upgraded to hydrocarbons; catalysts will be assessed for improved product specificity and yield. Approaches include rare earth oxide catalysts to ketonize vapor-phase carbonyls to more upgradeable species, tuning heteropoly acid acidity for alkylation selectivity, and using fractional condensation of vapors to remove coke-forming heavy species prior to upgrading.

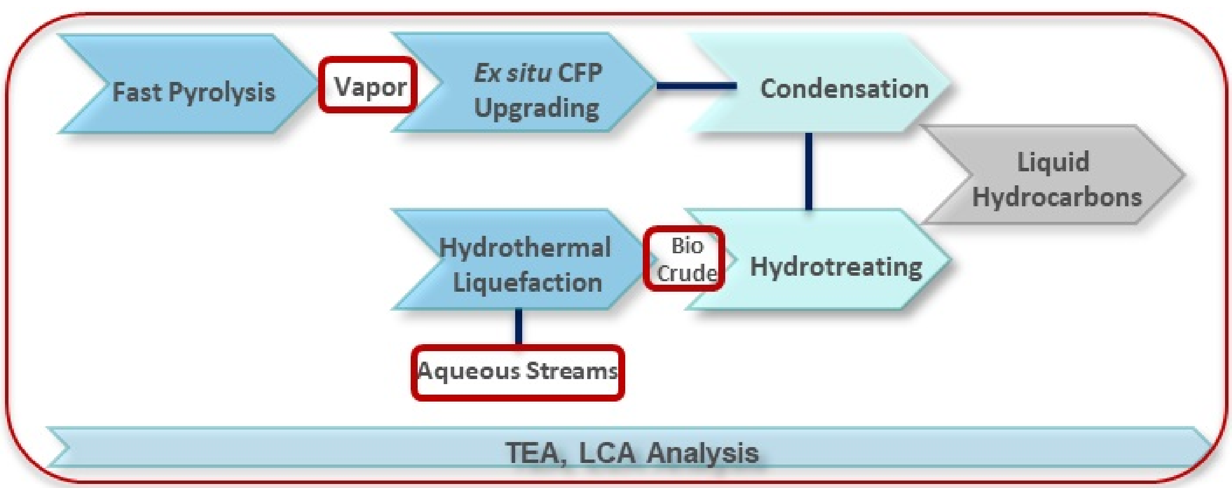


Photo courtesy of Bioprocessing Separations Consortium

OVERALL IMPRESSIONS

- Team is well organized and focused on needs of BETO. The only question here: is it worth diluting efforts on the main product stream separations by spending effort now on waste treatment filtration recovery of carbon? However, when considering the environment, this approach is the right thing to do.
- The thermochemical efforts of the BioSep have presented several viable methods for purification of thermochemical process streams. Further, it is more focused than the biochemical effort. More specifics on which technologies hold the greatest promise, or alternatively, a rationale for why multiple processes are needed, would be helpful.
- Project is making good progress but needs a link to valorizable outcomes, which at this time look challenging.
- The removal of low-level contaminants from thermochemical processes is a highly sensible strategy to improving downstream operations. Progress is on track and some piloting work has been performed successfully. A more thorough discussion is needed to ascertain the scalability and commercial acceptability of the technology.
- Really great, thorough, and clear presentation with lots of details on the approach of the R&D. Very clearly explained. Well-organized project management plan and clear understanding of risks. Critical success factors were well defined and the description on commercial relevance and viability was well understood by the research performers. Focusing on catalyst preservation, feed cleaning, and carbon valorization are the three challenges that seem appropriate.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their insightful and useful comments. The comments for the three thermochemical separation projects that address contaminant removal from biomass-derived process streams (cleaning and conditioning biomass fast pyrolysis vapors through CHGF and removing bio-oil contaminants via selective sorbents prior to hydrotreating or valorizing carbon from aqueous waste streams via selective membrane separation) were insightful and focused on three areas, including more closely tying each project to a valorizable outcome, assessing process scalability and commercial potential, and developing defined progress measures for the sorbent and membrane projects. The CHGF project currently is focused on producing enhanced vapors for downstream upgrading to fuels and chemicals. Future work will focus as well on vapor phase separation of valuable monomers (cresols). Bio-oil cleaning valorization will produce clean feed for hydrotreating to biogenic fuels with demonstrated improvement in catalyst lifetime. Aqueous stream valorization comprises capturing and concentrating acetic acid and ammonia from biomass waste streams. Waste handling from each approach was also identified as a potential significant cost component that is/will be included in each TEA. The IAB review of scalability was suggested and this will be included in the next BioSep meeting with the IAB. The process for downselecting projects is discussed in the overview presentation summary and will be used for the thermochemical separations projects.

BIOPROCESSING SEPARATIONS CONSORTIUM – ANALYSIS

Bioprocessing Separations Consortium

PROJECT DESCRIPTION

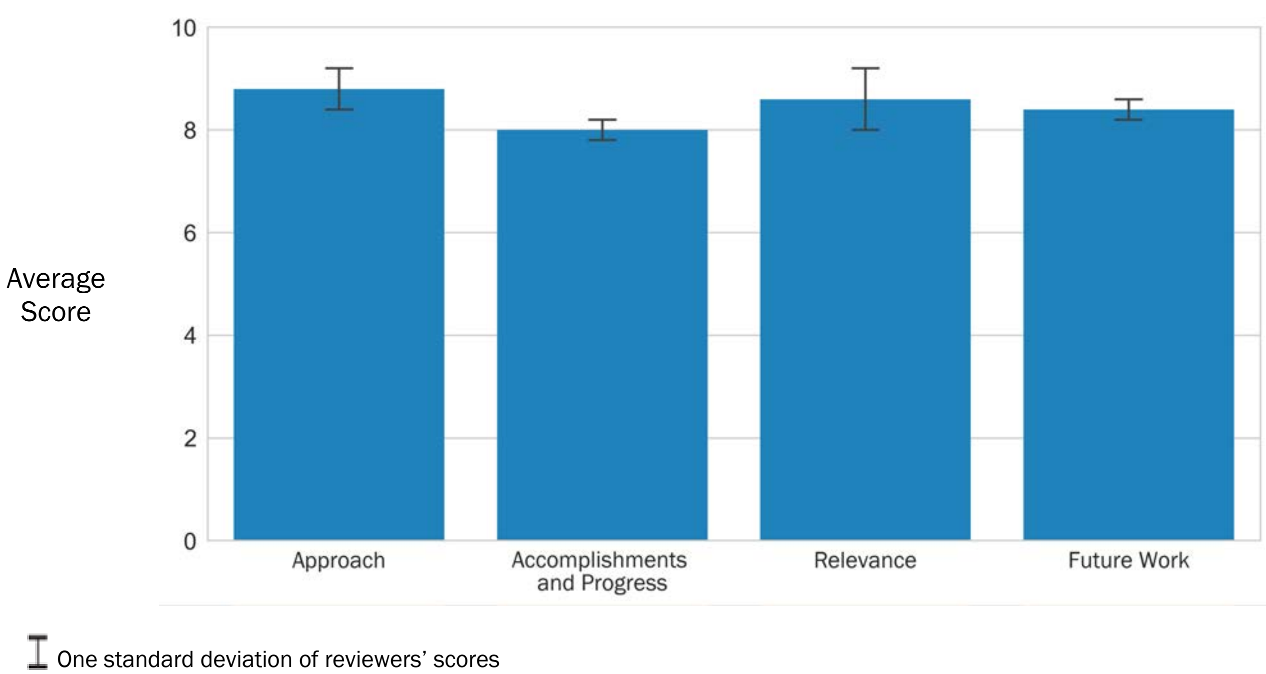
WBS:	2.5.5.501d
CID:	NL0031310d
Principal Investigator:	Dr. Mary Biddy
Period of Performance:	5/1/2016–9/30/2019
Total DOE Funding:	$1,190,000
DOE Funding FY16:	$500,000
DOE Funding FY17:	$400,000
DOE Funding FY18:	$175,000
DOE Funding FY19:	$115,000
Project Status:	Ongoing

Research in the BETO-supported BioSep is leading to new separation strategies designed specifically to address the challenges and scales of biorefinery technologies. This collaborative project integrates eight national laboratories, bringing a broad range of separation techniques to address biorefinery needs, including reducing impurities in intermediates that impede downstream biological and chemical catalysts to the recovery and conversion of dilute carbon. All strategies are developed by targeting high-efficiency processes that are both economically viable and sustainable.

The goal of the integrated analysis project in BioSep is to provide an analysis-based foundation to support and guide the research strategies being pursued. The collaborative team from NREL, PNNL, and ANL are developing TEAs and LCAs for each of the strategies being pursued under the integrated consortium. The analysis project works closely with the research teams to develop process designs for each strategy and supports each team by outlining cost and sustainability drivers, as well as key metrics that must be achieved for process scale-up that are critical to the ultimate success of the integrated consortium. One of the biggest challenges the analysis team faces is that the novel technologies being developed are significantly different from the off-the-shelf designs common in industry such that information on capital costs and scale-up performance are often limited. To overcome this challenge, the

Weighted Project Score: 8.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



analysis team works closely with the IAB to review the analysis approach and to vet the results of the designs, economics, and sustainability assessments.

The overview of this project will provide examples of how TEA and LCA have been integrated to support the R&D of novel separations technologies in the consortium and how these analyses inform research directions and highlight key strategies to enable the production of bioderived fuels and chemicals. Future work plans for this analysis project, including publications, will also be outlined.

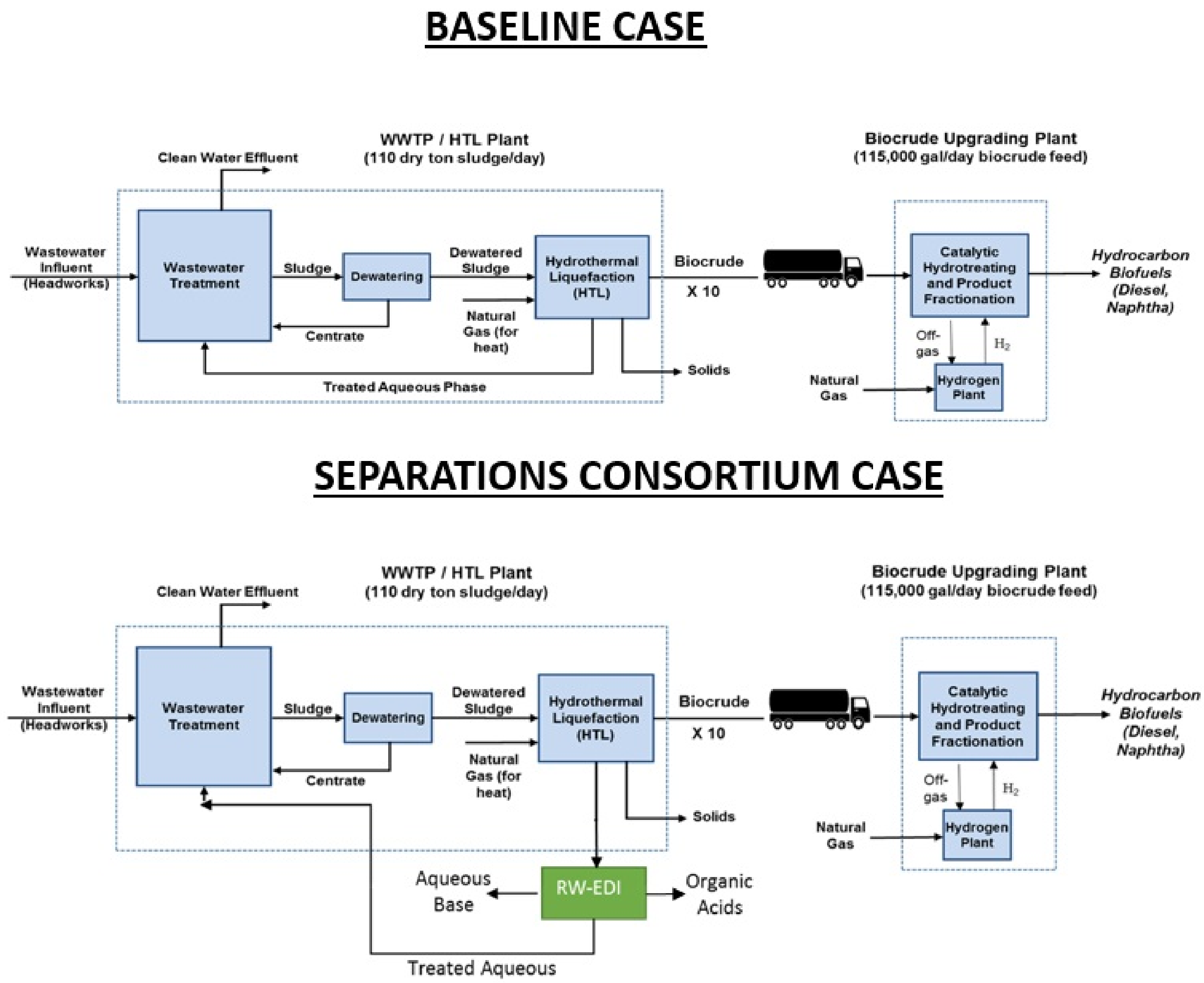


Photo courtesy of Bioprocessing Separations Consortium

OVERALL IMPRESSIONS

- This team provided excellent work results. This type of analysis in industry is routine and often starts early in large projects. The value of such analysis work at early-, middle-, and late-stage projects is critical to BETO programs. These analyses increase dramatically the speed of development, providing information on where to focus future efforts to drive down cost or where to stop working when further refinement is not impactful. The only question is, can BETO provide some level of techno-economics to even smaller start projects to make sure that the original strategy has the ability to succeed? The only other comment is that funding for plant capital for new technologies typically, from my experience, is not a 20-year payout but more like 10 years, thus only true for the n^{th} plant. Also, I've never known a plant to come in on original capital cost estimates. Some confidence on calculation information (i.e., ± x%) would be helpful as well for reviewers.

- This part of BioSep is *the* most important.
- The analysis team provides a critical service function to the entire BETO effort. Although this presentation focuses on separations, the broader contributions to the BETO program and the researchers is also vital to the success of the research in an industrial context. Better understanding of actual industrial benchmarks and the viability of different separation techniques at scale will be important as this effort proceeds.
- This project makes the case for baselines, design cases, and meaningful TEAs and LCAs to focus separations projects on high-value strategies as a critical steering tool across BioSep.
- This work is highly relevant to inform how the program/technology area is meeting the objectives of BETO, as cited in the *Multi-Year Plan*. The project performer considered applications of the expected outputs, which are informed by an IAB. The project performer presented the relevancy of this project and how successful completion would advance the state of technology and could have a significant positive impact on the viability of commercial biorefinery applications.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Reviewer comments on the overview of the consortium were very helpful and focused on three main points. First, reviewers suggested additional members be added to the IAB such that the board covered more ground with expertise in separations materials, petroleum refining, and existing separations technologies. The consortium will seek to enhance the expertise on its board through addition of members with these areas of expertise. The second set of suggestions centered around the importance of crosscutting analysis towards a defensible evaluation of reducing the contribution of separations costs below 50%, which is the case for some pathways based on literature sources, including by the PI.[1] The final group of comments regarded how the consortium selects projects. BioSep selects projects based on identification of separations in industry based on input from industry and BETO's existing research into bioprocessing. Input from industry is obtained through mechanisms such as listening days, special sessions at conferences, and the directed funding opportunity. Subsequently, we evaluate whether the consortium has the expertise and capabilities to address the challenge. We then leverage existing analyses or evaluate anew the possibility of the project to reduce overall bioprocessing separations costs. If these factors are favorable, the project is a strong candidate for inclusion in the consortium.

[1] Biddy, Mary J., Ryan Davis, David Humbird, Ling Tao, Nancy Dowe, Michael T. Guarnieri, Jeffrey G. Linger, et al. 2016. "The Techno-Economic Basis for Coproduct Manufacturing to Enable Hydrocarbon Fuel Production from Lignocellulosic Biomass." *ACS Sustainable Chemistry & Engineering* 4(6): 3196–3211. http://doi.org/10.1021/acssuschemeng.6b00243.

BIOPROCESSING SEPARATIONS CONSORTIUM – OVERVIEW OF CRADAS

Bioprocessing Separations Consortium

PROJECT DESCRIPTION

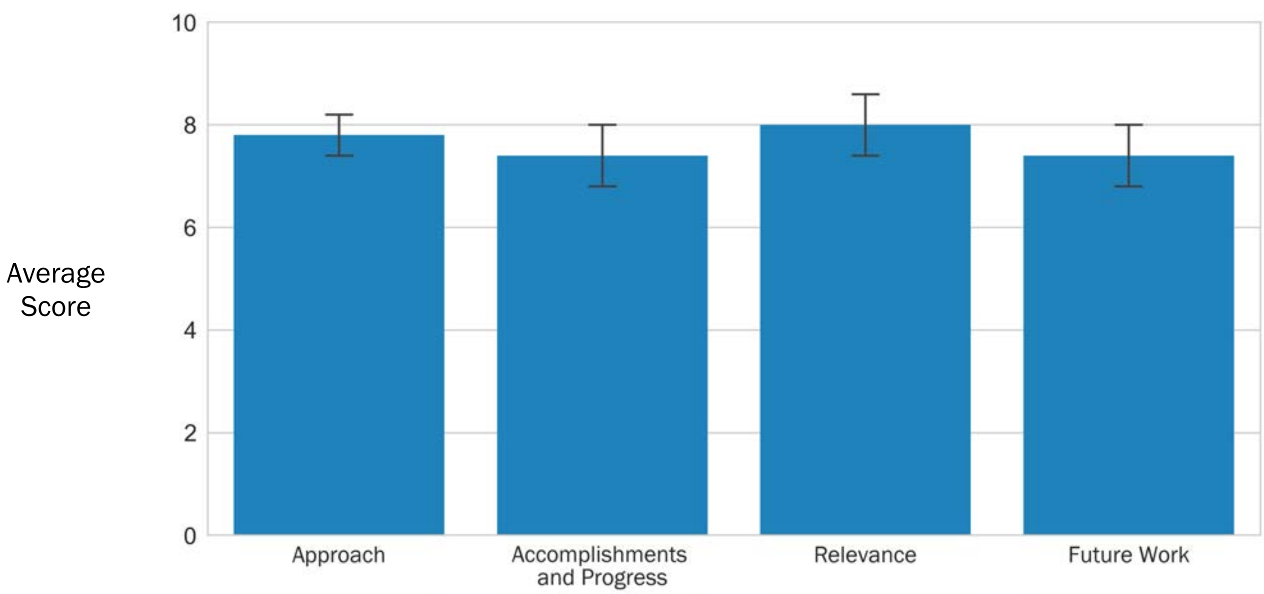
WBS:	2.5.5.501e
CID:	NL0031310e
Principal Investigator:	Dr. Todd Pray
Period of Performance:	10/1/2018–9/30/2019
Total DOE Funding:	$1,000,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$1,000,000
Project Status:	Ongoing

A key component of the BioSep is to engage with industry for both stakeholder input and to develop collaborative projects. To achieve the second aim, the consortium team solicited project proposals in an open call. One million dollars in funding was made available by BETO to be spent at the labs in support of industry collaborations.

Potential industry participants teamed up with different national lab partners from BioSep. Ultimately, five collaborative projects were selected to be awarded after review by external subject-matter experts. Proposals were scored based on the following criteria: Challenges Addressed and Research Approach (30%); Impact of Proposed Research on the Biofuels and Bioproducts Industry (25%); Benefit to Bioprocessing Community (10%); Key Personnel, Resources, and Bioprocessing Separations Consortium Capabilities (20%); and Requested Budget, Milestones, and Appropriateness of Government Funding (15%). The consortium's steering committee also provided input on the proposals related to topic area diversity, capability diversity, relationship to existing annual operating plan (AOP) work, national lab diversity, collaborative projects across national labs, and industry partner diversity.

Weighted Project Score: 7.7

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%

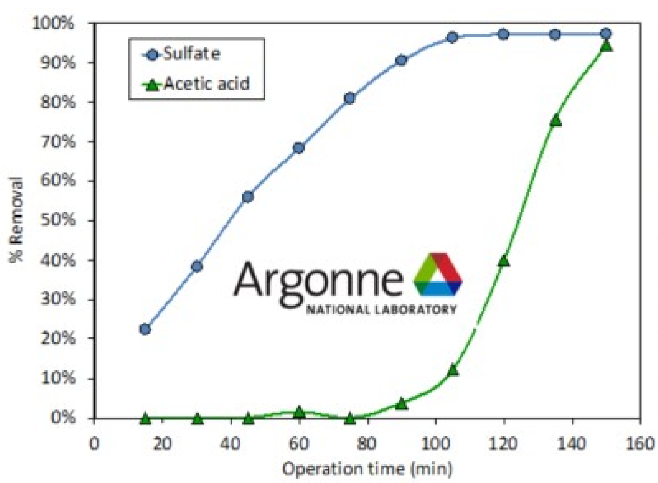


One standard deviation of reviewers' scores

The funds from these projects—$200,000 each—are being deployed at the national labs to utilize their unique capabilities. The industrial participants are providing in-kind cost share and expertise to help achieve project goals. The awarded projects are with the following organizations:

- DMC Biotechnologies is partnering with a team led by ANL along with LBNL. The goal is to maximize production of high-value terpenoids from microbial fermentations through an adsorptive product recovery process.
- HelioBioSys is partnering with a team led by LBNL along with Sandia National Laboratories [SNL] and NREL. The goal is to develop a cost-effective and efficient protocol for separation and purification of extracellular polysaccharides from marine cyanobacterial culture broth.
- Kalion is partnering with a team led by ORNL along with NREL and ANL. The goal is to develop novel, low-cost means of water removal in Kalion's glucarate glucaric acid purification process.
- Mango Materials is partnering with the team at LBNL. The goal is to dewater lysed cells produced from waste biogas and recover the biopolymer, polyhydroxyalkanoate, using industrial-relevant equipment to help the company reach commercial-scale production.
- Visolis is partnering with a team led by ANL along with LBNL. The goal is to determine the efficiency and viability of extracting their hydroxy acid product from fermentation broth while minimizing the ionic contaminants in the captured aqueous stream.

Each of the above projects will be contracted under a CRADA with the participating national labs. The consortium's steering committee and BETO will monitor progress toward milestones and provide input to help achieve project goals, as stated in the overall consortium.



Demonstration of sulfate – acetic acid separation using RW-EDI at ANL

Purification of carboxylic acids from mixed broth at ABPDU using wiped-film evaporation

Photo courtesy of Bioprocessing Separations Consortium

Note: RW-EDI = Resin Wafer–Electrodeionization

ABPDU = Advanced Biofuels and Bioproducts Process Development Unit

OVERALL IMPRESSIONS

- Program work results were excellent. My only question was that the project only has small-scale industry partners, albeit highly relevant to the biomass type project separation arena.
- Early-stage interactions with real-world ideas are good. The costs are relatively modest in relation to a diverse set of challenges.
- The concept of seed grants to increase industrial participation in BETO projects is useful and could serve as a model for other portions of the program. The funding levels seem low, and BETO would benefit from limiting the number of partners that could be involved on any single grant.
- The selected proposals represent a good diversity of topic areas, feedstocks, products, and separation technologies that are under development. The selection of earlier-stage companies and projects is high risk, but of significant mutual benefit to the innovation cycle because it provides an early process development opportunity that small companies cannot otherwise implement on their own.
- Amazing job putting together such a strong consortium and CRADAs with industry in some innovative areas with such little funding.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The consortium team appreciates the general overall positive feedback from the reviewers. The small companies that were awarded as part of this first cohort of industry partners will hopefully set the stage for larger partners as well in later years. During the selection process we focused on developing a diverse and robust set of partners, and the early-stage companies ended up submitting the most meritorious proposals.
- Moving forward, the BioSep team will work to expand the pool of applicants and potential funding for these CRADA projects. By expanding industry outreach efforts and demonstrating successful outcomes from the first cohort of projects, we expect to attract more and larger corporate partners with relevant technical challenges.
- An added approach to generating a larger and even more robust applicant pool, which the team will work with BETO to prioritize, will be to expand the capabilities and process and materials R&D approaches that the team develops as part of its core BETO pathway and product work. The team will also work with BETO to attempt to find additional resources to support more and larger CRADA projects.

MELT-STABLE ENGINEERED LIGNIN THERMOPLASTIC: A PRINTABLE RESIN

Oak Ridge National Laboratory

PROJECT DESCRIPTION

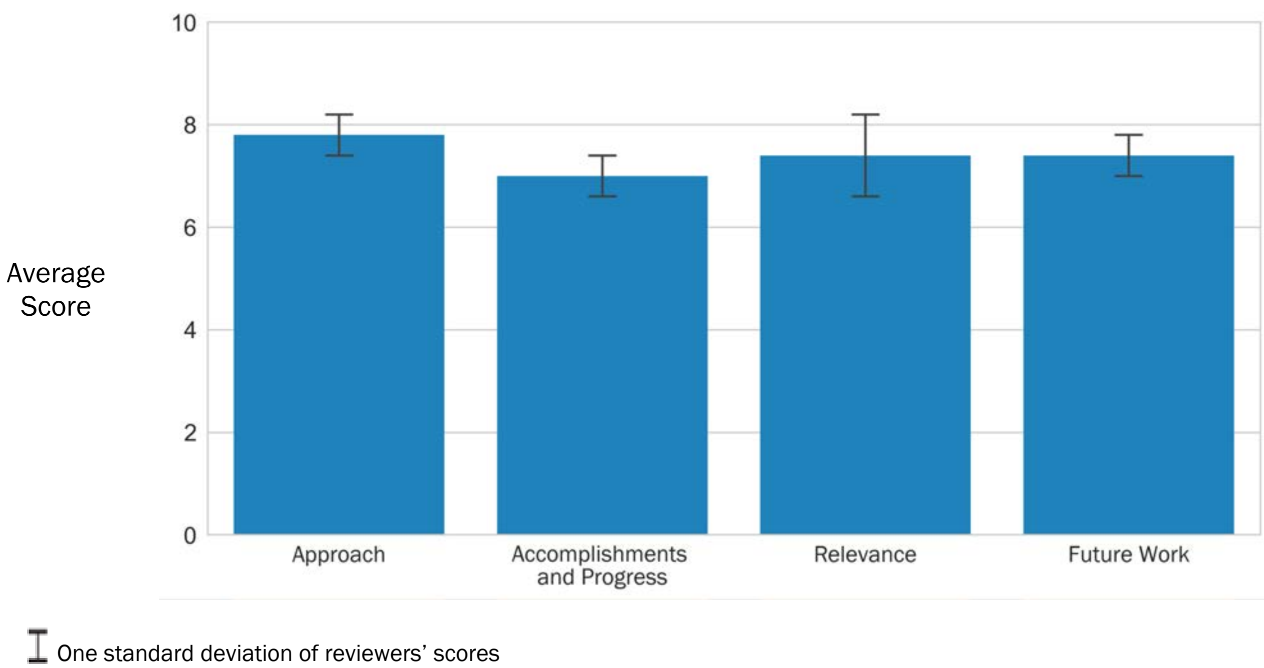
The proposed research develops a novel family of commercial-ready, lignin-based thermoplastic polymers and polymer composites suitable for high-volume applications, specifically those that are inherently recyclable, high-speed moldable, and 3D printable, with the capability to retain their exceedingly high mechanical properties after repeated thermal processing. The objective of this research is to produce and commercialize lignin-derived, industrial-grade polymers and composites with properties, including printability, exceeding current petroleum-derived alternatives. Technologies that enable high-value uses of lignin—a biorefinery waste stream—are important to enable the cost-competitive production of biofuels.

WBS:	2.5.6.103
CID:	NL0031314
Principal Investigator:	Dr. Amit Naskar
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$1,860,000
DOE Funding FY16:	$500,000
DOE Funding FY17:	$500,000
DOE Funding FY18:	$460,000
DOE Funding FY19:	$400,000
Project Status:	Ongoing

We are developing a green processing technology using various lignin fractions. A new fractionation method is introduced in this research to separate functionally graded lignin. High lignin contents in the polymeric products have been aimed at incentivizing biorefining process.

Weighted Project Score: 7.4

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



OVERALL IMPRESSIONS

- Outstanding project with great learnings and milestone. One suggestion would be to provide some initial stabilization of a small amount of sodium borohydride. I have seen polymeric materials with reactive end groups that can often be treated with low levels of sodium borohydride to stabilize them to color formation and degradation. Lignin-reactive parts are external and the most sensitive to heat and processing because most of the lignin is H-bonding internally to form structures, as discussed. This applies to other teams working on lignin. This may only cost on order of a few cents per pound for low-level pretreatment for initial stabilization if it has not already been tried.
- The project looks promising. What are the key/best target opportunities to hone in on?
- The PIs present an interesting project that is well based in science, but also has a clear target market and potential impact. The project would be greatly strengthened by a better description of the overall yields during lignin extraction, the assumptions underpinning the economics, and an indication of which polymers have the greatest opportunity.
- The use of lignin as a copolymer has significant merit and market potential, especially given that the investigators have demonstrated that advantaged properties can be accessed. The fact that several licensing deals have been closed speaks to significant product pull from industry. It will be important to receive input back from industry to continue to formulate copolymers with desirable properties, protect them (e.g., with patents), and get them into the hands of partners.
- This project is gaining a better understanding of the different lignin characteristics and their potential impacts on properties of lignin-based thermoplastics that can outperform commodity automotive-grade polymers and other petrochemical-derived plastics.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- This is a great suggestion! Sodium borohydride will be able to reduce the carbonyl chromophore, which was shown to be prone to induce photo yellowing and degradation. Although our product is already colored (originates from lignin's brown color), we can use it to enhance the stability of the product. We are glad that the reviewer recognizes the cost issue associated with this and a minimal dosage can be used. We will follow the recommendation.
- Although we find promise with several types of lignin-based polymers (printable plastics, thermoplastic elastomers, self-healing rubber, and adhesives), we may find immediate applications of lignin-based thermoplastic elastomers in automotive interiors. Organosolv lignin will not have an odor issue for such applications. We also recognize a penetration in the automotive market is difficult and currently we are reaching out to several industrial partners on that goal.
- In the future, we will present more details about yield. Our ongoing work not only focuses on yield increase, but also on the application of the extraction residue. We envision complete utilization of lignin. Functional fraction of lignin will deliver the toughest and strongest thermoplastic elastomer and self-healing rubber that will have higher value (≥$5,500/t). Non-fractionated lignin can go to printable plastics with polyamide or acrylonitrile butadiene styrene. Intermediate-value materials such as elastomers can be made from extract residues. Fibrous residues can be used in a common plastic matrix that are used for low-cost composite applications.
- This is a great suggestion! We are religious about intellectual property protection and feedback from licensees. Also looking forward to the long-term joint development program for targeted industrial products.
- Glad to see this comment. We are indeed targeting automotive-grade polymers. This suggestion itself answers one of the earlier comments.

BIODERIVED MATERIALS FOR LARGE-SCALE ADDITIVE MANUFACTURING

Oak Ridge National Laboratory

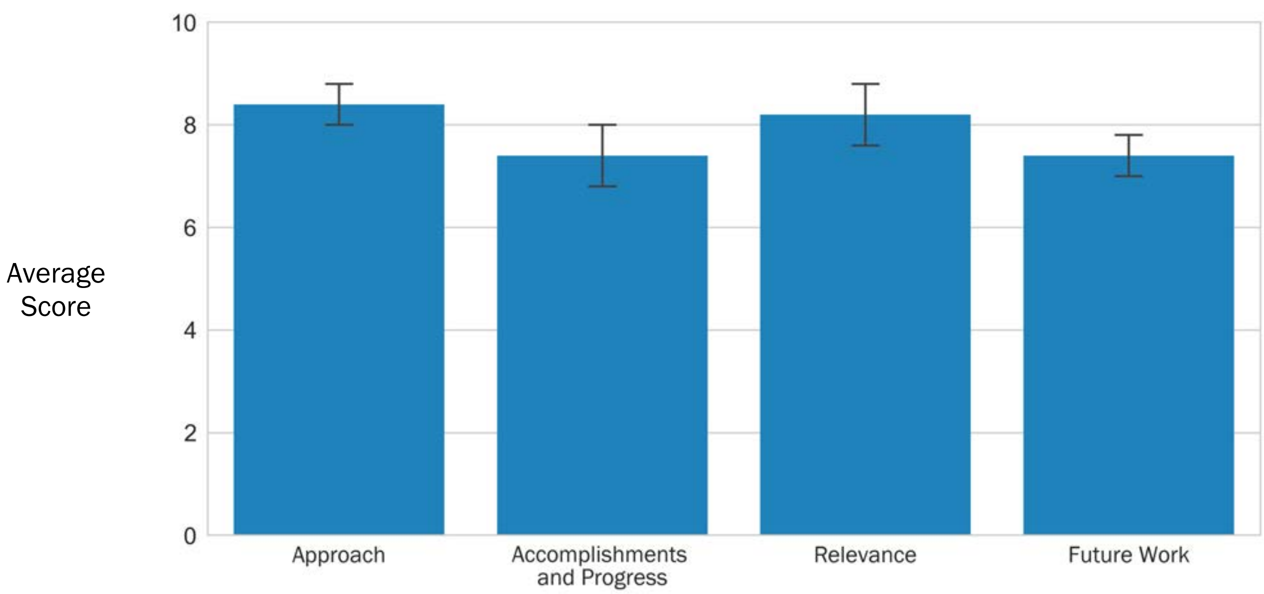
PROJECT DESCRIPTION

WBS:	2.5.6.105
CID:	NL0033558
Principal Investigator:	Dr. Erin Webb
Period of Performance:	10/1/2017–9/30/2020
Total DOE Funding:	$692,960
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$346,460
DOE Funding FY19:	$346,500
Project Status:	Ongoing

This project will improve economic viability of the biofuels industry by adding a new high-value revenue stream for biomass supply chains—bioderived composites for the rapidly expanding large-scale additive manufacturing industry (i.e., 3D printing). With recent innovations in printer technology and materials development, large-scale 3D printing has transitioned from a prototyping method to an advanced manufacturing technique. The market for 3D printing with polymers is growing rapidly. Among polymer 3D-printing approaches, large-scale additive manufacturing is 200 times faster than conventional desktop 3D-printing equipment and can reach deposition rates comparable to today's high-volume production methods such as injection molding. The most common material for large-scale 3D printing is a composite consisting of acrylonitrile butadiene styrene (ABS) plastic resin impregnated with roughly 20% carbon fiber (CF ABS). Carbon fibers provide the necessary overall strength and dimensional stability for the composite structure. Priced around $6.00/lb, CF ABS plastics for large-scale 3D printing are limited to high-value products that require the superior strength of carbon fiber.

Weighted Project Score: 7.8

Weighting for Ongoing Projects: Approach - 25%; Accomplishments and Progress - 25%; Relevance - 25%; Future Work - 25%



One standard deviation of reviewers' scores

A large untapped market exists for 3D printing with composites that are less expensive than CF ABS to enable expansion of the additive manufacturing industry. The current market price of carbon fiber is $15.00/lb. With current biomass prices in the range of $100.00–$250.00/dry ton, composites with biofiber reinforcement can meet this demand. In fall 2016, ORNL printed a pavilion and seating designed by Shop Architects of New York City for the prestigious Design Miami show using a composite of polylactic acid and bamboo particles. Bamboo has very desirable printability properties, but it poses some sustainability concerns as it is not domestically produced at scale. Growing bamboo in the United States is a challenge because most varieties are invasive species and others do not exhibit high yields in U.S. conditions. Rather, in this project we are using domestically sourced bioenergy feedstocks with a positive environmental footprint and rural economic development potential to create a flexible feedstock-to-product stream that optimizes the economic feasibility of both feedstock-to-fuel and feedstock-to-manufacturing pathways.

The central hypothesis of this project is that minimally processed biomass fibers can be used in large-scale additive manufacturing as a low-cost, sustainable alternative to carbon fiber reinforcement. Successful completion of this project will provide a new, high-value feedstock coproduct stream that reduces biofuel costs by sharing feedstock supply-chain resources, and thus costs, with bioenergy feedstocks. Much like conventional refineries can alter their product ratios based on current market prices, flexible biomass-processing strategies (milling and particle size separation) developed in this project will allow for optimum profit from biomass feedstocks.

In printing tests to date, we have produced poplar polylactic acid composites with a tensile strength of 75% CF ABS with superior printability. In future work we plan to test additional feedstocks (namely pine and switchgrass), optimize and scale up feedstock size reduction and fractionation operations for larger-scale printing tests, and match biocomposites with the best applications. Currently, we are targeting tooling—specifically molds—for manufacturing. Current estimates of the U.S. tooling market value are billions of dollars annually. While the cost of 3D printing is not feasible for mass production, it is ideally suited for producing molds that are notoriously expensive and time intensive to construct. 3D printing reduces production time of molds from years or months to weeks. Bioderived composites are well suited for tooling as they do not require the superior strength of carbon fiber and could reduce the costs of molds even further.

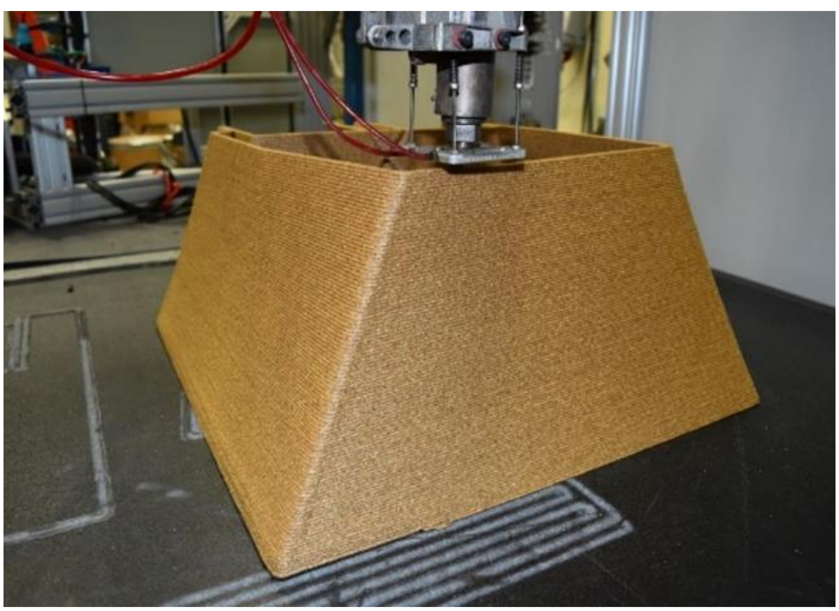


Photo courtesy of Oak Ridge National Laboratory

OVERALL IMPRESSIONS

- Excellent team effort to make value-added construction material for footprint reduction. Question: has the team tried to connect with companies like ICON who are looking at and claiming 3D-printed homes for $4,000.00 in 24 hours and working with charity organizations already? I am skeptical about the price of their printed homes currently, but this could fit with the larger DOE goal around the social aspect talked about as an overarching impact on the United States through providing homes for the homeless in cities with homeless population challenges. One concern to address is that the density of the material prepared was quite high versus standard lumber materials, as this cost per cubic foot could be a project killer when trying to compete in the market with other moldable materials from petroleum.

- It's not clear how this project is following a scientific approach. It was not clear who they are working with in the building material space to further develop products. Surface coatings would need to be added to the product, but it was not clear how this was included in the cost analysis. Specifically, how do we know the industry would use this material? Could this project have an IAB similar to other projects? It was not clear what the market size is of these desired end products. It was difficult to connect their research results back to the highest impact application areas.

- The PIs present an interesting, straightforward, and easily understandable project that has the potential to affect a number of markets by the 3D printing of formed materials made from biofibers and polylactic acid. Moving forward, a greater understanding of interfacial interactions and molecular-level investigation could further improve the properties—and thus the areas for application—of their products. A better connection between the potential and reality of eventual industrial use would be helpful.

- This is a very encouraging project. It would be timely to get investors involved.

- This project represents a low-intensity process for valorization of lignin, using minimally (mechanically) processed lignin as an additive for manufacturing. Polylactic acid-lignin mixed polymers have been demonstrated to have structurally useful properties, perhaps best suited for applications where the full strength of carbon fiber is not needed and lower cost is desirable, such as in the 3D printing of manufacturing molds. The work needs to focus on optimization of particle size, testing other feedstocks to improve yields, and matching biocomposites with other applications. This project is an excellent effort, especially for the relatively low amount of funds currently dedicated to it.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project team would like to thank the review panel for the encouraging and highly constructive feedback. The reviewers noted our trial-and-error discovery approach employed thus far in this project. We acknowledge that characterization of our approach in the first 18 months of the project was designed to answer two questions: (1) can biomass be a suitable replacement for petroleum-derived carbon fiber reinforcement in large-scale 3D printing, and (2) can this new biomass coproduct reduce biofuel feedstock costs? Now that we have proved both to be true, we are eager to delve into the science of how and why biomass works in this application. We appreciate the reviewer suggestions to explore the molecular interactions between polylactic acid and biomass fibers and to better understand how these interactions determine strength, dimensional stability, and printability. The reviewers also noted that this project would benefit from industry interaction to assess and develop “market pull” for large-scale, bioderived materials. We agree and are optimistic that our success thus far will be useful in capturing the interest of industry partners. Other observations by reviewers were that aligning the scale of biomaterial and biofuel supply chains and scale-up of the biomass processing for biomaterials could be a challenge. We agree with this assessment and are considering how to better address these questions in year three of this project.