CATALYTIC UPGRADING

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Catalytic Upgrading 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 March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 27 projects were reviewed in the Catalytic Upgrading session by six external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $53,638,660 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 6.2% 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 15–45 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 Catalytic Upgrading 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 Dr. Jeremy Leong as the Catalytic Upgrading Technology Area Review Lead, with contractor support from Mr. Trevor Smith (Allegheny Science & Technology). In this capacity, Dr. Leong was responsible for all aspects of review planning and implementation.

CATALYTIC UPGRADING OVERVIEW

The Conversion Research and Development (R&D) Program Area focuses on technologies and processes that break down biologically derived feedstocks and reassemble them into useful products. BETO's current strategy reflects an approach that more broadly enables a wide variety of potential processes by performing early-stage, applied R&D to overcome technology barriers. The associated processes and steps are grouped into the broader categories of deconstruction, fractionation, synthesis, and upgrading.

The Catalytic Upgrading session included projects focused on overcoming the various challenges and barriers associated with synthesis and upgrading. Specific challenges include improving catalyst lifetime, increasing yields from catalytic processes, and decreasing the time and cost to develop novel, industrially relevant catalysts. These projects address these challenges through a combination of specific, pathway-focused projects with industry, universities, and at individual national laboratories, as well as consortia that combine the unique capabilities of several national laboratories in collaboration with industry via technical advisory groups and joint projects.

The Catalytic Upgrading session covered projects addressing challenges related to the catalytic upgrading of intermediates from both high- and low-temperature processes. Core catalytic technology development projects include upgrading of lignin, carbohydrates, and other biologically derived intermediates (e.g., lignocellulosic ethanol), upgrading of synthesis gas and synthesis-gas-derived intermediates (e.g., C1/C2 oxygenated intermediates), and hydroprocessing and upgrading of catalytic fast pyrolysis (CFP) bio-oils and electrocatalytic and thermocatalytic carbon dioxide (CO_2) utilization. Enabling capabilities and cross-cutting projects included those related to analysis, modeling, characterization, and other guiding R&D.

The bulk of the session featured projects that are part of the Chemical Catalysis for Bioenergy Consortium (ChemCatBio). ChemCatBio is a national lab-led R&D consortium dedicated to identifying and overcoming catalysis challenges for the conversion of biomass and waste resources into fuels, chemicals, and materials.

The second-largest part of this session included projects with industry partnerships through directed funding awards (DFAs). DFA projects mirror the ChemCatBio but include industrial partners that were funded to specifically address their needs by utilizing world-class national laboratory capabilities which they could not otherwise access.

The final component of the session featured four competitive funding opportunity projects within the Conversion R&D portfolio that aim to enable the bioeconomy more broadly where their technology focus utilized catalytic upgrading processes.

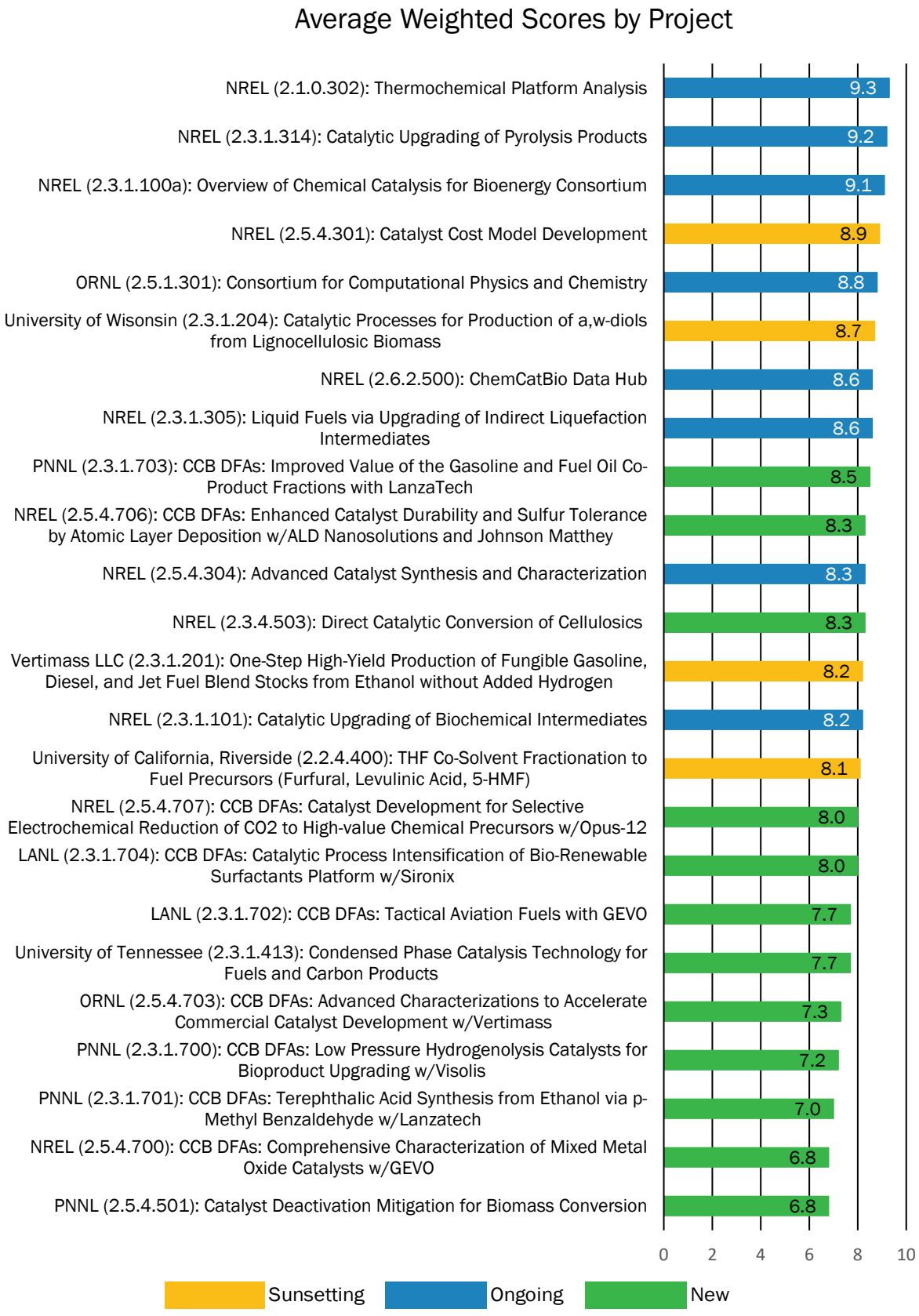
CATALYTIC UPGRADING REVIEW PANEL

The following external experts served as reviewers for the Catalytic Upgrading Technology Area during the 2019 Project Peer Review.

Name	Affiliation
Lorenz Bauer*	LJB Chemical Consulting
Cory Phillips	Phillips 66
Jesse Bond	Syracuse University
John Regalbuto	University of South Carolina
Viviane Schwartz	U.S. Department of Energy - Office of Science
Chris Bradley	U.S. Department of Energy - Office of Science

*Lead reviewer

TECHNOLOGY AREA SCORE RESULTS



CATALYTIC UPGRADING REVIEW PANEL SUMMARY REPORT

Prepared by the Catalytic Upgrading Review Panel

Our efforts in reviewing the catalytic upgrading portfolio and summarizing the outcomes of projects therein are dedicated to the memory of Dr. Lorenz (Larry) Bauer. His leadership, clear thinking, technical depth, and private-sector experience sharpened our focus, and working with him improved our understanding of the challenges facing commercial deployment of bioenergy technologies. Perhaps most importantly, his boundless enthusiasm for renewable energy was an inspiration to all. The words are ours, but the vision is Larry's.

The catalytic upgrading session summarized progress within the portion of the BETO research portfolio focused on enhancing the economic potential of catalytic technologies for converting biogenic carbon into fuels and chemicals. Projects in this portfolio include those within BETO's Annual Operating Plan (AOP), which are led by the national laboratories; those awarded to external investigators through competitive Funding Opportunity Announcements (FOAs); and those awarded through DFA programs, which partner private-sector ventures with national laboratories to accelerate commercial development.

Research within this portfolio has made a significant impact on bioenergy technologies by demonstrating clear reductions in minimum fuel selling price (MFSP), accelerating catalyst design cycles, delivering a new suite of bio-based fuels and chemicals, and advancing bioenergy R&D. Innovations herein are numerous and have resulted in novel material designs and catalyst formulations, both of which are serving to enhance selectivity and decrease costs associated with catalytic processing. Further, research efforts have generated scientific insights that will impact other programs in BETO. More broadly, these insights advance the field, which benefits academic and industrial stakeholders working in similar areas. Synergies are apparent throughout this portfolio. Research projects leverage national laboratory capabilities as well as those of external partners from academia and industry. Project teams are collaborating effectively to accelerate material and process design. These efforts combine to support the overarching focus of this program, which is to enable commercially viable production of bio-based fuels and chemicals. This central theme is appropriate to the goal of increasing the market share of renewable carbon, and the commercialization potential of projects within this portfolio is strong. For example, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates and Catalytic Upgrading of Pyrolysis Products are both rapidly approaching the 2022 BETO target of producing biofuels at $3/gasoline gallon equivalent (GGE). High-value coproducts in particular have the best near-term commercial potential, and they are emerging as enabling technologies to facilitate cost-effective biofuels.

IMPACT

From a technical perspective, impacts within the catalytic upgrading portfolio arise from accelerating catalyst design cycles and enhancing commercial potential for bio-based fuels and chemicals. These are evidenced by new catalysts with improved activity, stability, and cost; continuous reductions in MFSP for core technologies; and demonstration of new pathways to high-value coproducts to enable near-term commercialization. From a general perspective, this unique, well-executed portfolio is impactful in that it provides a model architecture for cross-cutting, consortium-based research. In many respects, the catalytic upgrading program defines best practices in facilitating commercial deployment of integrated biorefineries. Specifically, this portfolio includes programs in techno-economic analysis (TEA), advanced catalyst synthesis and characterization (ACSC), and computational physics and chemistry, all of which enable the comprehensive set of individual, technology-oriented core research projects.

Advancing the Industrial State of Technology

Current research efforts are responsive to guidance from an external industrial advisory board. This has ensured that all projects prioritize work-breakdown structure and take active steps toward addressing existing hurdles to industrial deployment. By doing so, research within this portfolio is advancing the industrial state of technology. Projects have accelerated the catalyst design cycle by identifying material properties that

positively impact reactor performance and reduce operating costs. Advances have driven MFSP estimates close to 2022 BETO targets primarily by focusing research on mitigating cost drivers and expanding the suite of accessible coproducts within an integrated biorefinery.

Two clear examples of improved MFSP estimates are the projects Catalytic Upgrading of Pyrolysis Products and Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates. Both have identified novel catalyst formulations relative to benchmark materials. Their new materials improve stability, enhance selectivity, reduce cost, and/or deliver high-value coproducts, thereby bringing MFSP estimates in line with targets of roughly $3/GGE.

Another outstanding example of advances in the state of technology is the Catalytic Upgrading of Biochemical Intermediates (CUBI) project, which continues to push the boundaries in synthesis and applications for bio-based platform molecules, such as furfural, 2,3-butanediol (2,3-BDO), and hydroxymethylfurfural (HMF), which are all produced by selective fractionation of biomass. The CUBI program has also highlighted the importance of lignin valorization in achieving cost targets. In doing so, the CUBI project is responding to guidance from past program reviews—specifically, that BETO should focus on technologies that fractionate biomass to maximally leverage each component instead of relying only on thermochemical front-end technologies for single-stage deconstruction of whole biomass.

It is also worth highlighting DFA projects in this discussion. They provide commercial ventures access to the powerful tools and domain expertise available within BETO. In this way, they directly impact the current state of industry, and they advance technologies along the development pipeline. This is a nice synergy because nascent ventures lack in-house access to the suite of analytical tools accessible to a national laboratory. Further, startups may be unable to dedicate resources, personnel, and time to elucidating the scientific insights necessary to accelerate catalyst and reactor design. At the same time, industrial partners provide crucial access to industrial catalyst formulations and commercial structures (e.g., extrudates and engineered materials), as well as data generated in pilot and/or demonstration-scale facilities.

DFA projects leverage strengths from all partners in moving technologies toward commercial deployment, and they represent one of the clearest demonstrations of how research within BETO is helping to advance the industrial state of the art. A good example of such a partnership is the project Enhanced Catalyst Durability and Sulfur Tolerance by Atomic Layer Deposition (ALD). Catalyst instability is a grand challenge in biomass upgrading, particularly in liquid media. Issues like metal leaching, sulfur tolerance, and particle sintering remain largely unresolved, and they continue to hinder the economic viability of catalytic upgrading process technologies. This project is a collaboration between the National Renewable Energy Laboratory (NREL) and commercial catalyst manufacturers ALD NanoSolutions and Johnson Matthey, and it has allowed the team to rapidly deploy ALD to design a more robust, sulfur-tolerant catalyst for selective hydrogenation of muconic acid. The resultant platform is versatile, and it can be easily adapted for broad applications in biomass processing.

In another example, the Improved Value of the Gasoline and Fuel Oil Coproduct Fractions with LanzaTech project highlights the productive and rewarding partnership between Pacific Northwest National Laboratory (PNNL) and LanzaTech. This collaboration has been successful in generating technologically viable bio-based aviation fuels, ultimately delivering a demonstration flight with Virgin Atlantic. Presently, they are focused on producing higher-value fractions, namely high-octane gasoline additives and lubricants, from ethanol. This will enhance their economic potential and move the field closer toward practical, bio-based aviation fuels.

Focus in Light of Private-Sector Investments

In terms of technology readiness level (TRL), research in this portfolio ranges from early to middle levels. At the lower end, projects include bench-scale research to explore novel catalysts and upgrading technologies. At the higher end, projects aim to reduce MFSP estimates by improving catalyst stability, decreasing noble metal loadings, and optimizing coproduct synthesis. As a whole, BETO projects are moving successful proof-of-

concept demonstrations down the development pipeline, and they are aiding industrial partners in resolving hurdles to commercial deployment.

At lower TRLs, private-sector investments are unlikely to support the early-stage, basic research necessary to discover new materials, chemistries, and technologies, nor will the private sector support efforts to elucidate the fundamental origins of catalyst or reactor performance. These steps are crucial to accelerating the design of catalytic materials and catalytic processes, and BETO support at this TRL is accordingly justified. At higher TRLs, one finds mature projects, such as Catalytic Upgrading of Pyrolysis Products, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates, and CUBI. While their core technologies are capable of delivering a range of biofuels and/or biochemicals, they are as yet unable to generate profits alongside oil and natural gas. This makes it difficult to attract private-sector investment to transition these processes to pilot, demonstration, and/or commercial scales. Continued support from BETO is thus critical to ensuring continued development of technologies that have long-term promise but face a presently unfavorable investment climate.

Standout Projects

Several projects stand out for bringing their MFSP estimates in line with 2022 BETO targets. Catalytic Upgrading of Pyrolysis Products has appropriately leveraged TEA to direct research toward reducing the primary cost drivers in pyrolysis-based fuels. For example, to decrease catalyst costs associated with pyrolysis oil upgrading, the project team designed an active, low-metal platinum (Pt)/titanium dioxide (TiO_2) catalyst. This was a major improvement to the first-generation materials synthesized at the outset of the project. To address the issue of a low selling price for commercially available, paraffin-rich fuels, the team optimized coproduction of higher-value aromatic oxygenates like phenol and catechol. These efforts have the potential to reduce MFSP to $2.50–$3/GGE, and the work has largely set the current state of technology for pyrolysis-based transportation fuels.

The Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates project leverages a robust liquefaction frontend for biomass deconstruction and offers a suite of downstream upgrading options that improve upon well-known catalytic chemistries (methanol synthesis, methanol to hydrocarbons, and alkene oligomerization). In this way, the project offers flexible fuel production from a range of biomass or waste feedstocks. The indirect liquefication (IDL) team has demonstrated a process development trajectory allowing for a near-continuous decrease in their MFSP estimates. While it may be difficult to commercialize an IDL-based biofuel facility in the near term due to oil and natural gas availability, this platform will almost certainly play a role in the long-term production of alkane fuels, and it remains a vital part of the catalytic upgrading portfolio.

The CUBI project plays a key role in advancing fractionation-based strategies to target production and upgrading of well-defined platform chemicals, such as furans or carboxylic acids, as opposed to the heterogeneous bio-oils sourced from pyrolysis and liquefaction. The CUBI project continues to enhance the commercial potential for bio-based platform chemicals, and the team has highlighted the importance of lignin valorization in achieving cost targets.

Some of the most important impacts of the catalytic upgrading portfolio come from the cross-cutting programs that enable other research projects. TEA is tightly integrated with laboratory research efforts across this portfolio. Formally, this is enabled by the Thermochemical Platform Analysis project. Throughout the biomass-processing community, their work has set an important, best-practice standard of using TEA to guide future research. The ability of TEA to identify primary cost drivers and its ubiquity in the catalytic upgrading program has been instrumental in expanding efforts in lignin valorization and production of high-value coproducts. These new directions have driven the rapid progress toward 2022 BETO dollar-per-GGE targets made by the Pyrolysis, IDL, and CUBI teams.

The Consortium for Computational Physics and Chemistry (CCPC) provides insights about fundamental physical and/or chemical phenomena that underlie the inherent performance of catalytic materials as well as the physicochemical dynamics of catalytic reaction engineering. The CCPC is a mature and well-coordinated

team that has made tangible and impactful contributions within the catalytic upgrading group and across the BETO portfolio. It should serve as a model structure for future consortia launches and subsequent development. The ACSC team provides the synthesis capabilities necessary to deliver well-defined, active, and stable materials, as well as the characterization tools and expertise necessary to understand how catalyst structures evolve under working conditions. These consortia are effective at reducing redundancies across BETO. At the same time, they ensure that adequate technical depth exists to support core technology projects while also generating significant scientific impact. All technology-focused projects effectively leverage these programs. This is a powerful, cross-cutting approach to the complex and multidisciplinary research necessary to advance commercialization of biofuels and biochemicals.

In addition to the projects cited above, the Catalyst Cost Model Development project and the ChemCatBio Data Hub are noteworthy for their far-reaching impact, both internal to and outside of BETO. The former is a robust tool that facilitates estimation of commercial catalyst cost to inform TEA. This tool is therefore able to guide early-stage catalyst design toward utilization of lower-cost and earth-abundant materials as well as less-complex synthesis methods. The developers have demonstrated that this tool is secure, accessible, and sufficiently robust to allow new users to generate realistic cost estimates. Further, they provide tutorials and case studies, and they have undertaken a broad outreach effort within the catalysis community through webinars and workshops at the American Chemical Society (ACS) and American Institute of Chemical Engineers (AIChE) national meetings. These efforts have yielded a quantifiable increase in this tool's use over the past year.

The ChemCatBio Data Hub is a relatively new project, but it shows incredible potential, especially in light of recent and pending advances in data science, machine learning, and artificial intelligence. The Data Hub will serve as a centralized repository for sharing characterization and performance data about materials designed, developed, and tested within BETO consortia. Further, the team aims to develop a catalyst design engine, which will allow users to leverage computational tools to explore the material design space for targeted reactions. Although an early-stage project, the Data Hub is headed in the right direction. In the short term, it will facilitate data sharing as a means to eliminate redundancies across the consortium. It will also allow machine-learning algorithms to leverage a massive set of data in order to improve predictive capabilities in material design. In addition to providing useful support within BETO, these projects will have far-reaching impact as they are intended for distribution to a broad audience, and they should see widespread adoption in the catalysis community.

INNOVATION

Innovations within this portfolio take many forms. We highlight projects that have resulted in new catalytic materials, new high-value fuel or chemical targets, or new fundamental insights into catalyst and reactor performance.

FOA projects are a clear source of innovation. They focus on lower TRLs and technologies that are as yet unproven; thus, BETO support is pushing the boundaries of known strategies for the production of bio-based fuels and chemicals. A good example is the project Catalytic Processes for Production of α,ω-diols from Lignocellulosic Biomass. 1,6-Hexanediol and 1,5-pentanediol are high value, have good market potential as polymer precursors, and are expensive to source in a petrochemical facility. These factors combine to make them attractive for near-term commercial development. Another example is the Tetrahydrofuran (THF) Co-Solvent Fractionation to Fuel Precursors (Furfural, Levulinic Acid, 5-HMF) project, which has delivered a novel approach to the long-standing challenge of biomass fractionation and upgrading. This technology achieves impressively high yields of C5 and C6 sugar dehydration products in an intensified process.

Projects supported through BETO's AOP continue to innovate, primarily through catalyst design and enabling production of high-value coproducts. For example, the Catalytic Upgrading of Pyrolysis Products team has developed a Pt/TiO_2 catalyst that offers improved activity and reduced cost. This effort toward a traditional, thermochemical approach to fuel production is balanced by efforts within the CUBI program, which is

advancing a route toward production of bio-based butadiene that leverages a hybrid biochemical and catalytic technology. In addition, several of the DFAs pursue new and exciting directions:

- Tactical Aviation Fuels with Gevo employs photo-initiated dimerization to produce targeted cyclobutane derivatives that have improved energy density and are appropriate for use in aviation fuels
- Catalyst Development for Selective Electrochemical Reduction of CO_2 to High-Value Chemical Precursors with Opus 12 is designing catalysts to facilitate electrochemical conversion of CO_2 into chemical targets
- Catalytic Process Intensification of Bio-Renewable Surfactants Platform with Sironix is commercializing an entirely new class of furan-derived surfactants that offer a number of performance benefits relative to conventional surfactants.

Overall, the portfolio is well balanced. It includes relatively mature technologies, such as upgrading oils generated through pyrolysis and liquefaction, while also pursuing new directions aimed at the production of high-value coproducts to support near-term commercialization. While the span of projects within the catalytic upgrading program is appropriate, the commercial success of efforts therein depend heavily on two efforts that do not fall within the core of the catalytic upgrading portfolio: lignin valorization and separations. TEAs consistently indicate that lignin valorization is a crucial component of an economically feasible technology, and it will be necessary to incorporate higher-value applications for lignin across the catalytic upgrading portfolio. Analogously, separations contribute substantially to capital and operating expenses, and their efficacy impacts impurity carryover, catalyst lifetime, and product quality. There are clear synergies with lignin valorization and separations consortia within BETO, and efforts therein are vital to decreasing MFSP estimates for technologies in the catalytic upgrading portfolio. Project summaries in the 2019 panel review only hinted at the scope of work in these partner consortia, and their impacts were not clearly quantified in TEA. We encourage continuing and strengthening interactions between catalytic upgrading, lignin valorization, and separations programs and highlighting synergies more clearly during reporting. This is particularly important in the discussion of TEA for individual projects. This will ensure that catalysts are developed with realistic purity specifications in mind and that critical separation stages are detailed in TEA.

SYNERGIES

The portfolio has many synergies that are effectively leveraged to benefit all stakeholders. A clear example is the critical need for TEA in all projects, which has resulted in the Thermochemical Platform Analysis team providing TEA support across the portfolio and driving research in appropriate directions. Similarly, the capabilities of the ACSC team impact nearly every project. They have the tools and expertise necessary to prepare well-defined materials and to characterize their working state, which is essential to understanding how structure determines function. The ACSC team thus enables a rational and scientific approach to accelerating the catalyst design cycle. Expertise in catalyst synthesis within the portfolio additionally leads to creation of the Catalyst Cost Estimation Tool, which is a nice synergy between TEA and the ACSC.

In terms of deepening scientific understanding, the Consortium for Computational Physics and Chemistry explores physical and chemical phenomena that dictate the performance of catalysts and reactors at micro-, meso-, and macroscales. In doing so, they both advance the state of knowledge and provide the hierarchical modeling that is critical at all stages of the development pipeline. At the atomic scale, electronic structure calculations confer understanding of reaction mechanisms and how the structure of a catalyst determines its activity, stability, and selectivity. At the macroscale, computational fluid dynamics simulations help to capture mass- and heat-transfer impacts on reactor performance, which become increasingly important in industrial processes. Finally, the ChemCatBio Data Hub centralizes data generated across the consortium in a single, searchable repository. This is essential to avoiding redundancy and ensuring that measurements and experiments have maximum impact. Projects supported through FOAs and DFAs exploit synergies between national laboratories, academic institutions, and the private sector. A good example is the pair of Gevo-

affiliated projects that are pursuing different strategies to enhance the value proposition of cellulosic ethanol by offering new, high-value products (cyclobutane derivatives) and by upgrading low-value byproducts (fusel oil). These two projects benefit from Gevo's expertise in cellulosic ethanol production, while also leveraging expertise in catalyst and process design at the national laboratories.

There are strong synergies with groups elsewhere in BETO, such as those working in lignin valorization and those working in separations. Lignin valorization and efficient, effective separations are critical components of a commercially viable technology; thus, outcomes from these partner consortia will directly impact the MFSP estimate for catalytic upgrading technologies. The catalytic upgrading portfolio should continue to leverage these programs to the maximum extent possible. This will generate process models that more accurately anticipate yields of lignin coproducts, feed compositions, impurity carryover, and product quality levels that are attainable at scale.

By partnering national laboratories with industry, DFA projects provide a unique opportunity for the catalytic upgrading program to access commercial catalysts and pilot facilities. BETO should seize these opportunities to research industrial catalysts and to enhance TEA models by incorporating data from industrial pilot or demonstration facilities. At the same time, industrial partners in DFA projects would clearly benefit from leveraging TEA capabilities in the Thermochemical Platform Analysis project as well as the modeling and simulations capabilities within the CCPC. DFA projects should additionally take advantage of the BETO industrial advisory board to help guide technology development.

A major strength of the catalytic upgrading portfolio is cross-cutting assets like the Advanced Catalyst Synthesis and Characterization, Thermochemical Platform Analysis, the Consortium for Computational Physics and Chemistry, the Catalyst Cost Estimation Tool, and the ChemCatBio Data Hub and its forthcoming Catalyst Design Engine. These programs are having significant impact within the catalytic upgrading portfolio and, more broadly, across BETO. They are further poised to have a longstanding impact on the field. It is important to maintain and support these initiatives such that they can continue to evolve and reflect both the state of the art and the needs of the field.

FOCUS

The focus on developing pathways that produce fungible transportation fuel components from biomass is appropriate. Although the portfolio supports a range of projects that consider diverse technologies, they share a goal of making integrated biorefineries commercially viable. Projects geared toward decreasing the MFSP estimate of biofuels toward the $3/GGE target align with the mandate to increase utilization of renewable carbon in the transportation sector. At the same time, the program also acknowledges the challenge in commercializing biofuels alongside inexpensive fossil carbon. The portfolio is smartly balanced by including technologies that pursue higher-margin commodities, such as select fuel additives or higher-value chemicals, which may be more commercially relevant in the near term. It is worth noting that this is responsive to recommendations raised in the 2017 BETO Peer Review of the Thermochemical Conversion program. Finally, this portfolio leverages experimental and computational research in material discovery. This is an appropriate focus considering the programmatic goal of accelerating the catalyst design cycle.

The majority of projects target hydrocarbon production, with fewer focusing on organic compounds functionalized by one or more heteroatoms (oxygen, nitrogen, etc.). Heteroatom-bearing chemicals are useful as fuel additives, solvents, chemical intermediates, and polymer precursors, which are all high value relative to alkanes. Further, they represent a class of chemical commodities where biomass may have a competitive advantage relative to oil or natural gas. Selective activation of alkanes to produce functionalized hydrocarbons is challenging, and it may be possible to leverage the inherent oxygen and/or nitrogen content of biomass for mild, selective production of functional intermediates. Although the markets for heteroatom-containing chemicals are small relative to transportation fuels, they may offer better near-term commercial potential, motivating additional focus in this area. As the consortium continues to leverage the synthesis capabilities within ACSC to accelerate the catalyst design cycle, it is important to address the transition from lab-scale

formulations (powdered catalysts, colloidal nanoparticles, etc.) to extrudates and pellets that are more characteristic of the commercially engineered materials used in industrial-scale reactors. Finally, the ChemCatBio Data Hub is poised for considerable impact. Additional emphasis should be placed on developing the Data Hub such that it is accessible to and can accept input from external users, such as other Energy Materials Network consortia or researchers in industry or academic institutions. A straightforward, computational Catalyst Design Engine would have a tremendous impact on the field, and additional efforts in this direction should be emphasized.

The 2017 BETO Peer Review raised concerns about continued reliance on pyrolysis to deconstruct whole biomass. This yields a low-grade crude that has, to date, struggled to find a commercially viable application. A major challenge with this approach is its reliance on hydrotreating, hydrodeoxygenation, and hydrogenation to stabilize low-grade bio-oils and promote oxygen removal. Because of their hydrogen demand, they remain too costly to deliver a commercially viable fuel. It is unclear whether continued research into catalyst and reactor designs for pyrolysis oil upgrading is improving the process sufficiently to enable commercialization; rather, it appears that the most dramatic improvements in MFSP estimates are coming from coproducts and lignin valorization. It may be possible that additional work in the area of catalyst and process design for pyrolysis oil upgrading will help to improve the state of technology, but the case should be clearly motivated by TEA.

It is critical that assessment and mitigation of catalyst deactivation comprise a central part of each research project that relies on catalytic chemistry. In general, each project currently appears cognizant of the need for this, and all appear well equipped to address catalyst stability in the course of their research. Although the standalone catalyst deactivation project could potentially serve as an enabling technology, it is unclear whether it will be able to provide the type of consortium-wide support envisioned at modest funding levels. Because catalyst deactivation is so complex and technology specific, it may be more appropriate to emphasize catalyst deactivation within individual research pathway projects rather than to outsource to a supporting consortium.

While exploratory work in catalyst design can have significant impact in terms of demonstrating the synthesis of a new material, having a rationale for new material selection is important to ensuring that catalyst design and synthesis efforts align with BETO's mission. For example, the ACSC is expanding its portfolio to include metal-organic frameworks (MOFs); however, it was not made clear which challenges MOF structures are intended to address, nor how this class of materials will uniquely enable commercial development.

TECHNOLOGY DEVELOPMENT PIPELINE

Projects span from early- to midscale TRLs, which seems appropriate to the organization's mandate. BETO's support for relatively early-stage research helps to transition projects away from bench scale and toward TRLs that generate intellectual property, leverage intellectual property through licensing agreements, and launch startups that accelerate commercial deployment. Although technologies at higher TRLs are relatively mature, BETO funding remains appropriate. Biofuel technologies based on liquefaction, pyrolysis, and syngas upgrading are established with respect to their technical art; however, they have struggled to gain a commercial foothold because of the large upfront capital investments required and the difficulty of competing in the low-margin transportation sector. There are clear ways that additional targeted research will benefit their economic potential. For example, the DFA project Terephthalic Acid Synthesis from Ethanol via *p*-Methyl Benzaldehyde provides LanzaTech with the capacity to convert a portion of their ethanol product to aromatic aldehydes. Although LanzaTech is an established venture, this targeted effort facilitates Guerbet condensation and shape selectivity to enable production of bio-based para-methyl benzaldehyde, which is a valuable coproduct. Success in this project will dramatically improve near-term economic potential. Further, by diverting a portion of their ethanol product to chemicals manufacture, this technology could help to mitigate the blend wall currently facing increased production of cellulosic ethanol. By funding research at these relatively mature TRLs, BETO occupies a critical niche in the technology development pipeline. Specifically, BETO supports projects that are too applied to be competitive in programs oriented toward basic science research (e.g., National Science Foundation or DOE's Basic Energy Science program). At the same time, these technologies have not yet achieved adequate economic potential to attract investment from the private sector. By supporting

mid-scale TRL projects, BETO is helping relatively mature processes to identify (through TEA) and resolve or mitigate the major cost drivers in their technology.

The integration of TEA throughout the ChemCatBio portfolio is clearly working to identify major cost drivers. There is pressure to meet dollar-per-GGE targets, and most technologies that are approaching these targets rely heavily on projected sales of high-value coproducts; however, details on higher-value coproducts were often sparse in project reports, particularly for those products sourced through lignin valorization. Based on summaries during the program review, it was not clear if robust markets exist for these coproducts, which may be problematic if a low MFSP estimate depends on producing these coproducts at scales commensurate with transportation fuels.

The panel accordingly raised the question of whether TEA estimates are sufficiently conservative, or if they reflect an overly optimistic forecast at the conceptual process design level. TEA is appropriate as a relative gauge of whether the economics of the process are improving, but it may not be representative of actual production costs incurred upon initial commercial-scale deployment. Although dollar-per-GGE estimates will look less attractive, it may be helpful to consider the economics of the standalone process (i.e., without coproducts) and to separately highlight the scale and impact of valorized coproducts. This would make clear the extent to which achieving dollar-per-GGE targets for a given process will depend on, for example, lignin valorization, which has been historically challenging. Along these lines, many technologies within the portfolio are bio-based analogs of mature industrial processes. For example, Liquid Fuels via Upgrading of Indirect Liquefaction Intermediates relies on syngas upgrading, and the economic potential of those technologies using methane or coal are well established. Similarly, the Improved Value of the Gasoline and Fuel Oil Coproduct Fractions with LanzaTech project appears to rely heavily on olefin oligomerization for the production of high-octane gasoline. These projects (and others within the portfolio that are relying on technologies with a clear fossil carbon analog) would benefit from a more thorough consideration of the history of these technologies, their MFSP estimates, and their commercial potential. This would be helpful in benchmarking the bio-based technology against fossil-upgrading processes to inform and de-risk commercial deployment.

Catalyst improvements have advanced two pathways—CFP and IDL—and are approaching MFSP estimates at or below $3/GGE, which stands as an example of helping to orient technologies toward successful adoption by industry.

RECOMMENDATIONS

The panel's most important recommendations that would strengthen the portfolio in the near to medium term include:

1. The Thermochemical Platform Analysis project is providing critical support across the catalytic upgrading portfolio. It should be formally considered as an enabling technology within ChemCatBio, similar to the ACSC and CCPC, and it should continue to be refined and expanded as necessary to support research across BETO.

2. The ChemCatBio Data Hub will play an important role in accelerating the catalyst design cycle, particularly as the role of data science continues to evolve. This effort should be further emphasized and expanded to support the development of more tools, such as the Catalyst Design Engine, and to accept data input from external users, as well as interface with other Energy Materials Network consortia or stakeholders from industry and academia.

3. BETO should increase focus on technologies that deliver higher-value products to benefit near-term commercialization. All high-value products are of interest, and TEA indicates that lignin valorization is particularly critical to achieving dollar-per-GGE targets.

CATALYTIC UPGRADING PROGRAMMATIC RESPONSE

INTRODUCTION/OVERVIEW

The Conversion R&D Program would like to take the opportunity to thank the six Catalytic Upgrading session reviewers for their time and careful review of the projects presented in this session. We recognize that this was a challenging review process where other presentations/sessions were difficult to attend due to scheduling and time constraints. BETO is committed to continuous improvement of the peer review such that all reviewers have opportunities to engage other areas within BETO to further their understanding related to specific areas they have been asked to review.

BETO appreciates the review panel's recognition of the successes of consortium-based research, acceleration of the catalyst design cycle, and tight integration of TEA throughout the portfolio. Additionally, the review panel recognized the program's continued efforts in addressing previous recommendations to focus on technologies that fractionate biomass to maximally leverage each component towards higher-value fuels and coproducts, as well as leveraging strengths from consortium and industrial partners in moving technologies towards commercialization. BETO intends to continue to support industry partners by leveraging national lab capabilities through the various consortium national laboratory-led projects, DFAs, and competitive funding opportunities.

The review panel specifically noted the appearance of fewer projects focusing on organic compounds functionalized by one or more heteroatoms (oxygen, nitrogen, etc.) as an area that could benefit from more emphasis within the portfolio. While the majority of projects reviewed within this session are focused on hydrocarbon production, the Performance Advantaged Bioproducts Consortium is in its second year of activities and has the stated mission of exploiting biomass properties for higher-value chemicals that could support near-term commercialization efforts. Similarly, the Advanced Development and Optimization Program has begun an early effort to address the transition from lab-scale catalyst formulations (powdered catalysts, colloidal nanoparticles, etc.) to extrudates and pellets that are commonly used at larger scales. Both of these areas were reviewed in different sessions of this peer review due to time constraints. These efforts will continue to be supported by BETO and results will be tightly integrated through TEA activities and guided R&D.

The review panel noted that continued R&D associated with "low-grade" pyrolysis oil upgrading and the reliance on hydrotreating, hydrodeoxygenation, and hydrogenation (and the associated high hydrogen demand) do not appear as impactful as coproduct and lignin valorization efforts (and associated separations impacts) on overall TEA outcomes. Specifically, they noted that it was unclear that continued research into catalyst and reactor designs for pyrolysis oil upgrading is improving the process sufficiently to enable commercialization. BETO is currently focused on higher-quality bio-oils and will continue to leverage TEA activities to target the most impactful areas for future R&D. For example, in pursuit of the larger goal of achieving a $3/GGE cost target by 2022, the Catalytic Fast Pyrolysis project will evaluate impacts of lower-cost feedstocks, extending catalyst time on stream, maximizing carbon yield to the oil phase, and capturing and purifying individual components from the light oxygenate stream to generate coproducts, as well as evaluating the potential to couple remaining light oxygenates to increase octane/cetane ratings of fuel blendstocks generated from hydrotreating of the CFP oil. While focus on future catalyst development has already been deemphasized within this project, critical tradeoffs remain between multiple variables within these complex systems, where iterative catalyst development may be required. BETO recognizes the limitations of pyrolysis oil upgrading but remains committed to the thermochemical pathways that can deliver high yields to both fuels and products.

The review panel noted the critical importance that assessment and mitigation of catalyst deactivation play within each individual project reliant on catalytic chemistries, and that each project appears well aware of these factors. The review panel questioned the ability of the standalone Catalyst Deactivation project to provide sufficient support to an entire portfolio at modest funding levels. BETO recognizes that all projects involving catalytic research must include deactivation and mitigation components that are tailored to the individual technologies and will continue to require milestones that target these areas. BETO's support of this new project was intended to develop a broader framework of tools and capabilities that could support new technology approaches that use similar catalyst systems, as well as produce more general publicly available tools and publications to assist researchers who work with biomass but do not use the catalyst systems currently funded by BETO. Initial focus for the project will be on a small suite of catalysts and pathways to determine if similar deactivation research can be applied to alternate approaches.

The review panel noted the potential impact of catalyst development efforts but questioned the specific challenges the ACSC intends to address with MOFs. BETO recognizes the lack of a clear pathway to overcome specific commercial challenges associated with MOFs at this time. While not emphasized in the review presentation, this specific activity was funded as a seed project and will be retired in FY 2020.

The following sections specifically address the three top recommendations from the review panel:

Recommendation 1: Expansion of the Thermochemical Platform Analysis project as an enabling technology within ChemCatBio.

The review panel recognizes BETO's commitment to using TEA to guide future R&D, but it was noted that the reliance on coproducts and associated details were not well presented and raised questions about assumptions related to markets, pricing, and impacts of required scale-up efforts. The panel suggests a more "level playing field," where a standalone process without coproducts is evaluated through TEA with separate assessments for scale and coproducts, especially where a technology approach is intended to compete with an analogous commercial process.

BETO agrees that better communication of TEA assumptions and results, specifically separate consideration of the relative impact of coproducts, would provide a more transparent assessment of a particular technology. For all new-starts, an initial TEA is already required to demonstrate proof of concept, compare various process assumptions (e.g., inclusion of coproducts vs. standalone), and assess near-term research objectives. Additionally, TEA activities are included as specific tasks/goals within every technology project. The Thermochemical Platform Analysis project is funded based on joint milestones within those projects and BETO will continue to support TEA activities in all phases of research within the portfolio. BETO will discuss and consider ways to "level the playing field" through more uniform presentation of TEA assumptions and coproduct integration for future peer reviews.

Recommendation 2: Expanded support of the ChemCatBio Data Hub.

BETO agrees that the ChemCatBio Data Hub project will play an important role in accelerating the catalyst design cycle, especially as data science continues to evolve. The Data Hub project is in its first year of activities and began with the expectation that efforts could expand with demonstrated results. The development of additional tools, such as the Catalyst Design Engine (that can leverage materials R&D data), represents excellent stretch goals for the near term and will be considered in future strategy development. BETO has also committed additional resources to more high-performance computing power in future fiscal years and anticipates that projects like the ChemCatBio Data Hub will greatly benefit from increased access to these resources.

Recommendation 3: Focus on higher-value products.

BETO appreciates this recommendation and recognizes the potential for higher-value products to overcome barriers to commercialization. The Biochemical Conversion technology area (including lignin valorization), Performance Advantaged Bioproducts, and Bioprocessing Separations Consortia have specific goals targeting

the identification and synthesis of high-value products, and these efforts are expected to continue. Each of these areas had separate peer-review sessions, and while some crosscutting efforts (Biochemical Platform Analysis project and CO_2 Utilization: Thermo- and Electro-Catalytic Routes to Fuels and Chemicals) were presented in the Catalytic Upgrading session, BETO will consider additional means to communicate those impacts at future reviews.

THERMOCHEMICAL PLATFORM ANALYSIS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

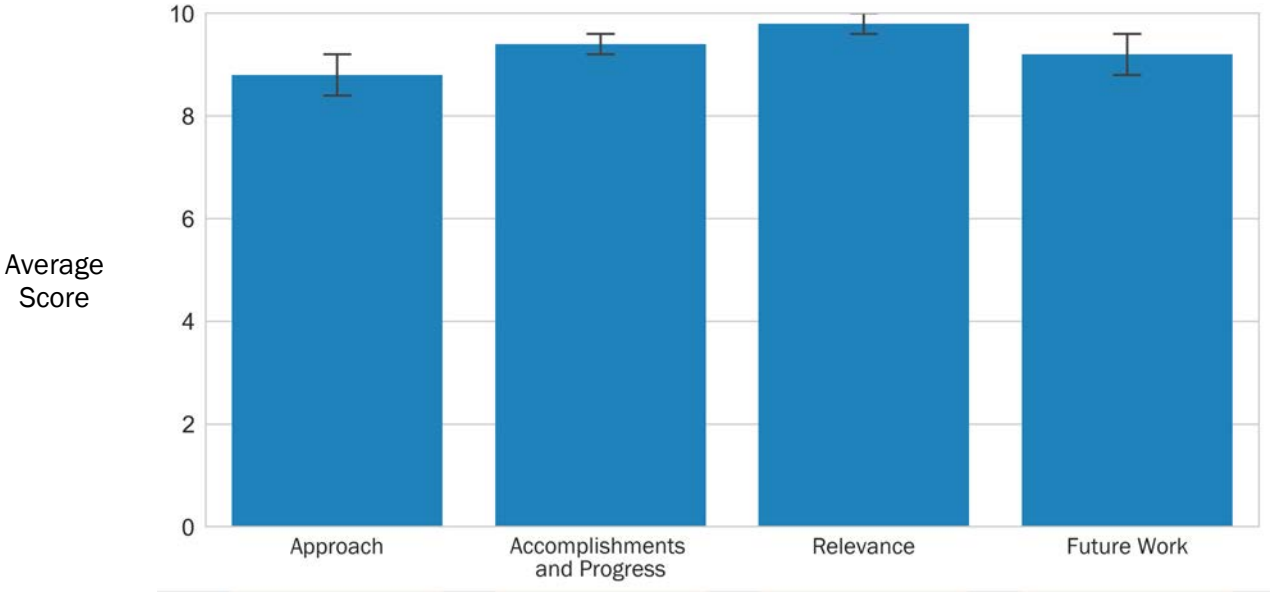
The objective of this project is to inform and guide R&D priorities for thermal and catalytic conversion processes by providing process design and TEA. This is achieved through close collaboration with researchers and external experts, along with the use of both commercially available modeling tools and the development or use of partner-developed and domain-specific tools and resources, such as refinery integration, kinetic and reactor models, phase equilibrium models, and pertinent bioproduct market studies.

WBS:	2.1.0.302
CID:	NL0008191
Principal Investigator:	Dr. Abhijit Dutta
Period of Performance:	10/1/2016–10/1/2019
Total DOE Funding:	$5,250,000
DOE Funding FY16:	$1,900,000
DOE Funding FY17:	$1,950,000
DOE Funding FY18:	$700,000
DOE Funding FY19:	$700,000
Project Status:	Ongoing

This project is directly aligned with BETO goals—this includes the reduction of projected conversion costs for biomass-derived fuels and products by enabling research advancements. TEA-guided research has helped achieve significant modeled cost reductions for the *ex situ* CFP pathway since the previous 2017 Peer Review and we have identified specific research steps to help reduce the modeled MFSP to less than $3/GGE by 2022. Further cost reduction through refinery integration, development of valuable coproducts, and other options are being identified for future research to help reduce the modeled MFSP to $2.50/GGE by 2030. Additional priorities anticipated in the future, such as the use of renewable electricity for liquid fuels and products, as well as emphasis on waste utilization, are also being explored in conjunction with research on catalytic utilization of syngas and other gases. Industry-relevant

Weighted Project Score: 9.3

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



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parameters are given deliberate attention as part of the work done under this project to help answer questions important for future commercialization.

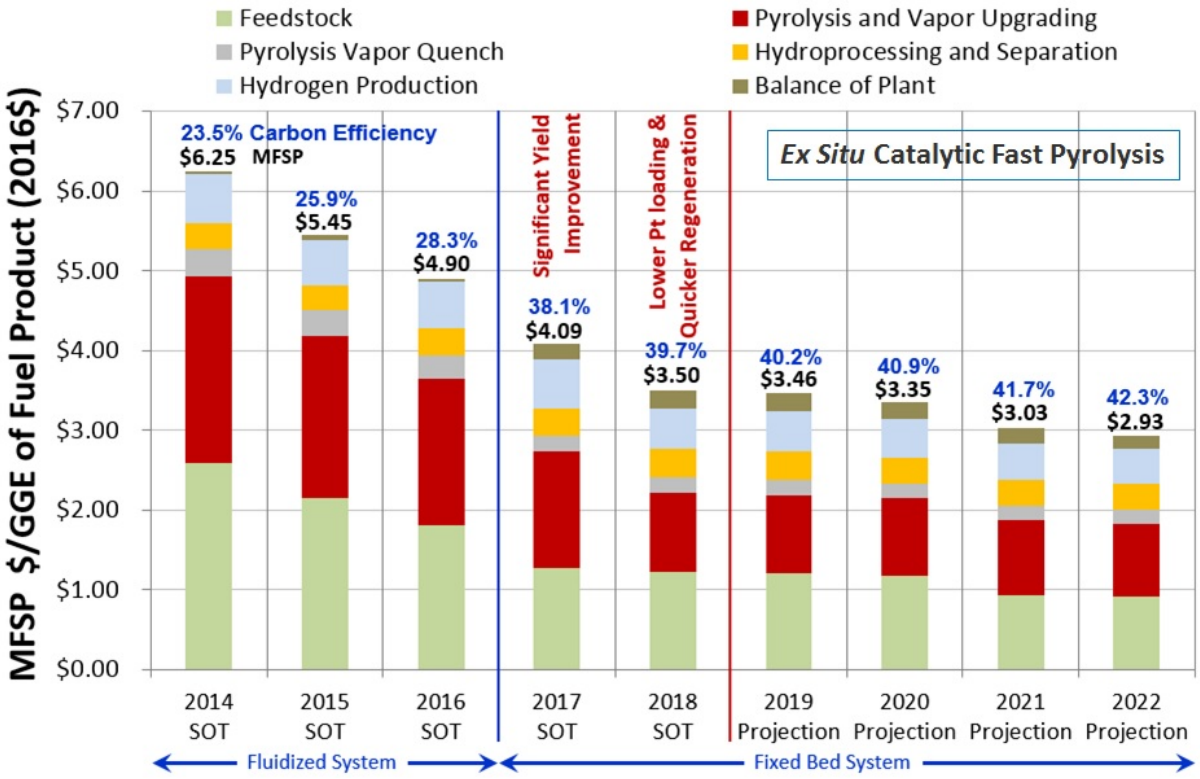


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- This is a very critical component to the activities of ChemCatBio as a whole. Milestones were met throughout the prior funding periods and the near- and long-term milestone planning seems appropriate.

- Overall, this is a very important enabling technology for emerging biomass-processing technologies. My only concern based on past exposure to TEA is that they are based on a large number of assumptions and often may invoke the most optimistic case rather than most likely cases. The team may want to consider that attainable yields, selectivities, and rates are probably uncertain and should forecast that impact (e.g., Monte Carlo-based TEA to consider uncertainty).

- Overall, this is a strong, well-managed project with solid deliverables thus far. The TEA work is probably the most impactful work to BETO because of its influence on R&D direction. It is extremely important to get this right. I would encourage the project team not to settle on the current tools and continue to explore ways of enhancing the modeling capability that allows multiple scales to be incorporated into the analysis. Please continue to harmonize this work with the Biochemical Platform Analysis project. The less-severe conditions and shape-selective catalyst pivot away from methanol-to-gasoline is small and the premise is still the same: small alcohol conversion over modified zeolites. This is a winning formula.

- The thermochemical conversion team has produced significant advances over the past two years and now appears to be on target to meet BETO cost and sustainability objectives. The new process scheme and catalysts have performed as predicted. The next steps would be to address operability issues that have plagued other efforts. A detailed feasibility study by an independent outside group would confirm these results. The project shows great synergy with other groups such as Idaho National Laboratory (INL),

Argonne National Laboratory (ANL), National Institute of Standards and Technology, and others. The outputs included technical metrics, life cycle assessment (LCA), MFSP, reports, and journal articles. The TEA shows a path for biomass to fuel of less than $2.50/GGE, however, it should be noted that this is a comparative number valid for comparing DOE projects. The initial costs of the fuel produced by early plants is likely to be significantly higher. The progress made by this project is impressive; the thermochemical conversion team addressed many of the comments from the 2017 Peer Review and has found new catalysts and other improvements that greatly improve the likelihood of success.

- The TEA and LCA specialty of this work has an application to all BETO processes. One wonders if the CCPC can subsume its modeling efforts on the sunset of the project. This superb work must be continued not only for the CFP platform, but across ChemCatBio projects.

- This is a central effort supporting the technical programs within the consortium. TEA has proved to be a powerful resource to guide research and is undoubtedly a key asset that should continue throughout the years. LCA provided by the collaboration with ANL is also a key portion of this effort and should continue, as it seems to work well. It is important that they keep up with the emerging technologies as described by their presentation. The feedback loop between this effort and the technical efforts are an important approach, and examples presented show the value of TEA providing alternative R&D pathways. CFP timeline and accomplishments presented are impressive examples of how well this effort interacts and is synergistic with the technical projects.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback.

- The projections for future research, presented in design reports, are based on researchers' and reviewers' feedback about attainable performance goals. We include sensitivity analysis to show the impacts of various parameters and the effects of overperformance and underperformance compared to the baseline analysis. The state-of-technology assessments are based on experimental data, but at smaller scales compared to the conceptual designs. We thank the reviewer for the comment and will continue to emphasize and expand on areas where we need to assess uncertainty (Monte Carlo analysis may be helpful at times but may not always help develop additional insights as compared to single-point sensitivities).

- We work with the CCPC, which does multiscale modeling. We will continue to pay attention to their work and include any tools that are useful for TEA into our work. An example of such a collaboration is the development of a one-dimensional entrained reactor model compatible with the TEA modeling framework. We will continue to harmonize with the Biochemical Platform Analysis project; please note that we use the same set of assumptions and modeling frameworks as the work done under that project, and our tools and methods have the same genesis.

- We appreciate the comments and agree with the reviewer about operability issues, which we plan to address through pilot-scale tests. Although higher costs and problems associated with pioneer plants are not explicitly mentioned, we are working closely with other groups, including the Feedstock-Conversion Interface Consortium, to understand and address those uncertainties.

- We will continue to work with the CCPC to find synergy between that work and the TEA modeling under this project.

- We will continue to address emerging technologies under the broad scope of the analysis of catalytic conversion under this project.

THF COSOLVENT FRACTIONATION TO FUEL PRECURSORS (FURFURAL, LEVULINIC ACID, 5-HMF)

University of California, Riverside

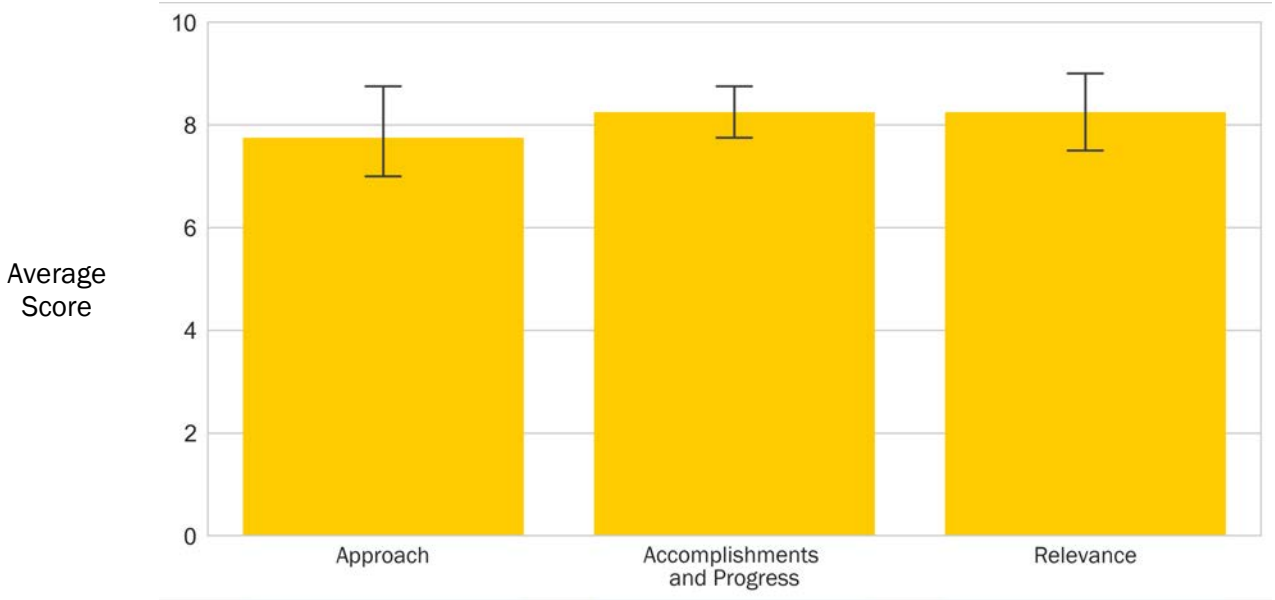
PROJECT DESCRIPTION

WBS:	2.2.4.400
CID:	EE0007006
Principal Investigator:	Dr. Charles Wyman
Period of Performance:	10/1/2015–9/30/2018
Total DOE Funding:	$1,060,000
Project Status:	Sunsetting

The goal of this research project is to advance transformative cosolvent-enhanced lignocellulosic fractionation (CELF) to first achieve high yields of fuel precursors (FPs) such as furfural (FF), 5-hydroxymethylfurfural (5-HMF), and levulinic acid (LA) from hardwood poplar biomass, and to further convert the FPs to fungible fuel blendstocks (methylated furans). Concurrently, we aim to capitalize on CELF's extremely high lignin extraction to produce aromatic platform chemicals to increase process revenues. TEA analysis will inform process design to reduce fuel costs.

Weighted Project Score: 8.1

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



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OVERALL IMPRESSIONS

- This project focused on developing a simple, intensified process for biomass deconstruction and upgrading into methylfuran and dimethylfuran, as well as converting lignin into high alkanes that might blend into jet fuel. Achieving <$2/GGE for conversion of biomass into fuels is impressive.

- This was a nice, tight project with well-defined objectives and division of labor. It appears that all but the fourth task was ably completed. The reviewer does not know, despite the fine success of the first three tasks, if the process met the goal of <$3/GGE.

- The THF cosolvent to fuel precursors was a hard project to review. On face value, it describes an integrated process to produce low-cost fuels. However, it is difficult to follow the TEA analysis, which is critical for evaluating the process. The MFSP was calculated to $1.50/GGE, which would exceed the BETO target. An independent evaluation by the DOE TEA team would provide a more systematic approach. Typically, solvent and chemical cost of multistep processes like the CELF process have been found to produce products with higher costs than other approaches. Organic solvent extraction processes have been shown to work technically but have not been commercialized due to the complexity and requirements of multiple conversion and recovery steps. The products obtained, particular LA, may themselves have value as products, if the costs are lower than the current approaches. The PI reported commercial interest by at least four companies. If this is confirmed, the project can be viewed as a success.

- The project is divided in four sequential tasks that are clearly complementary, and the group has made significant progress with their process. In general, it is well outlined; however, the presentation could have benefited from a greater focus on addressing the use of THF as the solvent in the process while also providing more details regarding the economic analyses.

- The value of the project is clear for the BETO mission, as the aim is to develop a new process that is also evaluated economically to convert lignin fractions. Patents and a license have resulted from this project. TEA using the BETO-derived tool is a plus.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

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

OVERVIEW OF CHEMICAL CATALYSIS FOR BIOENERGY CONSORTIUM

National Renewable Energy Laboratory

PROJECT DESCRIPTION

WBS:	2.3.1.100a
CID:	NL0024509a
Principal Investigator:	Dr. Josh Schaidle
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$300,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$150,000
DOE Funding FY19:	$150,000
Project Status:	Ongoing

Catalysis plays a central role in converting biomass and carbon-rich waste feedstocks into fuels and chemicals; however, critical catalysis challenges exist that are limiting commercialization of emerging bioenergy technologies. By leveraging unique DOE national laboratory capabilities and expertise, the Chemical Catalysis for Bioenergy Consortium (ChemCatBio) seeks to overcome these catalysis challenges and accelerate the catalyst and process-development cycle. The foundation of the consortium consists of an integrated and collaborative portfolio of catalytic and enabling technologies, which positions ChemCatBio to address both technology-specific and overarching catalysis challenges across the development cycle from discovery to scale-up. The core catalysis projects target technological advancements for specific conversion processes, such as catalytic upgrading of biochemical process intermediates, CFP, indirect liquefaction, and CO_2 upgrading, while the enabling technologies provide access to world-class capabilities and expertise in computational modeling, materials synthesis, advanced *in situ* and *in operando* catalyst characterization, and catalyst design tools.

Weighted Project Score: 9.1

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

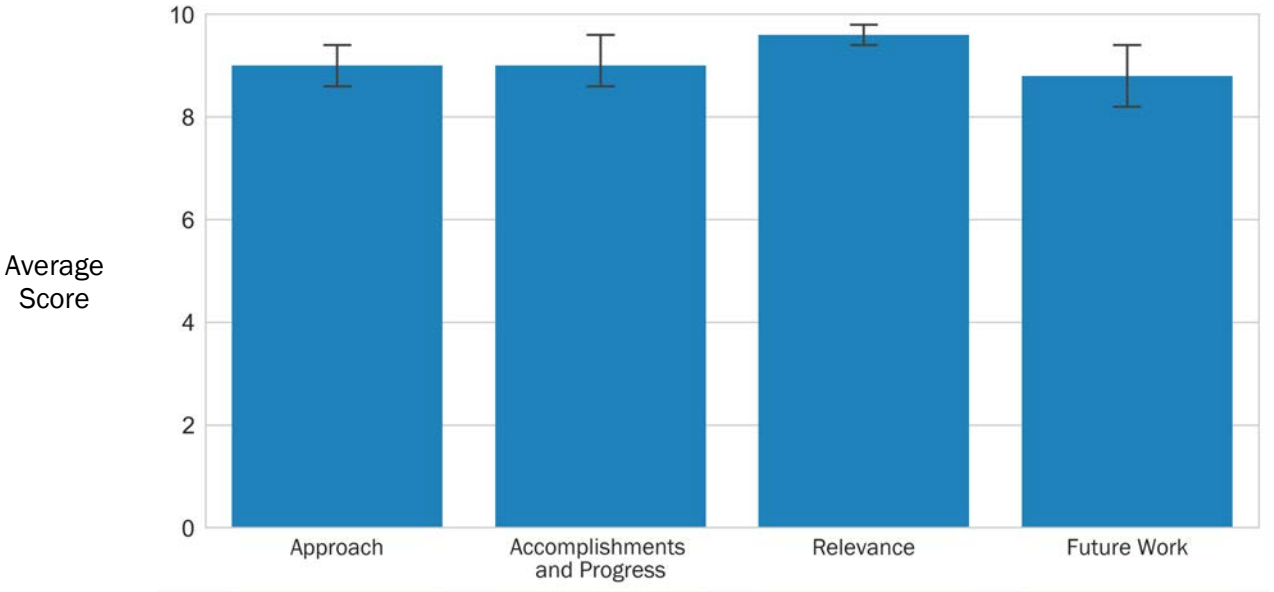

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Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- This presentation provides proper context for the ChemCatBio consortium as a whole. The structure, overall objectives, and future directions provide an excellent framework for the collective and provides the ability for interfacing between labs and researchers in the basic science, applied, and industrial areas. Opportunities to better demonstrate the ChemCatBio synergy and expand the impact of the center to university settings should be considered.

- This is an overview of the ChemCatBio consortium, and it provides a snapshot of outcomes in individual research thrusts. Overall, this is a nice consortium that was established with direct guidance from industrial partners. It broadly unites DOE labs, academic partners, and industrial partners, and it has a pretty impressive footprint with respect to the breadth of research. I think the heavy reliance on TEA for guidance is a strength; however, when assessing an individual technology, it would be beneficial to me to see less focus on leveraging coproducts to achieve DOE cost targets and more focus on how the specific research on a given conversion chemistry is impacting the bottom line. It would also be informative to have a more detailed consideration of carbon economy, as it was unclear in certain technologies like BDO synthesis.

- ChemCatBio was launched in 2017 after following up on the BETO 2015 Peer Review feedback similar to these comments on the need to "establish an experimental catalysis consortium." The consortium should be proud of themselves and deserve to be congratulated for conceiving such a multi-lab collaboration, successfully launching it, and now reaping tangible deliverables as a result. This is a highly intelligent, productive, and capable consortium for the bioenergy community. The leadership is strong, and the members are talented. I strongly recommend continued funding, and everyone involved in 2015 reviews that helped make the feedback clear to BETO should celebrate this achievement. ChemCatBio is an incredible BETO success story and should be celebrated. A sophisticated level of teamwork and technical collaboration was demonstrated here that should be highlighted at the DOE level. It is impressive how the stakeholder feedback was actually used along with other programmatic drivers at the DOE level to inspire the formation of ChemCatBio. The same model can be used for data, separations, engines, infrastructure, etc. It takes organizations of people to do this properly and sometimes making the right partnerships is more important than the early technical achievements. The catalyst design engine coming out of the computational group will be a major deal, especially when the proper back casting is incorporated into the analysis.

- The ChemCatBio consortium is a successful cross-government lab project. The consortium works on problems that are of critical importance. For example, the CFP change in catalyst, coupled with process design facilitated by changes, are making it conceivable to obtain less than $3/GGE in the near future. The consortium can access a vast amount of expertise and equipment acquired by the national labs and allows them to focus on these critical challenges across sites. Involvement of commercial groups provides an outlet for commercialization. The presentation cites that catalyst costs are 10% of the

production costs of biofuels. This number understates the impact of catalysts, which also are major determinants of yields, product selectivity, required feedstock properties, and overall throughput and operational times. The projects use realistic feeds and are TEA driven. They have kept the project overhead low while coordinating the projects between sites with regular meetings. The project has successfully incorporated industry input by involving an industrial advisory board. While the TEAs reported are internally consistent, they can give an impression the product costs are lower than they would be for initial projects. In part, this may be due to overstating the estimated operational time, which is not included in the TEA. Also, the TEAs and catalyst cost models do not include a projection of potential market changes due to increase supply of product versus demand and possible effect of increased metal use versus the global supply.

- In this age of shale oil, gas, and global warming, it is a delight to see such a comprehensive and deep research consortium as ChemCatBio. I can't imagine another consortium in the world that is working as hard and effectively on bio-based fuels and chemicals. I certainly don't know of one. This stokes my pride at being an American researcher involved in this effort. Decades of management experience at DOE must explain how the whole thing can operate so effectively. Virtually every project sets difficult goals and has made substantive progress. What's working: good structure of the ChemCatBio consortium, an effective matrix of catalytic technologies, enabling capabilities, and industry partnerships underpinned by cross-cutting support. What's not working: TEA may not be utilized to a sufficiently broad extent.

- The goal of this project is to overcome catalysis challenges for the conversion of biomass and waste resources into fuels, chemicals, and materials by leveraging unique DOE national laboratory capabilities. It is a collaborative, lab-led project. It also aims to facilitate industry access to national laboratory capabilities and expertise. The overview is clear and carries a large umbrella. The overarching goal is highly meritorious as it tries to tackle an important and emergent technology of high-energy impact. The effort is impressive and well coordinated with a solid management plan. Cross-cutting support is adequate to help with management and coordination of such a big effort. Cross communication among the different projects is highly encouraged and a formal mechanism to improve, encourage, and measure collaboration among the groups should be pursued. The work involves realistic bioprocess streams but there is no indication of coordination with groups involved with the R&D of feedstocks, which would also be beneficial. It is good to see the industrial partners utilizing unique national laboratory capabilities and the new research directions that can result from these new partnerships. Evidence of high demand for industrial partnerships is another relevance of the impact and relevance of the work. The reviewer only wonders if some of these industrial partnerships/projects could be done as effectively with the utilization of Small Business Innovation Research program resources. ChemCatBio should continue to look for opportunities to demonstrate the consortium's synergy and strategic alliances with university researchers who can augment the existing strengths and capabilities of the consortium.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We would like to express our appreciation to the reviewers for their thoughtful analysis and constructive feedback. Moving forward, we will continue to build upon the collaborative foundation of the consortium and our early-stage technical successes by (1) maintaining our responsiveness to stakeholder feedback; (2) emphasizing carbon utilization as a key metric for all catalytic conversion technologies; (3) strengthening existing partnerships and developing new partnerships, especially with universities; and (4) developing tools that broadly enable the research community to accelerate the catalyst and process-development cycle for bioenergy technologies.

CATALYTIC UPGRADING OF BIOCHEMICAL INTERMEDIATES

National Renewable Energy Laboratory

PROJECT DESCRIPTION

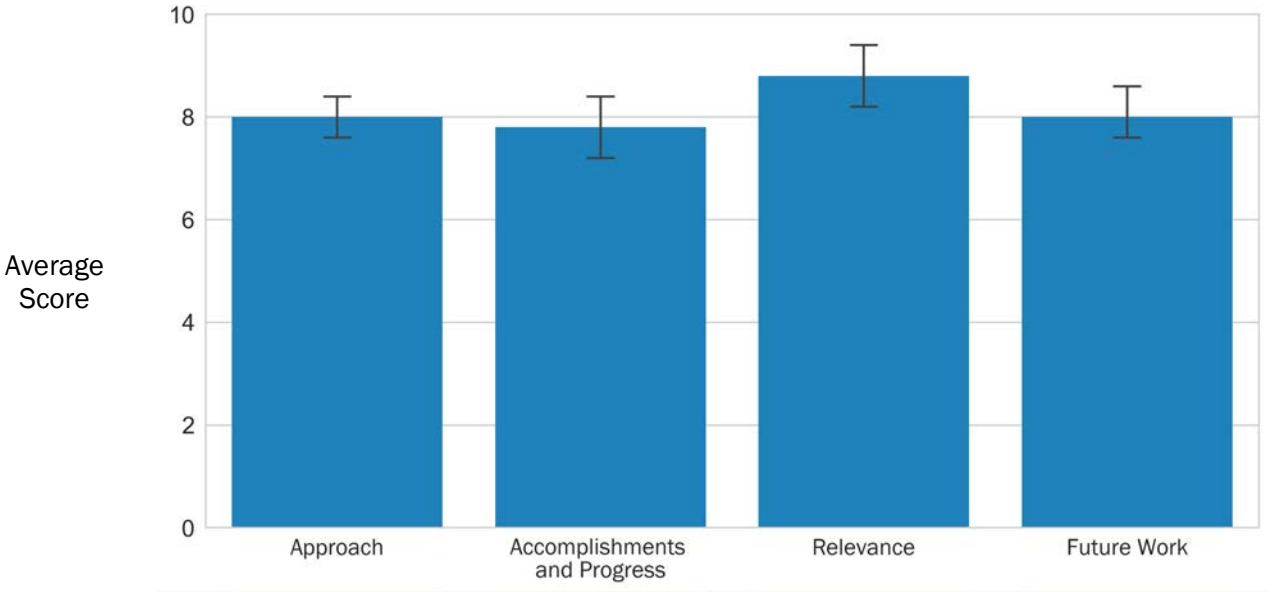
WBS:	2.3.1.101
CID:	NL0026681
Principal Investigator:	Dr. Richard Elander
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$5,410,593
DOE Funding FY16:	$1,200,000
DOE Funding FY17:	$1,381,000
DOE Funding FY18:	$1,529,593
DOE Funding FY19:	$1,300,000
Project Status:	Ongoing

The CUBI project is a multi-lab effort within ChemCatBio that is specifically focused on catalytic upgrading of sugar-related intermediates from biochemical deconstruction and/or biologically derived (i.e., fermentation) intermediates to hydrocarbon fuels. As several companies are developing catalytic upgrading routes from clean sugars, this project will help facilitate a transition to catalytic upgrading of such intermediates by providing a quantitative performance and economic assessment of several catalytic-upgrading approaches using biochemical deconstruction fermentation intermediates. While there are strong reasons for use of biochemical conversion-appropriate feedstocks and deconstruction methods, numerous challenges exist, including integration of biochemical upstream and catalytic downstream operations; understanding inhibitory impacts on upstream and downstream operations; developing specifications for biochemically derived feed streams to catalytic processes; and quantifying impacts of such feed streams on catalyst durability, lifetime, efficiency, and selectivity.

Specific catalytic upgrading routes are being investigated within the CUBI project, including: (1) catalytic upgrading of fermentation-derived 2,3-BDO; (2) catalytic upgrading of fermentation-derived carboxylic acids; and (3) catalytic upgrading of lignocellulosic sugar-derived sugars and associated intermediates, including

Weighted Project Score: 8.2

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



I One standard deviation of reviewers' scores

furfural and 5-HMF. These routes represent key technology pathways being investigated within BETO's biochemical conversion portfolio. The CUBI project is closely linked to numerous projects within that portfolio, most of which are being reviewed in the "Biochemical Conversion" session of the 2019 Peer Review. Additionally, as one of the core catalytic technology projects within ChemCatBio, the CUBI project interacts with ChemCatBio-enabling projects by utilizing analysis, characterization, modeling, and economic tools to develop improved catalysts and understand reaction and inhibition mechanisms associated with these specific catalytic-upgrading routes.

Driven by the findings from a mid-project go-no-go milestone that identified key areas for R&D focus in order to achieve commercial-scale economic viability (defined as the ability to achieve an MFSP of ≤$3/GGE), key technical approaches for each process route being investigated within the CUBI project are briefly summarized below. Yield and selectivity data for each route have been generated, along with a fuel property characterization for generated samples.

Catalytic Upgrading of 2,3-BDO: Catalytic upgrading approaches via (1) Cu-zeolite core-shell catalysis to C3+ mixed olefins (primarily butenes), followed by oligomerization and hydrogenation; (2) $ZnZrO_x$ catalysts for olefins production via methyl ethyl ketone (MEK) condensation and decomposition; (3) In_2O_3 catalysis to methyl vinyl carbinol (MVC) and acid catalysis to butadiene; and (4) single-step conversion to butadiene using CsH_2PO_4 SiO_2 catalysts.

Catalytic Upgrading of Carboxylic Acids: Mixed (C2–C4) and single (C4) conversion of fermentation-derived carboxylic acids via ketonization, condensation, and hydrodeoxygenation (HDO) to generate branched fuel-range hydrocarbons.

Catalytic Upgrading of Sugars and Derived Intermediates: Aldol condensation of furfural and HMF from mixed C5–C6 sugars followed by HDO to produce C14–C16 hydrocarbons. Additionally, HDO optimization in continuous-flow systems (for this route and other routes involving HDO reactions) is being developed.

Upon the completion of this project, the main outcome will be to quantify the catalytic upgrading performance of these routes using biochemical process-derived intermediates (including an inhibition mechanism assessment) in a fully integrated TEA model, with the identification of further R&D needed to achieve a modeled commercial-scale MFSP of ≤$3/GGE.

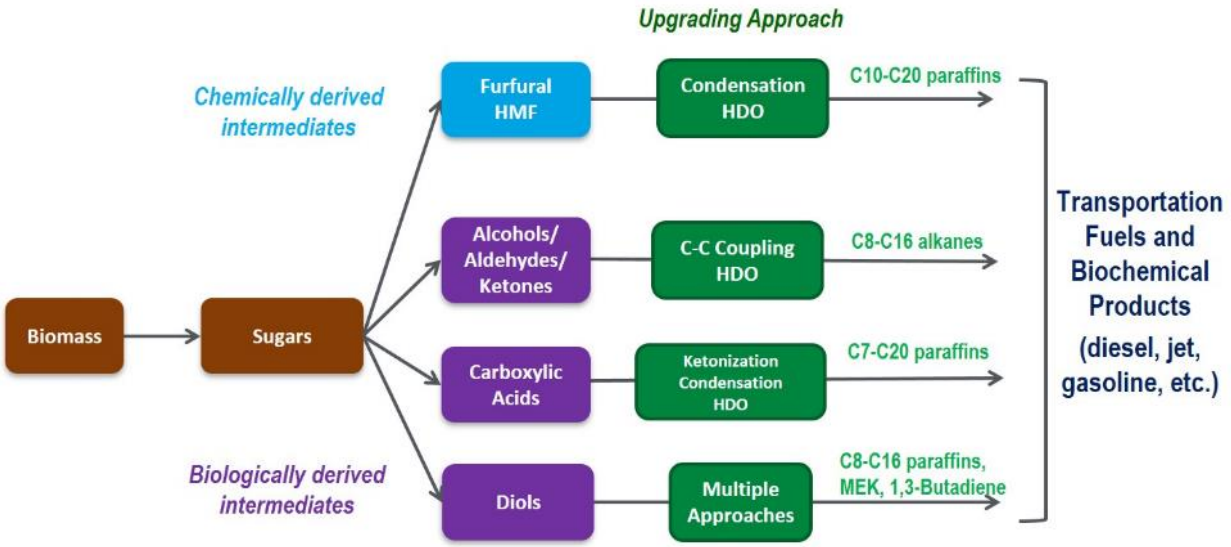


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- This project successfully assembles a range of projects and integrates them in a very logical way. The structure provides for a cohesive effort. Significant progress appears to have occurred across tasks, and future work has clear metrics established across the portfolio. The relevance to BETO and potential for this technology is clear.

- This program has been very productive, with several routes being identified and promising catalyst-upgrading results achieved by the team. The comments involving lignin valorization requirements to reach a $4–$5/GGE offset cost were honest and revealed how challenging "pathway work" can be. Overall, CUBI has been a solid, successful program taking information from TEA, creating highly organized tasks, operating cross-functionally, taking advantage of resources from several laboratories, focusing on using BETO-derived feedstocks and not model compounds, innovating new catalysts (e.g., Zr, Zn, In) with promising performance, and sound and practical organic chemistry.

- Catalytic upgrading of biochemical intermediates derived from sugars is aligned with BETO's goal of producing lower-cost biofuels with dependency on success of the lignin valorization project. The chemical conversion route provides an alternative to fermentation that has the potential to produce hydrocarbons directly, as compared with other routes that are focused on ethanol as the main cellulose conversion product. Comparison of the competing routes for the catalytic upgrading of biochemical intermediates will provide useful guidance to developers in the future. The project is guided by TEA and looks at several alternative routes that maximize the chances of success. However, the initial MFSP and relative importance of the lignin conversion process are not quantified. The team should consider switching the goal to producing value-added chemicals in place of fuels; as long as these products replace fossil fuel-derived products they will contribute to greenhouse gas (GHG) reduction and increase the cost effectiveness of the process.

- This project summarizes a broad effort in moving a family of technologies for fuel and coproduct production toward commercial development and is driven by TEA-informed decisions that steer the work toward dollar-per-GGE targets. The suite of technologies seems very appropriate to the types of feedstocks available. While TEA is helpful for assessing progress toward dollar-per-GGE targets, the impact of specific catalytic technologies may be somewhat obscured. Such heavy reliance on coproducts may be of concern: it isn't clear if the technologies have been demonstrated yet, and it isn't clear if, for example, lignin coproduct markets are commensurate in size with fuel markets. It would be helpful to make the case for producing fuels plus coproducts, versus fuels alone, versus coproducts alone.

- This is a quintessential ChemCatBio project, taking in biochemically derived intermediates and further converting them with chemical catalysis, all under the watchful eyes of the TEA team. The bar appears to be set high in all the tasks and the overall impact of the project will be commensurately high at sunset later this year. What's not working: while TEA has been used to indicate that each of the main four pathways has potential to reach the goal of <$3/GGE, the actual current value of the dollar-per-GGE has not been presented. This would provide valuable information.

- This is a large effort involving many labs and four different tasks around a very important topic and many different processes. It is very comprehensive work involving many skills and resources, and one of the backbones of the consortium. It would be beneficial to have a clear definition of the range of products that are being targeted and the state of the art in many of these processes. Routes are being evaluated with comprehensive TEA. It is necessary to relate costs not only to catalyst performance but also to other factors, such as solvent selection and downstream separation process. The relevance to BETO and potential for technology development is clear.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the comment on producing value-added chemicals to enable biofuels production. We are aware of the market volume challenges for specific coproducts. Envisioning the future bioeconomy, there will many coproducts via sugars, along with fuel production. The initial MFSP and importance of the lignin conversion process has been determined and presented in the biochemical conversion session presentations. We will also include more TEA scenarios, including fuels only, coproducts only, more than one coproduct, etc. For 2,3-BDO upgrading, we envision a flexible process where 2,3-BDO could be converted to either fuels and/or value-added chemicals (e.g., 1-butanol, isobutanol).

- The TEA was conducted within the first six months of effort for some upgrading pathways. Significant progress has been made by each catalytic-upgrading route within the last 18 months and the TEA will be updated in Q4 FY 2019 and will further inform opportunities for cost reduction.

- We thank the reviewers for their positive comments. We appreciate concerns regarding the cost dependency on the production of lignin-derived coproducts and will show the cost of producing the sugar-derived products with and without lignin valorization.

ONE-STEP, HIGH-YIELD PRODUCTION OF FUNGIBLE GASOLINE, DIESEL, AND JET FUEL BLENDSTOCKS FROM ETHANOL WITHOUT ADDED HYDROGEN

Vertimass LLC

PROJECT DESCRIPTION

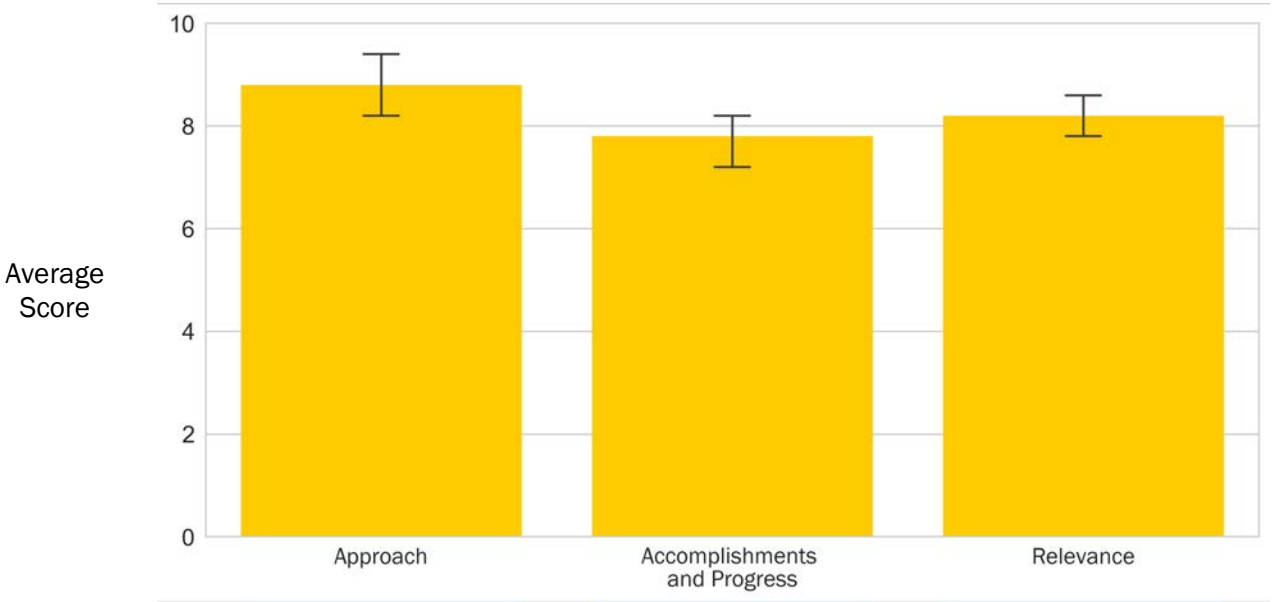
WBS:	2.3.1.201
CID:	EE0006875
Principal Investigator:	Dr. John Hannon
Period of Performance:	7/15/2015–5/31/2019
Total DOE Funding:	$1,650,000
Project Status:	Sunsetting

Most fuel ethanol is currently produced from starch in the United States and cane sugar in Brazil, and new technologies are emerging for production of ethanol from cellulosic biomass such as wood, grasses, and agricultural and forestry residues. However, U.S. ethanol is used primarily as 10% blends with gasoline, and current U.S. ethanol production has virtually saturated that market. The resulting "blend wall" and limited infrastructure to supply or use higher ethanol levels inhibit expansion of bioethanol production.

Vertimass LLC—through an exclusive license from Oak Ridge National Laboratory (ORNL)—seeks to commercialize novel catalyst technology to convert ethanol into gasoline blendstocks compatible with the current transportation fuel infrastructure and higher-value chemical coproducts, such as benzene, toluene, ethylbenzene, and xylene (BTEX), that provide valuable offsets, especially in low-oil environments. The gasoline blendstocks produced are anticipated to still fall under the Renewable Fuel Standard at the same level as feedstock ethanol. This catalytic process benefits from (1) production of minimal amounts of light components, (2) relatively mild temperatures and pressures, (3) ability to process 5% to 100% inlet ethanol

Weighted Project Score: 8.2

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



I One standard deviation of reviewers' scores

concentrations, (4) product flexibility to respond to changing market demands, and (5) no need to add hydrogen.

In this project, Vertimass has taken major steps in advancing this technology to date to include (1) scaling up the process 300 times; (2) maintaining 100% conversion yields of ethanol; (3) increasing liquid yield product distribution from 36% to 82%; (4) moving from powder to pelletized and now commercial catalyst formulations; (5) running ethanol feedstocks with no dilution; and (6) decreasing metal loadings while maintaining performance, resulting in less-expensive catalysts. These technology advances through this project have enabled the economic feasibility of a Vertimass bolt-on for industrial application.

Commercialization of this novel technology would overcome fungibility issues that limit ethanol use in gasoline for light-duty vehicles and partially contribute to mitigating climate change in offering more than 90% GHG reductions. Vertimass plans to partner with ethanol producers (with particular emphasis on emerging cellulosic ethanol plants) as rapidly as possible to overcome the blend wall and also allow the airlines to achieve Federal Aviation Administration targets of one billion gallons of renewable aviation fuel by 2018. This technology would expand opportunities to use more sustainable fuels in the United States. BETO funding will accelerate the scale-up of this technology to realize important goals of reduced GHGs, enhanced energy security, and domestic jobs.

OVERALL IMPRESSIONS

- This project has set up an effective commercialization pathway model for BETO to accelerate towards its targets while carrying out all the great, exciting fundamental research and elegant science and engineering activities required to discover the new pathways. In this parallel multiscale development model, pilot-scale campaigns may be led by an engineering, procurement, and construction (EPC) contractor and a catalyst original equipment manufacturer (OEM) using existing developmental catalyst materials with both surrogate and real feedstocks in ample supply while lab-scale catalyst development takes place. The catalyst OEM must be able to quickly modify and provide small batch extrudates based on informs from ChemCatBio and incorporate in the next pilot plant run campaigns. This model establishes the technology developmental pipeline from the atomic-scale modeling level with CCPC through the ACSC lab-scale synthesis and characterization activities to the commercial-scale process simulation level with the TEA team as oversight to the EPC operating the pilot plant and making iterations to the feedstock work. These types of accelerated commercialization projects should follow the general partnership model demonstrated in part here by Vertimass from inception and should include: catalyst optimization with ChemCatBio (e.g., ACSC, TEA, Co-Optimization of Fuels & Engines [Co-Optima] initiative), a proven EPC with close enough design experience and pilot-to-commercialization experience, a catalyst OEM, an inspection company, an additive company with access to engine dynamometers, and taxi fleets.

- At a high level, this project is impactful because it provides a value add for ethanol producers. Specifically, it can allow ethanol to be converted to higher hydrocarbons and BTEX, which could increase bio-carbon injection into the transportation sector and improve the overall economics of a cellulosic ethanol facility. In terms of a project report, details were sparse, and the presentation is relatively nonspecific, so it is difficult to assess technical merit. Many of the milestones seem arbitrary and it was not clear how this project is leveraging capabilities at the national laboratories.

- This is a targeted sunsetting project with relevance to BETO objectives. The scale-up continues to seem promising from a technical perspective, though the direction of the system is somewhat unclear (e.g., is increased BTEX fractions a key to make the process economically competitive?). The target of ethanol to hydrocarbons, aside from closing a potential loop of bioconversion to fuels, needed stronger argumentation for a cost-competitive implementation.

- This is a nice project on scaling up an active catalyst for ethanol conversion and appears successful so far in terms of product yield at larger scale. The only thing missing is the TEA needed to allay doubts that starting with a relatively expensive feedstock like ethanol can still meet the <$3/GGE target of DOE.

- Vertimass production of BTEX from ethanol is an example of a successful DOE-sponsored project. A viable commercial process resulted from initial work at a government lab that was licensed to a startup. The startup leveraged their work with a partnership with a catalyst manufacturer and engineering construction firm. They are working to provide an additional outlet for renewable ethanol production that is a value-added product that has no blending limit.

- The goal is to produce liquid hydrocarbons from ethanol using the catalyst licensed from ORNL. Their interest was to increase yield and scale up the process. The scale-up continues to seem promising from a technical perspective, though the impact of the coproduct on viability is somewhat unclear (i.e., is increased BTEX fractions key to making the process economically competitive or could this be an issue given the scale of a fuel-producing process?). Utilizing a technology developed at a national laboratory is of particular value. The advantages of the technology were mild conditions and one-step conversion. Management is clear and involves another two companies besides ORNL. The technology is relevant to the BETO mission. It is not clear how the knowledge acquired during this project could be transferred back to the lab and researchers involved within the consortium.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for this positive feedback. Vertimass chose to work with those with solid capabilities in the fields relevant to the project to avoid delays for purchasing and setting up equipment and analytical support, training of personnel, and startup of systems. Vertimass also greatly benefited from the expertise of these partners in terms of solving problems (e.g., substantially increasing yields from those realized at ORNL), transitioning to commercially relevant conditions (e.g., use of catalyst extrudates instead of powder), and providing a platform for rapid commercialization (e.g., ability to scale up to commercial operations from laboratory pilot/demo operations).

- Vertimass is working with the national laboratories for smaller-scale isotherm reactions that assist in directing pilot runs at pilot scale at TechnipFMC. Vertimass is also leveraging the catalyst characterization tools at national laboratories to examine the catalyst in its various states (e.g., fresh, run and regenerated, run and not regenerated, spent catalyst). Some details of the process and progress could not be presented at this time to protect potential patent applications.

- Utilizing the Vertimass bolt-on to make hydrocarbons from ethanol depends on the ethanol, gasoline, BTEX, and renewable identification number pricing. These prices are in constant motion though windows of opportunity, open where the ethanol produced can realize significant margin increases by using the Vertimass technology. In general, BTEX commands a premium as a chemical over fuels, so it is generally economically advantageous.

- Our TEA was presented and we displayed the detailed conversion cost transition from the start of the project ($1.10/gal ethanol), intermediate validation ($0.28/gal ethanol), current technology ($0.14/gal ethanol), and our target of $0.10/gal ethanol.

- Thank you for this positive feedback. We feel we are well positioned working with an engineering construction firm and a commercial catalyst manufacturer.

- Historically, BTEX has commanded a 40%–60% premium over fuel products, so it is generally economically advantageous.

CATALYTIC PROCESSES FOR PRODUCTION OF ALPHA-OMEGA-DIOLS FROM LIGNOCELLULOSIC BIOMASS

University of Wisconsin

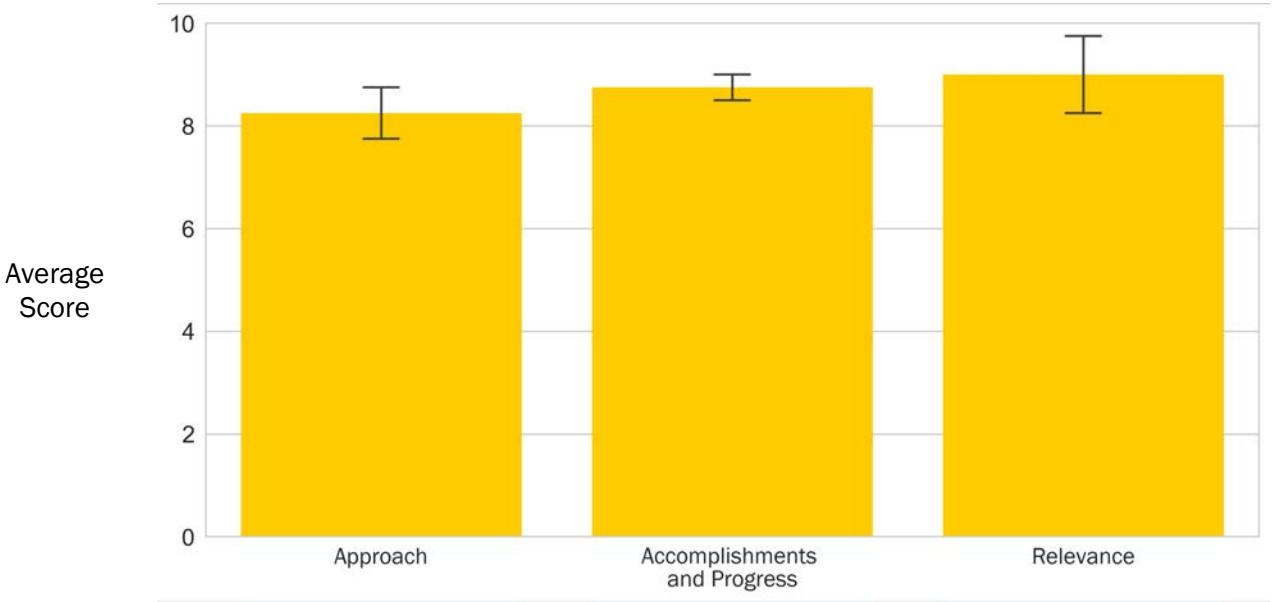
PROJECT DESCRIPTION

WBS:	2.3.1.204
CID:	EE0006878
Principal Investigator:	Dr. George Huber
Period of Performance:	2/1/2015–6/1/2018
Total DOE Funding:	$3,004,132
Project Status:	Sunsetting

In this project, we have demonstrated and developed a multistep catalytic process for production of 1,5-pentanediol (PDO) and 1,6-hexanediol starting from white birch. First, lignocellulosic biomass was converted into cellulose, furfural, and solid lignin via the TriVersa Process™ developed by Glucan Biorenewables, LLC (GlucanBio). GlucanBio fractionated biomass into a solid high-purity stream of cellulose (90% purity and 90% recovery) and a concentrated liquid phase of solubilized hemicellulose (90% of hemicellulose solubilized). The hemicellulose was then converted into furfural (85% yield) without any purification step. Furfural was converted into 1,5-PDO by four catalytic steps: (1) furfural was hydrogenated into tetrahydrofurfuryl alcohol (THFA), (2) THFA was dehydrated to dihydropyran (DHP), (3) DHP was hydrated to 2-hydroxytetrahydropyran (2-HY-THP) and 2-HY-THP dimers, and (4) 5-hydoxyvaleraldehyde (5-HY-Val) was hydrogenated into 1,5-PDO. This pathway will be referred to in this report as the dehydration, hydration, and hydrogenation (DHH) route. A total yield of more than 80% 1,5-PDO was achieved via this new DHH pathway, which surpasses the 50% 1,5-PDO yields over traditional noble catalysts.

Weighted Project Score: 8.7

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



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OVERALL IMPRESSIONS

- The goal of this project was to develop a catalytic process for converting woody biomass into 1,5-PDO and 1,6-hexanediol that makes economic sense. The diol market offers a multibillion-dollar product capture opportunity. The process design involves a number of units and synthesis steps, and the project team provided excellent thorough TEA analysis with transparent, believable capital expenditure hurdles on the order of several hundreds of millions of dollars for grassroots conceptual design estimates. The synthesis chemistry was elegant and provided numerous precursor opportunities for alternative routes and pathways. The project team was able to prove the synthesis route at the lab scale in flow reactors. The project team was able to spin off a company, Pyran LLC, to commercialize 1,5-PDO products produced from woody biomass. Mechanistic elucidation for interaction of diols within zeolitic frameworks and pore cavities was accomplished and coupled with computational and experimental agreement. Overall, this was an impressive project with sizeable market potential and its success reaching all of the key milestones.

- Production of α,ω-diols from lignocellulosic biomass project is a great example of what is required to prepare an early-stage commercialization proposal, including a thorough TEA. This TEA was done independently from the DOE and would need to be validated; however, it does indicate that the overall process is feasible. The estimated cost of the plant is $770,000,000. This is a very large investment for a grassroots startup even if the return on investment is achieved. It will be difficult to raise this capital without a major development project and demonstration of the key steps at scale. It is difficult to believe that a process with a catalyst with 10% platinum loading would be viable. However, the PI realized this issue and made sure to focus on critical steps that could be independently developed to use high-value chemicals and an intermediate (dihydropyran) which could be used as a platform for preparing bioadvantaged chemicals. This point was made in the prior peer review and was recognized by the PI.

- The conversion of lignocellulosic intermediate chemicals into diols presents a nice connection of development of a new technology, intimate study of the reaction mechanisms and catalyst operation, and attempts to transition the processes to a higher TRL. The TEAs are encouraging for incorporation of the one-diol conversion into cellulosic ethanol production. While the background materials and approach were sparse, the milestones and other achievements, including both technology transfer and several publications, were well detailed and indicate a strongly operated project that has successfully met its objectives. The relatively large body of publications, plus patents and spinoffs, are evidence of new knowledge being generated and the relevancy of the work to the BETO mission.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

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

LIQUID FUELS VIA UPGRADING OF INDIRECT LIQUEFACTION INTERMEDIATES

National Renewable Energy Laboratory

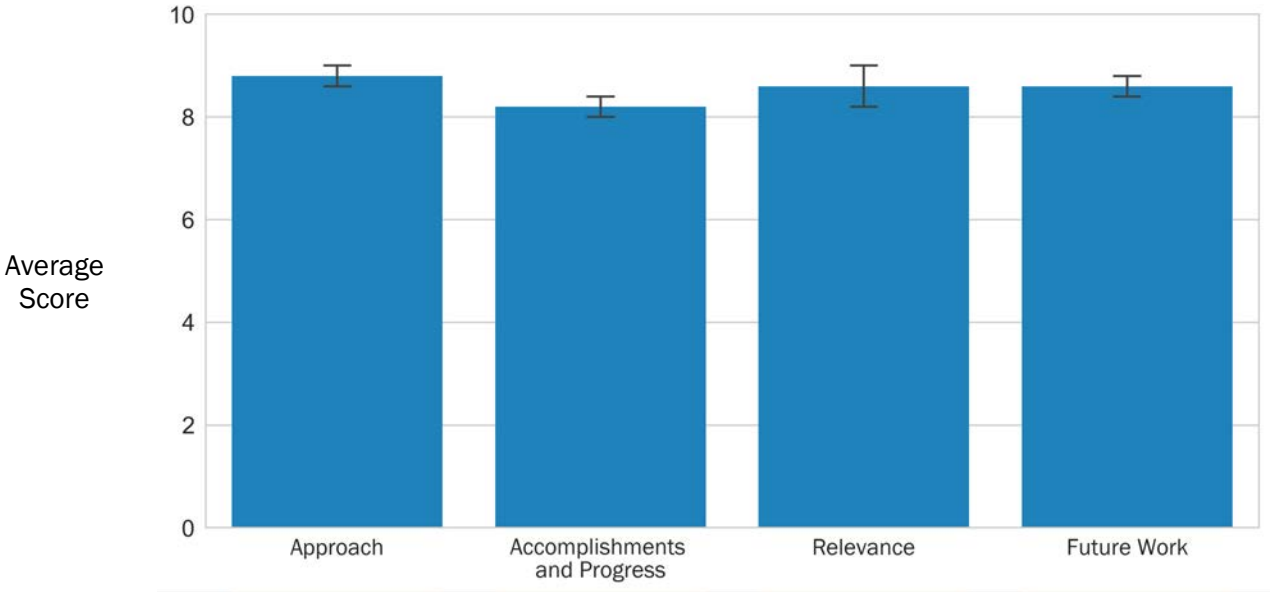
PROJECT DESCRIPTION

WBS:	2.3.1.305
CID:	NL0013383
Principal Investigator:	Dr. Dan Ruddy
Period of Performance:	10/1/2016–10/1/2019
Total DOE Funding:	$11,550,000
DOE Funding FY16:	$3,950,000
DOE Funding FY17:	$3,200,000
DOE Funding FY18:	$2,200,000
DOE Funding FY19:	$2,200,000
Project Status:	Ongoing

This project seeks to develop a responsive, integrated biorefinery concept based on IDL technologies that produces a suite of fuels and coproducts and provides control over the product distribution such that process operation can be adjusted to meet the shifting gasoline-distillate fuel market demand. Advanced upgrading technologies from syngas are critically needed for the successful commercial implementation of fuel production at a scale relevant for biomass. Research tasks within this project leverage light oxygenate intermediates from syngas and focus on the development of new catalytic pathways with lower-severity conditions to achieve high-carbon yields of gasoline, diesel, and jet fuel with integrated routes to coproducts that can improve overall economics. Each pathway under investigation offers promise to generate high-quality fuels (e.g., high-octane gasoline with low aromatics, and desirable jet- and diesel-range hydrocarbons) and to achieve favorable cost targets by 2022. Finally, research progress is compared against the Mobil Olefin to Gasoline and Distillate (MOGD) process, which also offers control over the gasoline and distillate products, as an industrial benchmark. The new pathways seek to exceed the fuel product yields and reduce the cost of production versus the MOGD process. Recent catalyst and process development accomplishments are highlighted by improvements in carbon

Weighted Project Score: 8.6

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



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selectivity to fuels and catalyst productivity for all three of the pathways under investigation, resulting in reductions to the modeled MFSPs of 10%–33%.

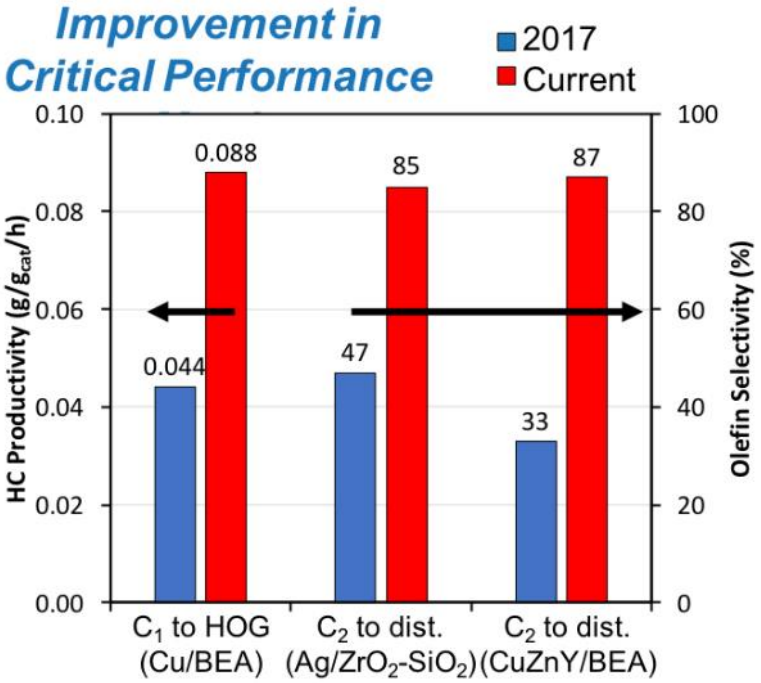


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- In general, the project has very focused tasks to develop a wide range of potential full candidates from low molecular weight oxygenates. The team successfully leverages interactions with many groups within ChemCatBio to enhance the project. The majority of the project has seen activity and selectivity metrics met, though room to improve catalyst reusability remains. In general, future studies appear to build on prior successes and will leverage capabilities in ChemCatBio to attempt to further catalyst performance. The project is productive in both connecting with fundamental science, publications in field-leading journals, technology, and several patents and a successful technology transfer with one of the processes.
- Overall, this seems like a comprehensive effort geared toward making IDL-based technologies commercially viable. It was not clear that the TEA estimates on biomass to liquids through the Fischer-Tropsch process and otherwise are presently realistic, and some comparison to commercial gas-to-liquids/coal-to-liquids would be useful, but that does not diminish from the work being done throughout this project.
- This project is making great progress already by delivering a promising pathway with several others to follow. This is the type of technology platform pipelining that BETO needs to continue funding in order to remain an innovative leader in bioenergy technology for the future. These types of processes that are rooted in alcohol conversion over modified zeolite chemistry will accelerate the progress toward the 2022 target. The information received from TEA and the CCPC make this project approach very robust. The team should stay vigilant and not trivialize the oligomerization chemistry and related unit operations required to drive the carbon-carbon bond formation to distillate-range material.
- Conversion of light oxygenates to drop-in hydrocarbon fuels is a flexible platform applicable to both biomass, CO_2 utilization, and natural gas, and as such is critical technology. There have been significant commercial efforts in this area; however, there are only a few operating plants even given the economies of scale. Improved catalysts could definitely facilitate the adoption of this approach, and the upstream

process, when integrated sustainably, would significantly impact GHGs. In the near term, it is unlikely that this approach will proceed without strong government support and mandates. However, in the long term this route is a likely component of future fuel supplies. The butadiene product produced and other intermediate olefins are more valuable than fuel and should be considered as the main product. The approach taken by the project team is extremely sound, allowing the comparison of multiple catalysts and routes in terms of both carbon efficiency and costs. Significant progress has made in the past two years and is likely to continue to be made going forward. The project with Enerkem would provide a potential near-term route to validate the new catalyst at a commercial scale.

- This is a heavyweight project at the heart of BETO's portfolio of catalytic technologies. It has made significant contributions to the field since its inception and will continue to do so as it sunsets.
- In general, the project has very focused tasks to develop a wide range of potential fuel candidates from low molecular weight oxygenates. The team successfully leverages interactions with many groups within ChemCatBio to enhance the project. The majority of the project has seen activity and selectivity metrics met, though room to improve catalyst reusability remains. In general, future studies appear to build on prior successes and will leverage capabilities in ChemCatBio to attempt to further catalyst performance. The project is productive in both connecting with fundamental science, publications in field-leading journals, technology, and several patents and a successful technology transfer with one of the processes. It involves NREL, PNNL, and a small portion (and more recent) to ORNL. Scaling is an important consideration on this project. It would be beneficial to evaluate modular processes as well and evaluate how synthetic catalysts work on large-scale processes.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that catalyst reusability remains an important part of our research. This is the focus of our end-of-year goal, where we will explore deactivation and regeneration in all three of our oxygenate conversion pathways.
- Comparative TEA is an important part of our approach, and we will revisit our analyses of benchmark processes (Fischer-Tropsch, MOGD, and other gas-to-liquids/coal-to-liquids) to ensure we have realistic estimates.
- Although our focus is on the catalyst development for oxygenate conversion to versatile hydrocarbon intermediates, the reviewer is correct that the oligomerization cannot be trivialized. Due to time limitations, these results were not presented. However, this is an active area of research in the project, and based on these comments, it will remain as such.
- The reviewer provides an excellent overview of the versatility of our research approach, the challenges, and the opportunities for successful implementation. We have previously considered butadiene and mixed olefins as value-added coproducts. At our last peer review, we were cautioned against considering them as the final products, in light of the strict purity requirements required in the chemical industry that may not be trivial to meet. In the near term, our goal is to develop a market-refinery biorefinery concept around these pathways, which would enable the production of fuels and chemicals. Thus, we seek to maximize the carbon efficiency to these valuable intermediates, and to further explore and develop chemistry to convert them to fuel products.
- In addition to our ongoing efforts around catalyst reusability, the reviewer presents a useful suggestion to consider varying scales and modular processes. Our initial assessment of smaller scales suggested less favorable process economics, as typically associated with small-scale gasification technologies. However, we acknowledge that the opportunity to utilize renewable carbon sources may someday favor modular systems, and we will consider how our technology scales.

CATALYTIC UPGRADING OF PYROLYSIS PRODUCTS

National Renewable Energy Laboratory

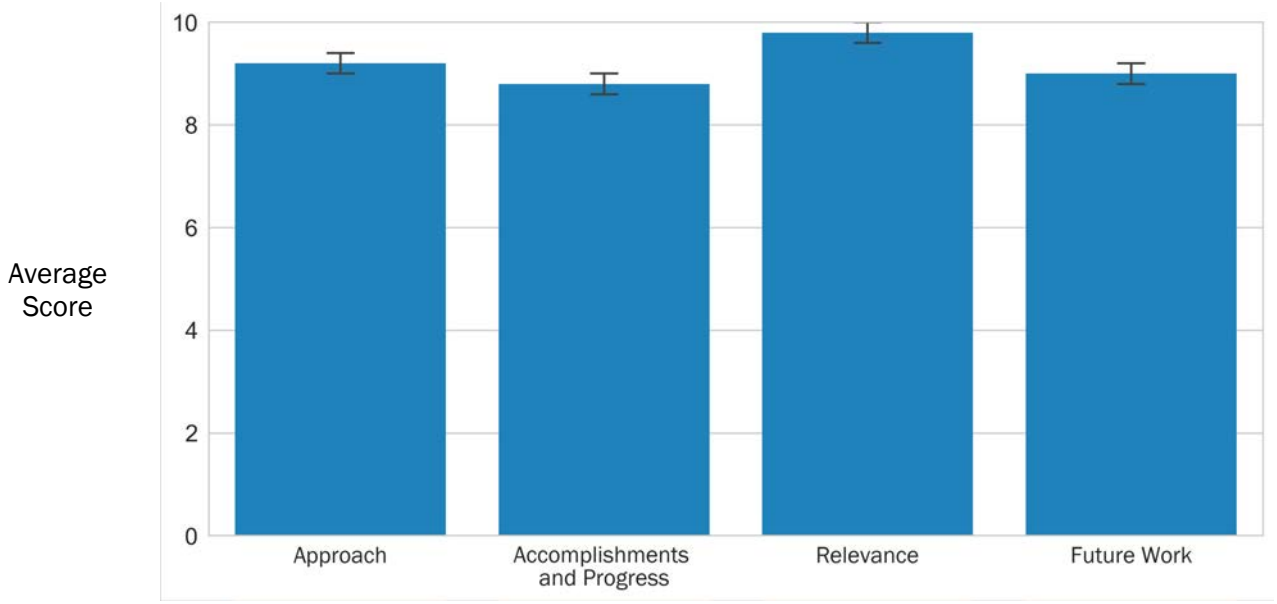
PROJECT DESCRIPTION

WBS:	2.3.1.314
CID:	NL0025579
Principal Investigator:	Dr. Josh Schaidle
Period of Performance:	10/1/2016–9/30/2019
Total DOE Funding:	$16,388,556
DOE Funding FY16:	$4,797,424
DOE Funding FY17:	$4,897,723
DOE Funding FY18:	$3,450,809
DOE Funding FY19:	$3,242,600
Project Status:	Ongoing

Fast pyrolysis of biomass is a promising route for converting lignocellulosic feedstocks into fungible biofuels; however, the resulting bio-oil must be upgraded prior to utilization as a fuel or blendstock. The focus of this project is to improve the fuel quality and stability of bio-oil through CFP, in which catalytic upgrading is performed in the vapor phase prior to condensation in either an *in situ* or *ex situ* configuration. The major challenge for CFP is to achieve high-carbon yields to the desired fuel-range molecules while operating under relatively harsh conditions that are conducive to catalyst deactivation via carbon deposition. To address this challenge, this project leverages a vertically integrated and collaborative approach, spanning from catalyst design to integrated bench-scale CFP. The overarching goal of this project is to reduce biomass conversion costs by developing catalysts and integrated processes for CFP that improve yield and enhance the fuel quality and stability of the resulting bio-oil by reducing the oxygen content (i.e., oxygen-carbon ratio), increasing the hydrogen content (i.e., hydrogen-carbon ratio), and increasing the carbon number into a range suitable for gasoline, diesel, or jet fuel. Ultimately, we seek to develop a CFP technology platform for an integrated biorefinery concept that is capable of producing both cost-competitive biofuels at greater than 75-GGE dry tons of biomass and high-value coproducts and can be market responsive by controlling the product distribution to meet market demand.

Weighted Project Score: 9.2

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



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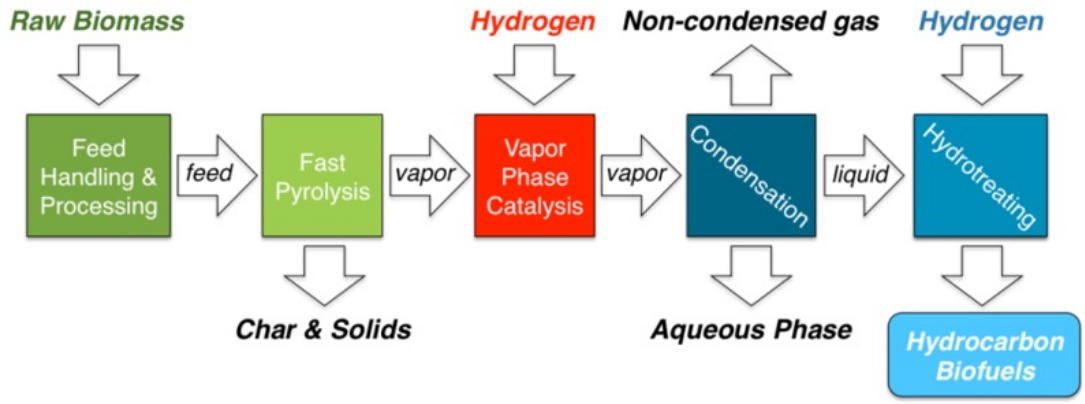


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Overall, this is a very nice project that is targeting the cost drivers in CFP.
- The project interactions approach to this work is commendable, involving the lab community, consortiums (ChemCatBio, Bioprocessing Separations), cooperative research and development agreements (CRADAs) with energy (Exxon Mobil Corporation), material and catalyst companies (Johnson Matthey), scale-up (Advanced Development and Optimization), and engine application (Co-Optima) functions. This has been a successful effort thus far with strong partners and steering efforts.
- This catalytic upgrading of pyrolysis products project has made significant advances since the last review. The CFP continues to be extremely attractive with an identified path to low-cost fuel when supplemented by separation of a value-added product. It is a role model for other projects in terms of progress and organization. The team has incorporated the feedback from past reviews into their plan and have made great progress. Significant additional development work is needed to commercialize the process. Improvements in yields and product quality are still likely, if work continues. The cost of the value-added products needs to be compared to that of the current products. The fixed-bed flow scheme with new catalysts has a good probability of successfully reaching the commercial targets.
- This is a difficult project. The devil is in the details and the details are being addressed. TEA shows the promise of $3.50/GGE. The work is at the heart of ChemCatBio and must be considered a crown jewel not only of ChemCatBio but of the entire BETO program.
- This is a successful, large-scale project with a rich history in BETO. Given the somewhat well-developed systems, the metrics are well defined and targeted to improve carbon efficiency, product distribution, and overall process costs. The recent progress is promising, and the future areas of focus expand on the recent successes to continue to improve catalyst performance and leverage coproducts effectively. Progress is heavily based on foundational science and the program is encouraged to leverage some of the work by coordination with other academic/national laboratory basic science programs. TEA and industrial relationships are important and working well. Feedstocks are key in their economic analysis and it is beneficial to encourage strong ties with bioenergy feedstock research partners.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their constructive feedback. We agree that CFP is a complex process and have sought to address this complexity through a collaborative approach leveraging both foundational science and applied engineering. Moving forward, we will continue to target improvements in carbon yield, catalyst performance, and product quality while identifying and developing routes to value-added chemical coproducts.

CONDENSED PHASE CATALYSIS TECHNOLOGY FOR FUELS AND CARBON PRODUCTS

University of Tennessee

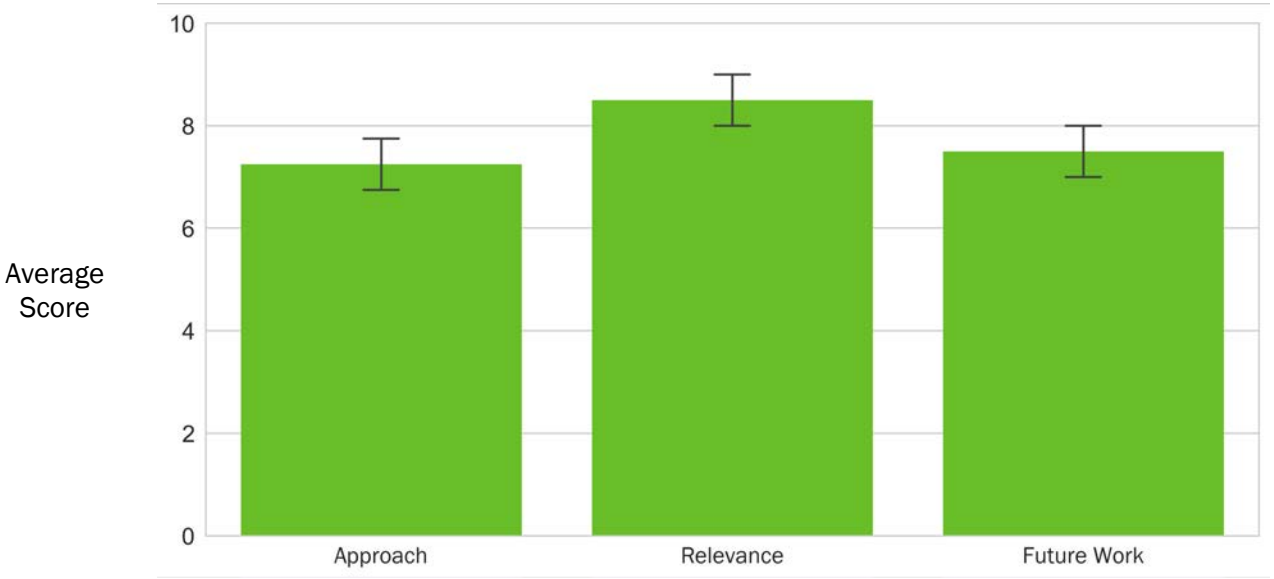
PROJECT DESCRIPTION

WBS:	2.3.1.413
CID:	EE0008353
Principal Investigator:	Dr. David Harper
Period of Performance:	8/1/2018–7/31/2020
Total DOE Funding:	$1,400,000
Project Status:	New

We propose a condensed phase catalysis technology with the biomass-derived solvent gamma-valerolactone (GVL) to deconstruct, fractionate, and upgrade lignocellulosic biomass to aviation liquid fuels (alkanes) and high-purity lignin. The lignin will be converted into functional carbon materials, such as activated carbon foams. Intermediate chemicals preceding the alkanes include furfural, high-purity cellulose, HMF, levulinic acid, and GVL. GVL is an effective solvent for biomass conversion because hydrolysis and dehydration reaction rates increase 100 time and 30 times, respectively, relative to water. Fast kinetics enable mild biomass deconstruction severity (time, temperature, acid concentration, and pressure) and lead to clean fractionation into concentrated liquid hemicellulose, solid cellulose, and lignin. The biomass fractionation produces high yield and purity for the C5, C6, and lignin streams at high biomass loadings, enabling downstream processing and product recovery with less energy. The fractionated biomass components are independently and simultaneously converted to products in GVL, leading to process intensification by reducing the number of separation steps. These capabilities are critical to achieve below a $3/GGE fuel cost target. The GVL-derived lignin readily converts into high-quality carbons. The GVL-enabled mild biomass digestion conditions produce lignin that has high purity, molecular weight, and glass transition temperature, yet also fusible. These characteristics are desirable for carbon materials with commercial applications. Our preliminary data suggest that we can use this lignin stream to create a range of carbon materials. Its high purity and low ash content make it ideally suited to produce high-temperature foam insulation, activated carbon, and

Weighted Project Score: 7.7

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



I One standard deviation of reviewers' scores

electrodes. Each of these products has high market value and will displace materials derived from fossil sources. Since roughly 25%–30% of lignocellulosic biomass is lignin, making biofuel production viable requires lignin valorization beyond its fuel price. Our goal is a continuous process integrated biorefinery that uses condensed-phase catalysis technology and the environmentally friendly biomass-derived solvent GVL to convert biomass into aviation fuel and functional carbon materials. By fully using and upgrading all major biomass components, the project will demonstrate the technical and economic feasibility of producing aviation fuel below $3/GGE.

OVERALL IMPRESSIONS

- Generally, the project seems well structured. The management appears adequate. Preliminary results are promising and suggest potential interesting science and a useful technology can result from the work. The relevance to DOE and BETO is clear. For a project ramping up, additional details about thoughts on overcoming potential challenges, non-catalysis aspects of the work (solvent recycling), and better-defined timelines of future work would have been beneficial.
- This project is definitely in the early proof-of-concept stage involving simple characterization of a few biomass feedstock options followed by a few solvency runs monitoring pH and temperature. The focus should be on the future work of screening more BETO-relevant feedstocks and accelerating the solvency testing to probe more fundamental characteristics and thermodynamics first principles. PIs should engage the BETO computational group on areas to focus the basic research part of this program. A related benchmark study from open literature would be helpful to improve the efficacy of the GVL solvent. There may be more opportunity in the economic analysis task to include a cellulosic ethanol partner and provide additional processing details.
- The condensed phase catalyst project is a high-risk and high-reward project. Achieving the target would provide a new commercial route to biofuels. However, the scope of the project is very broad, and it is likely under-resourced. The economic evaluation is critical and still remains to be done. Pieces of this approach have been evaluated by these and other researchers in the past, which reduces the technical risks. Cost reduction and simplification are the critical parameters, along with product quality and suitability for high-value applications. Two of the most important aspects are demonstrating the feedstock flexibility and developing higher-value products from lignin and should continue to be the focus. Feedstock flexibility is critical to the future of biofuels because lowering the costs will involve using lower-cost feedstocks.
- The approach to biomass utilization by breaking it down into C5 and C6 sugars and lignin is simple and tractable. Yield goals are high. The gathered team has world-leading expertise to successfully perform the work.
- The goal is to separate biomass into high-purity streams of its three main components—cellulose, hemicellulose, and lignin—in an integrated process to enable efficient and cost-effective downstream conversion processes. Eventually, the team should convert hemicellulose and cellulose to an aviation fuel (alkanes) through intermediate chemicals derived from biomass polysaccharides (i.e., furfural, levulinic acid). The goals are clearly relevant to BETO's mission. Partners are University of Wisconsin and GlucanBio. Tasks are clear and logically divided, including TEA, and management is adequate. It would be beneficial to have an analysis of how this process compares with the state of the art. For a project ramping up, additional details about thoughts on overcoming potential challenges, non-catalysis aspects of the work (solvent recycling), and better-defined timelines of future work would have been beneficial.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

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

CHEMCATBIO DFAS: LOW-PRESSURE HYDROGENOLYSIS CATALYSTS FOR BIOPRODUCT UPGRADING WITH VISOLIS

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

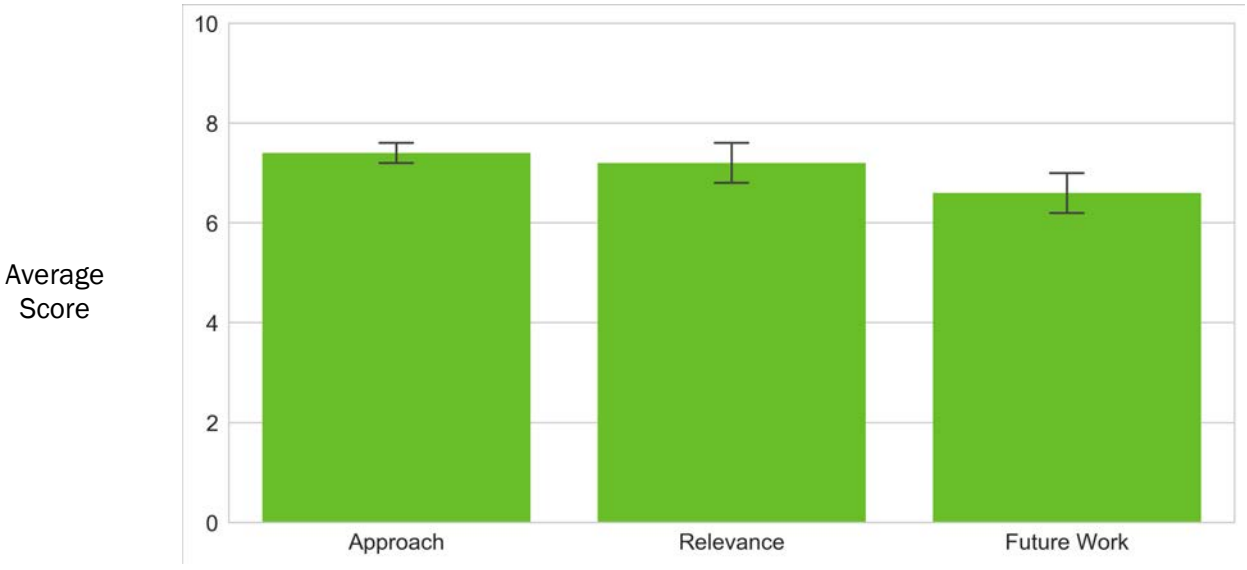
In late 2017, the ChemCatBio consortium invited industry to partner with national laboratories and leverage ChemCatBio capabilities. Visolis, a small company coupling bioengineering with chemical processing, answered the charge with a hybrid biothermochemical process to produce high-value monomers at near-theoretic yields.

WBS:	2.3.1.700
CID:	NL0033617
Principal Investigator:	Dr. Karthi Ramasamy
Period of Performance:	1/20/2018–12/31/2019
Total DOE Funding:	$525,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$525,000
DOE Funding FY19:	$0
Project Status:	New

Visolis has previously demonstrated demo-scale (6,000 L) fermentation to produce an intermediate with low projected costs at commercial scale. Development of hydrogenolysis to convert the bio-derived intermediate to the desired monomer was proposed to ChemCatBio. A major production cost in hydrogenolysis is the requirement for very high pressures—typical pressures for hydrogenolysis exceed 25 megapascals (MPa). In earlier work, Visolis and PNNL demonstrated complete conversion of the fermentation-derived intermediate with a selectivity of over 90% at 200°C and 12.5 MPa, but facilities capable of operating at such high pressures are expensive. Lower hydrogenolysis pressures improve capital and operating costs.

Weighted Project Score: 7.2

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



I One standard deviation of reviewers' scores

Objectives of the current effort are to develop and demonstrate a stable and robust hydrogenolysis catalyst by the end of FY 2019 for the conversion of the fermentation-derived intermediate to high-value monomer at ≥80% selectivity under 4-MPa pressure. The solution entails a bimetallic catalyst system, a challenge requiring the screening of hundreds of potential catalysts and to fine tune the catalyst to achieve the desired product yield and stability. The team will also provide TEA for pilot-plant design using ASPEN Plus process models and discounted cash flow analysis.

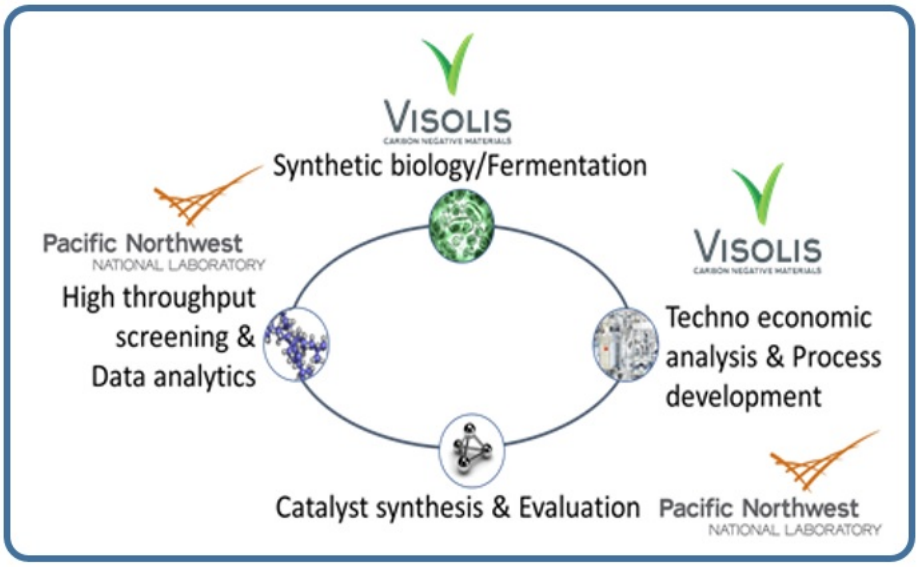


Photo courtesy of Pacific Northwest National Laboratory

OVERALL IMPRESSIONS

- This is a very targeted project with existing ties to PNNL catalyst development. Appears to be on track for meeting goals. More details could be provided regarding future work and justifying the fit with PNNL beyond the preexisting relationship.

- Overall, this is a good project in that it leverages high throughput synthesis and characterization abilities at PNNL to solve a relatively challenging selectivity issue (favoring reduction vs. carbon-carbon scission). Acknowledging this is a DFA, I understand that the level of detail has to be somewhat limited, but this also makes it very difficult for reviewers to comment on the relevance and quality of the work.

- The project team has done a wonderful job of showing how combinatorial catalytic research in bioenergy systems should be done. The high throughput screening apparatus should be used throughout ChemCatBio in every catalysis design project as a guide tool working parallel with rational *ab initio* design approaches simply for vector and ranking validation. The approach is sound by including commercial catalysts in the screening, working at real hydrotreating pressures near 1,800 psi. The presentation showed 100 catalytic materials, but it assumed that thousands have been screened. The project goal is highly relevant to BETO's objective of upgrading intermediate feedstocks from biocatalytic processing steps. In this case, C5 oxygenates produced by Visolis' demonstration-scale fermentation process are hydrotreated catalytically by PNNL to various alkanes of unknown speciation at 50% selectivity with a target of 80%.

- The PNNL/Visolis development of low-pressure hydrogenolysis catalysts for bioproduct found several new candidate formulations for improving the process. It would be easier to evaluate this project if more specific information was provided about the target products or catalysts. Presumably, intellectual

property protection is being prepared that will include this information. Hydrogenolysis catalysts that are active at low pressure and are water tolerant are highly attractive and could greatly facilitate the adoption of biomass conversion technology. The expertise gained can be applied to other BETO projects that require catalysts with similar functionality.

- This is a very sparse presentation, conveying some success at high throughput catalyst screening but offering no rationale for why these catalytic processes will give high yield as the pressure is lowered.

- Develop a low-pressure and water-tolerant hydrogenolysis catalyst to convert the fermentation-derived C5 oxygenate to a high-value monomer. A very targeted project with existing ties to PNNL catalyst development. The project appears to be on track for meeting its goals. More details could be provided regarding future work and justifying the fit with PNNL beyond the preexisting relationship. In addition, it is not clear what the lab and the consortium are learning from this project. One of the advantages could be data made available through the data hub.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The insightful comments provided by the reviewers are greatly appreciated. As pointed out by the review team, this project leverages the high throughput synthesis, screening, and characterization abilities at the ChemCatBio consortium to solve a relatively challenging issue in upgrading intermediate feedstocks from biocatalytic processing steps.

- We apologize for not being able to provide detailed technical information during the peer review presentation. This is due to the constraints of confidentiality with a commercial partner. Once the novelty is protected by patent, our goal is to make the information available to public and document all the information in the data management hub operated by ChemCatBio consortium.

- The commercial catalyst tested is designed to promote hydrogenolysis chemistry but is not specifically tuned to accommodate the bio-derived intermediate and feed composition. Thus, the commercial catalyst is not active to produce the high-value monomer of interest. The lessons learned from the commercial catalyst, through knowledge on the feedstock property and prior expertise in the hydrogenolysis chemistry, guided our team to develop an active catalyst that can operate at low pressure.

- Synthetic biology and fermentation are Visolis' core competencies, and this hybrid process requires heterogeneous catalyst discovery and development. PNNL's prior-demonstrated technical expertise in the hydrogenolysis catalyst development space and the equipment capability for heterogeneous catalyst development under the ChemCatBio consortium made PNNL the logical partner in accelerating this process.

- Even though the goal of this project is to develop a low-pressure and water-tolerant hydrogenolysis catalyst to produce a specific high-value monomer from a bio-derived intermediate, we strongly believe the successful outcome of this catalyst development with fundamental understanding will facilitate the adoption of other biomass conversion technologies that are under the BETO portfolio.

CHEMCATBIO DFAS: TEREPHTHALIC ACID SYNTHESIS FROM ETHANOL VIA *P*-METHYL BENZALDEHYDE WITH LANZATECH

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

To date, the only readily available renewable component of polyethylene terephthalate (PET) is ethylene glycol. Renewable terephthalic acid (TA) is a ready complement for renewable plastics (e.g., bottles and packaging films). In 2012, the global demand for TA was 47 million tons. The TA market is expected to grow continuously, reaching nearly 80 million tons in 2020. Ethanol could be a promising feedstock for renewable TA.

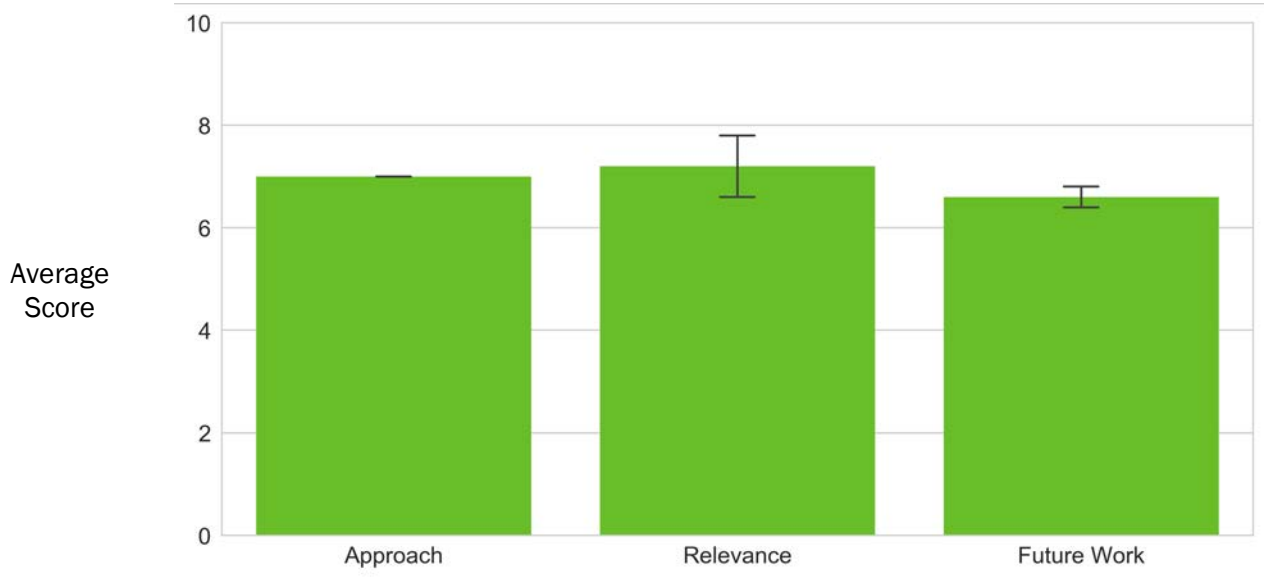
WBS:	2.3.1.701
CID:	NL0033621
Principal Investigator:	Dr. Karthi Ramasamy
Period of Performance:	4/3/2018–3/31/2020
Total DOE Funding:	$200,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$200,000
DOE Funding FY19:	$0
Project Status:	New

The development of ethanol-derived *p*-methyl benzaldehyde offers the possibility of producing 100% renewable PET from ethanol, adding flexibility and opportunities for a healthy industry that continues to grow. In addition, dehydrogenation of ethanol and the subsequent dehydrocyclization step in the *p*-methyl benzaldehyde synthesis generates hydrogen, which improves economics and life cycle impacts by reducing the need for external hydrogen for biorefineries having both a PET product line and a hydrocarbon fuels line.

The conversion of acetaldehyde occurs via a complex sequence of reaction mechanisms over a mixed-oxide catalyst. The complexity of the multistep cascade chemistry requires multifunctional catalysts with the acid base surface chemistry necessary for aldol condensation, paired with an active site that can promote the

Weighted Project Score: 7.0

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



I One standard deviation of reviewers' scores

dehydrocyclization step to achieve high conversion and selectivity. In addition to the multifunctionality, shape selectivity is required to maintain the high selectivity to the *p*-methyl benzaldehyde over the ortho isomer.

Objectives of the current effort are to develop and demonstrate the catalytic conversion of acetaldehyde (derived from renewable ethanol) to a methyl benzaldehyde(s) intermediate to establish the path to a marketable process for the economical and renewable production of TA and phthalates.

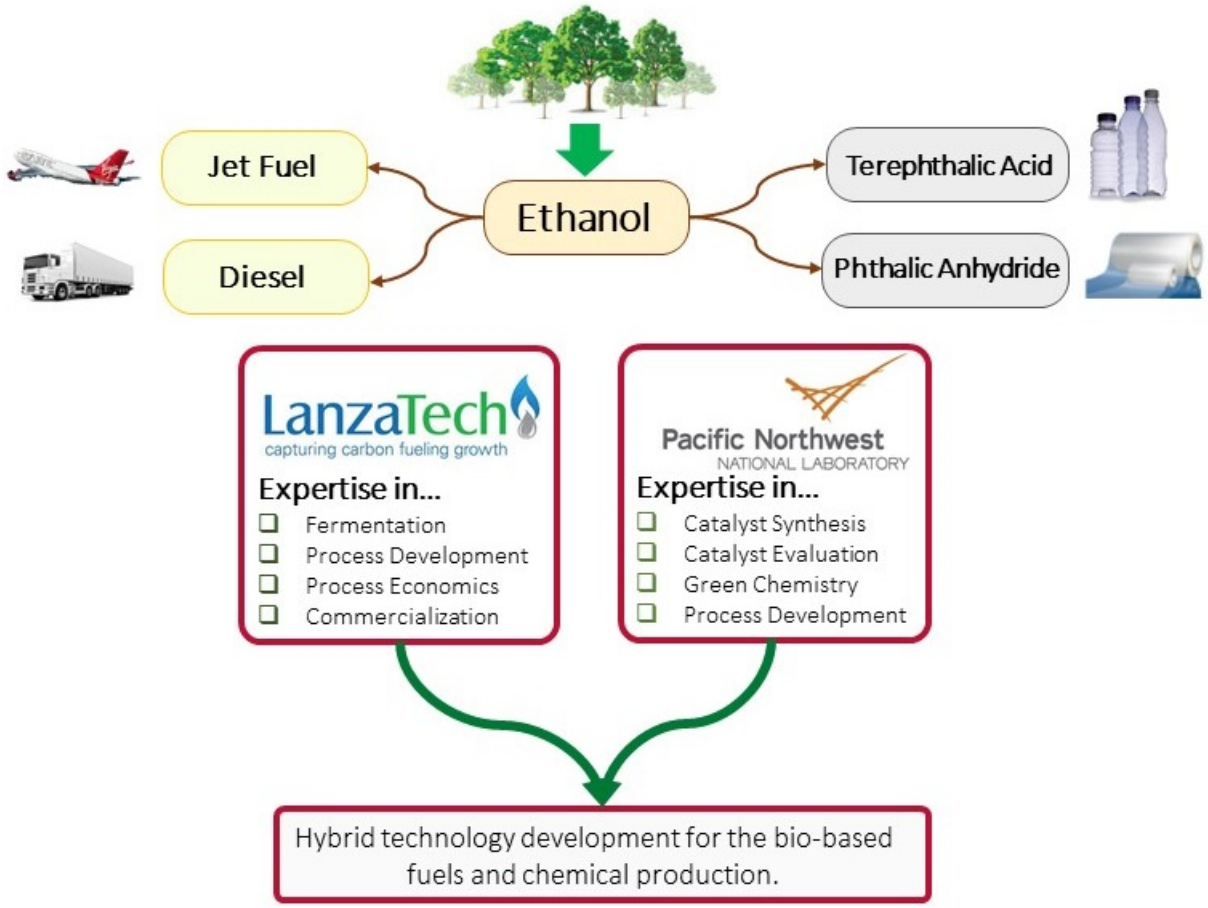


Photo courtesy of Pacific Northwest National Laboratory

OVERALL IMPRESSIONS

- A narrow focus effort with some level of productive results. Very little detail was provided on any aspect of the system, making this difficult to evaluate. Parts of the review criteria were omitted completely (i.e., a statement from the industrial partner).
- Producing aromatic aldehydes is an attractive addition to the ethanol upgrading portfolio. Consistent with other DFAs, it is difficult to assess the technical merit and progress due to a relatively high-level presentation, but overall, this seems like a technology that has some potential.
- Although this project is in the early stages, it feeds into BETO's long-term strategy for the flexible integrated biorefineries chemical pathway options. The project lead should continue to engage

ChemCatBio's resources and seek support for the next generation of catalytic materials in the future work.

- The PNNL/LanzaTech project to produce renewable precursors to terephthalic acid from ethanol is a route to a higher-value product that can lower the cost of coproduced fuels. Terephthalic acid is an important target because of the desire to create beverage and other containers with biomass-derived plastics. This project builds on the platform of finding higher-value use for biomass-derived ethanol. This project contributes to this effort; however, there are other approaches to preparing PET and other renewable substitutes that may be more attractive.

- Seed one-year project to verify if the chemical pathway proposed is viable for utilization of ethanol being produced by LanzaTech. The group seems to have a large degree of freedom in terms of selection of catalyst and process. New expertise and new processes for aldol condensation can be of advantage to the consortium despite the narrow focus that brings justification for BETO's investment. Parts of the review criteria were omitted completely (i.e., statement from the industrial partner).

- Initial results from the two-bed reactor system have demonstrated a very significant improvement in yield—from 10% or 20% to about 50%. The description of how additional improvement to the level of 70% yield was achieved was not provided.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The thoughtful comments provided by the reviewers are greatly appreciated. As mentioned by the reviewers, producing aromatic aldehydes is an attractive addition to the ethanol upgrading portfolio and the successful outcome of this project will feed into BETO's long-term strategy for the flexible integrated biorefinery chemical pathway options.

- We regret not including the statement from LanzaTech. As mentioned during the presentation, LanzaTech highly appreciates the PNNL collaboration and their statement is as follows, “This research has the potential to provide a high-yield pathway from ethanol directly to C8 aromatics without the yield loss to paraffins and higher aromatics. This pathway would provide an opportunity to leverage LanzaTech’s sustainable ethanol into the PET supply chain. This project is in the catalyst discovery phase, TRL 2–3. This type of work requires expertise, resources, equipment, and a skilled staff in the catalyst discovery space, to which LanzaTech does not have access.”

- We recognize the other renewable approaches to prepare PET. Compared to other routes, this process has advantage to produce C8 aromatics at high yield due to the nature of chemistry and mild operating temperature. In addition, the cogeneration of hydrogen from this chemistry enables the balanced biorefinery to produce fuels and chemicals in tandem. Current selectivity to the C8 aromatic aldehyde is ~60% and this is due to the generation of hydrogenated products from the feed and intermediates. Incorporation of gallium in the catalyst will reduce the hydrogenation and improve the product selectivity. A series of modified zeolites are being investigated to increase the *p*-methyl benzaldehyde to approximately a 20% level through isomerization.

- This project is in the early phase, so the work was not protected by patents at this time, and this made it difficult to present the technical details in the public forum. Our goal is to document all the information in the data management operated by the ChemCatBio consortium at the end of this project.

CHEMCATBIO DFAS: TACTICAL AVIATION FUELS WITH GEVO

Los Alamos National Laboratory

PROJECT DESCRIPTION

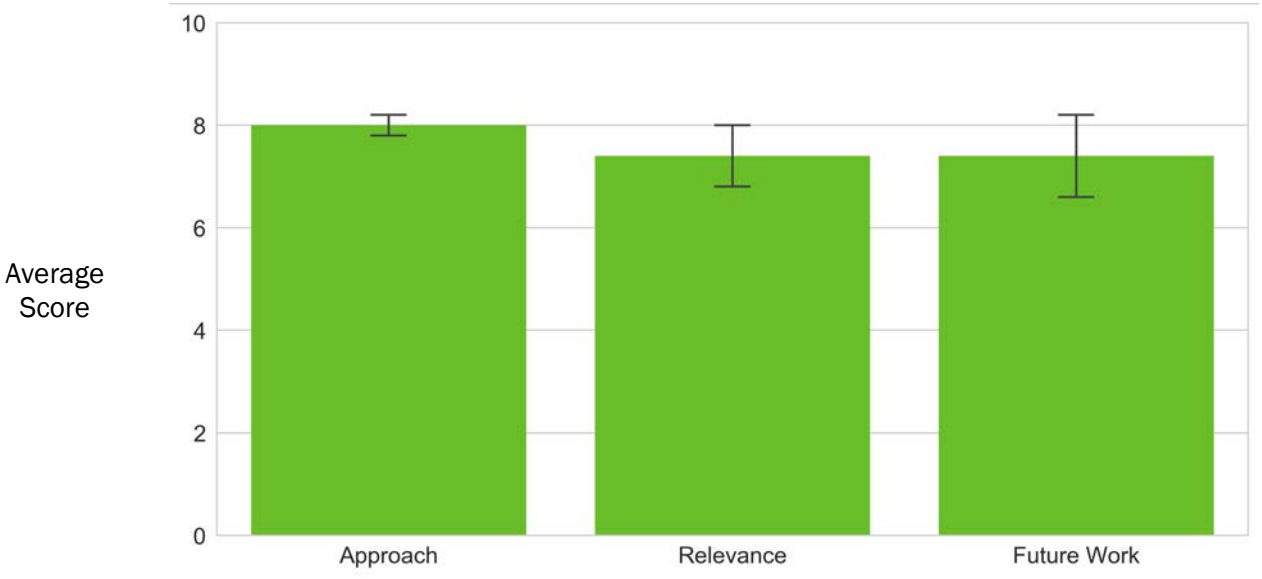
WBS:	2.3.1.702
CID:	NL0033622
Principal Investigator:	Dr. Andrew Sutton
Period of Performance:	4/1/2018–3/31/2020
Total DOE Funding:	$667,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$667,000
DOE Funding FY19:	$0
Project Status:	New

Increasing the energy density of an aviation fuel is nontrivial. Current branched-chain saturated hydrocarbons suitable for unleaded kerosene (Jet A-1) or Jet Propellant 8 (JP-8) applications produced by Gevo have a density of 0.76 g/mL and have an energy density of 33.44 MJ/L. While this exceeds the specification for ASTM D1655 7566 for aviation turbine fuel, performance advantaged fuels with higher energy densities are desirable. Increasing the density and energy density can be achieved through dimerization and cyclization reactions, and in particular through the formation of strained ring systems. For example, cyclobutanes can add approximately 100 kJ/mol of energy through ring strain alone and dimerization further increases the energy density. However, typical dimerization of olefins is performed industrially using strong acid catalysts such as sulfuric acid or hydrofluoric acid, which presents handling and environmental concerns and generates large quantities of corrosive waste to either dispose of or recycle.

We aim to use Gevo intermediates to produce higher energy density fuels in order to provide a performance advantage over current aviation fuels.

Weighted Project Score: 7.7

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



I One standard deviation of reviewers' scores

OVERALL IMPRESSIONS

- Overall, the project has some innovative ideas applied to upgrading of unfunctionalized alkenes to jet fuels. The link between the Los Alamos National Laboratory (LANL) performers and the company is clear. The multifaceted approach allowed some progress on this exploratory project. The path forward in both success areas and tasks needing improvement (copper sensitizers) is clear. Additional details about milestones, catalyst systems, and rationale for a photochemical over a thermal approach would have been valuable.
- This project aims to upgrade olefins from the Gevo process into targeted cyclobutene-type molecules to dramatically improve the energy density of jet fuels. This is based on some type of [2+2] addition reaction that is photoinitiated. It may be helpful to consider the scale of cyclopentenone availability (suggested to come from CFP) in comparison to Gevo alkenes and aviation fuel markets, which might provide a better assessment of whether the work will ultimately be practical at scale.
- The chemistry is interesting from a science-elegance standpoint, working through the enone-ene intermediate and then doing the coupling. The research appears to offer opportunities in solid alkylation conversions as well following a reducing step. Enone-ene production rates from Gevo should be disclosed and the other constituents present in an actual feedstream. More mechanistic details should be offered regarding the partial hydrogenation of the carbonyl group to produce the final cyclic alkane at the end via a phenol intermediate. If so, this is not a trivial step and the reactor exotherms may become dangerous at scale and difficult to control along with the catalyst. More information regarding the poisoning of this catalyst should also be gathered, especially those with the potential for trace metals like silicon or copper and some other things at parts-per-billion levels. The issue of ring strain in the presence of mostly straight molecules in kerosene hydrocarbon should be examined by fuel oxidation stability testing. Naphthenes may not be present at high amounts in some Jet A compositions and the influence of visible light on fungible mixtures should be determined.
- Production of high-performance tactical aviation fuels is an important target for both military and commercial projects. This is a very early-stage proof-of-principle project with a long road to commercialization. Photoreactors are not common in the chemical processing industry and are generally costly. However, gaining experience with photoreactors would significantly add to the repertoire of the laboratory. Production of less-costly alternatives to JP-10 is an important target for the national defense community and a side benefit of the program. The product would provide a source of income to Gevo while it is going through its development phase.
- This is something of a high-risk, high-reward project. If the [2+2] cross coupling can only be achieved with an external reagent, the impact will be severely lowered. It will be exciting to see if a photocatalyst (ultraviolet or visible) can be found to impact the homocoupling of the Gevo substrate.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their thoughtful and helpful responses to our project. We fully agree with them that this is a high-risk, high-reward project and we have tried to develop a stepwise approach towards increasing complexity as we progress to a set of building blocks that can be fully sourced from Gevo product streams. Our initial work was to demonstrate the [2+2] cycloaddition using bioderived molecules, such as cyclopentenone. While cyclopentenone can be produced in small quantities in CFP, it is a known product from furfural through a set of high-yielding and selective transformations. The efficiency of cyclopentenone cycloadditions led us to incorporate Gevo isopentenes in this reaction approach to produce strained ring molecules. The promising initial physical properties of the resulting cycloaddition products suggest they do have potential for application as high energy density fuels, assuming the long-term stability of these cyclobutanes can be demonstrated. Further expansion to use Gevo isopentenes as the sole carbon building blocks is ongoing and following analysis of these potential fuel molecules we will attempt to develop a feasible and economic strategy to produce these molecules at scale.

CHEMCATBIO DFAS: IMPROVED VALUE OF THE GASOLINE AND FUEL OIL COPRODUCT FRACTIONS WITH LANZATECH

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

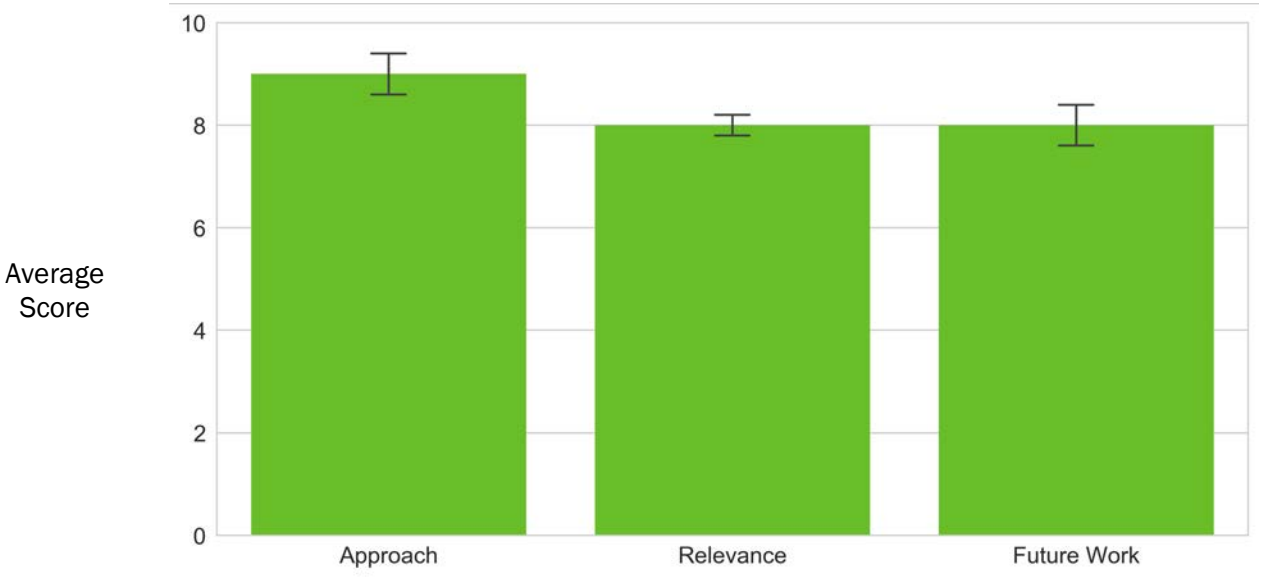
The ChemCatBio consortium invited industry to partner with national laboratories and leverage ChemCatBio capabilities in late 2017. LanzaTech, a small biotech company, led the charge to answer a challenge that all integrated biorefineries must face—finding a market or use for all carbon entering the plant, a necessity for economic and environmental sustainability. PNNL's alcohol-to-jet (ATJ) process primarily yields synthetic isoparaffinic kerosene in the jet range. This project is increasing the value of the gasoline (light) and fuel oil coproduct (heavy) fractions. The technical goals of this project are to (1) increase the research octane number (RON) of the lighter-than-jet gasoline fraction above 98 and (2) create a synthetic lubricant base oil from the heavier-than-jet fraction.

WBS:	2.3.1.703
CID:	NL0033624
Principal Investigator:	Dr. Rob Dagle
Period of Performance:	4/3/2018–3/30/2020
Total DOE Funding:	$600,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$600,000
DOE Funding FY19:	$0
Project Status:	New

To produce a high-octane RON gasoline blendstock, we are utilizing an intermediate stream from the current ATJ process that is rich in linear butenes. Low-temperature oligomerization of this intermediate has resulted in a lower-than-desired octane rating, restricted by limited branching. Thus, we are investigating high-temperature skeletal isomerization prior to oligomerization, which will result in more branched iso-olefins, thus increasing the RON of the mixture. For example, 2,2,4-trimethyl-1-pentene has an RON of 103, making it

Weighted Project Score: 8.5

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



I One standard deviation of reviewers' scores

a valuable gasoline blendstock component. We are targeting a 98+ RON blendstock that has a cost premium of 25% above gasoline. Shape-selective and non-shape-selective catalysts have been investigated for skeletal isomerization. After isomerization, controlled oligomerization using commercially available strong acid resin catalysts (e.g., Amberlyst-36) has been performed. Thus far, the RON of the gasoline fraction has been increased from 86 to 94. However, in order to reach the target RON of 98, further octane enhancement is required, and this will be accomplished through process improvements and/or by eliminating heavier constituents from the feedstock (e.g., C6+ olefins).

To produce lubricant, we have started to evaluate the isoparaffins that are produced by the heavier-than-jet-fuel oil fraction as a Group III base oil. Group III base oils with four centistokes viscosity have been valued from $3.80–$4.60 per gallon in 2017, a significant value improvement versus diesel spot prices of $1.40–$1.70 per gallon over the same period. Base oils are the name given to the hydrocarbon portion of fully formulated lubricants such as passenger car motor oils. Base oils typically consist of compounds with 18–40 carbons and boil between 288°C and 566°C. ASTM D6074 is the standard for characterizing hydrocarbon lubricant base oils. Group III base oil must contain more than 90% saturates, possess less than 0.03 wt % sulfur, and have a viscosity index (VI) above 120. Isoparaffinic content is a primary contributor to a significantly high base oil VI value. Hydrocarbons produced by the PNNL ATJ process are virtually all isoparaffinic and contain no sulfur. Thus, with minimal catalytic processing, we expect the material will classify as high-value Group III base oil. We are currently investigating hydroisomerization of the greater-than-jet-fraction in order to improve the viscosity index from 100 to greater than 120 and meet the specification as a Group III base oil.

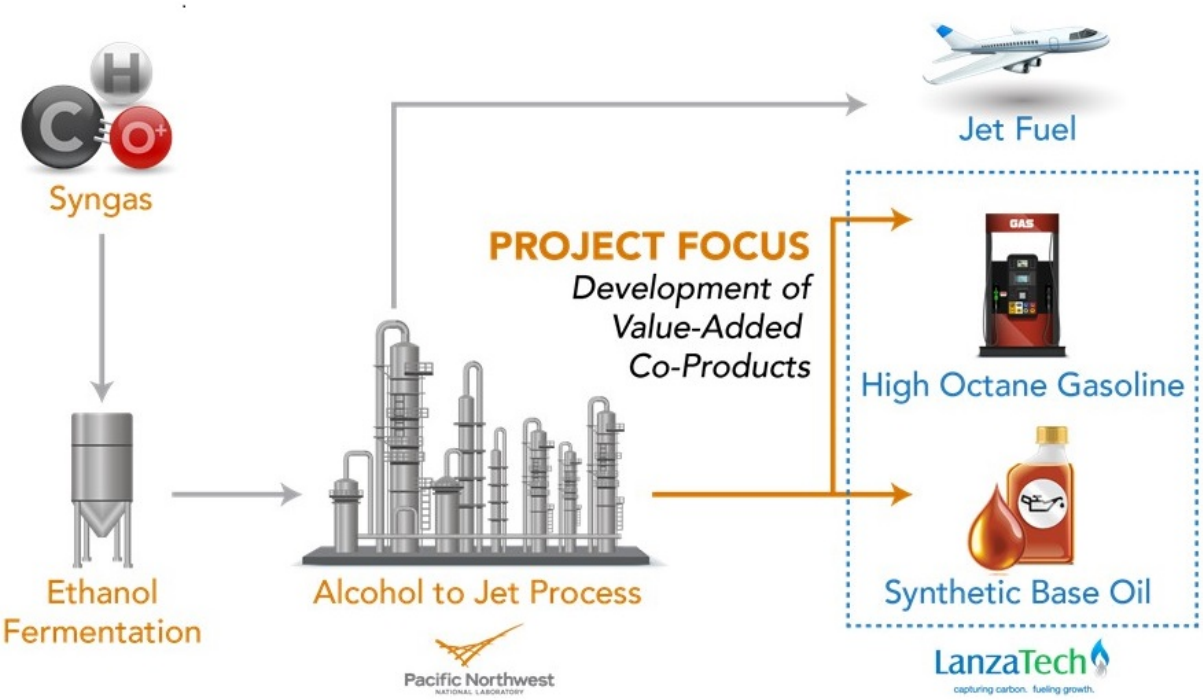


Photo courtesy of Pacific Northwest National Laboratory

OVERALL IMPRESSIONS

- The project continues a unique collaboration between LanzaTech and PNNL. The results look promising to complete the project milestones. There is clear perceived value of having PNNL participate in the studies. While some additional details of the system would contribute to a more thorough evaluation, this is still perceived as a well-organized and potentially successful project.

- I like the effort to make targeted oligomerization products that offer high RON and/or perform well as lubricants. I have some concerns that oligomerization-based chemistries can be very selective, particularly at high temperatures. I think carbenium-type oligomerization will, at these temperatures, probably lean toward a thermodynamically controlled distribution of oligomers, aromatics, cracking products, etc., and it wasn't clear that one could selectively target a specific class at 400°C. I think it might be possible to make isobutene at lower temperatures, provided one can find a way to turn on skeletal isomerization without encouraging too much oligomerization.

- In general, this work is headed in the right direction and is well done so far. The next phase is to work with real feeds that could exacerbate the coking and deactivation events. It is time to discuss the process options with LanzaTech from an engineering design perspective.

- The cooperative project between PNNL and LanzaTech to improve the quality of the gasoline and fuels made from ethanol has good commercial potential. It supports the technology that converts alcohol to hydrocarbons, which is a major potential route for producing biofuels from excess ethanol. Technically, the project should work, and a process can be developed; the questions are the cost versus the benefits. The production of renewable lube stocks is particularly attractive. The project furthers PNNL with LanzaTech, which is already licensing ethanol-to-hydrocarbon technology from PNNL.

- This project makes the most out of ethanol, addressing the previously unattended light and heavy hydrocarbon fractions from the LanzaTech jet fuel process. Strong teams give the sense that success is highly likely. The impact that improving the light and heavy fractions has on the TEA of the overall process would be interesting to see but has not been proposed.

- Develop new reaction routes and process to produce high-quality fuel/lubricants from fermentation-derived feedstocks from LanzaTech. Again, there is a clear advantage to both sides justifying BETO's investment: LanzaTech finds a new market to their product and the consortium creates new knowledge-based processes. Progress is appropriately demonstrated, and future work is commensurate to their goals. There is already a good relationship and technologies licensed from PNNL from work with LanzaTech. The partnership seems solid. While some additional details of the system would contribute to a more thorough evaluation, this is still seen as a well-organized and potentially successful project.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer’s positive comments and agree that this project continues a strong collaboration between LanzaTech and PNNL. This project builds upon the codeveloped alcohol-to-jet process being commercialized by LanzaTech. We appreciate the reviewer’s positive comment about our approach for making a targeted, oligomerized, high-RON coproduct and lubricant.

- We agree with the reviewer that at high temperatures the product distribution is more varied. Selectively producing isobutene at lower temperatures would be preferred; however, controlling selectivity against oligomerization is difficult indeed. Our approach has been to investigate both processing options, each with their own set of challenges. Results thus far indicate that at lower temperatures some degree of branching occurs but not enough to achieve our high-RON target. Operating at a higher temperature produces isobutene, but byproducts are formed, including aromatics—in fact a high-RON constituent—and undesirable cracking products and coke. Ultimately, both approaches will be evaluated with TEA. Here the tradeoff between a high-RON process—requiring more frequent catalyst regeneration and two-step processing—will be investigated versus a lower-RON process with a more simplified process scheme. TEA will also be performed for the lubricant processing and will be included in the final report.

- We agree that working with real feedstocks provided by LanzaTech will be important. We will verify RON and lubricant properties using ASTM methods. Additionally, we will evaluate catalyst stability when using real feedstocks, and study catalyst regeneration.

- We appreciate the reviewers' positive comments about this project having good commercial potential. This project aims to find coproduct opportunities and find value for all of the carbon in the plant. We agree with the reviewer that the production of renewable lubricant is particularly attractive. We note that at the time of the review we had just initiated the lubricant study, as the project began with development of the high-RON coproducts. We have since initiated hydroisomerization studies of the lubricant fraction using metal-promoted zeolite catalysts. We are evaluating the effects of the zeolite structure and acidity on resulting lubricant properties, particularly viscosity.

CHEMCATBIO DFAS: CATALYTIC PROCESS INTENSIFICATION OF BIO-RENEWABLE SURFACTANTS PLATFORM WITH SIRONIX RENEWABLES

Los Alamos National Laboratory

PROJECT DESCRIPTION

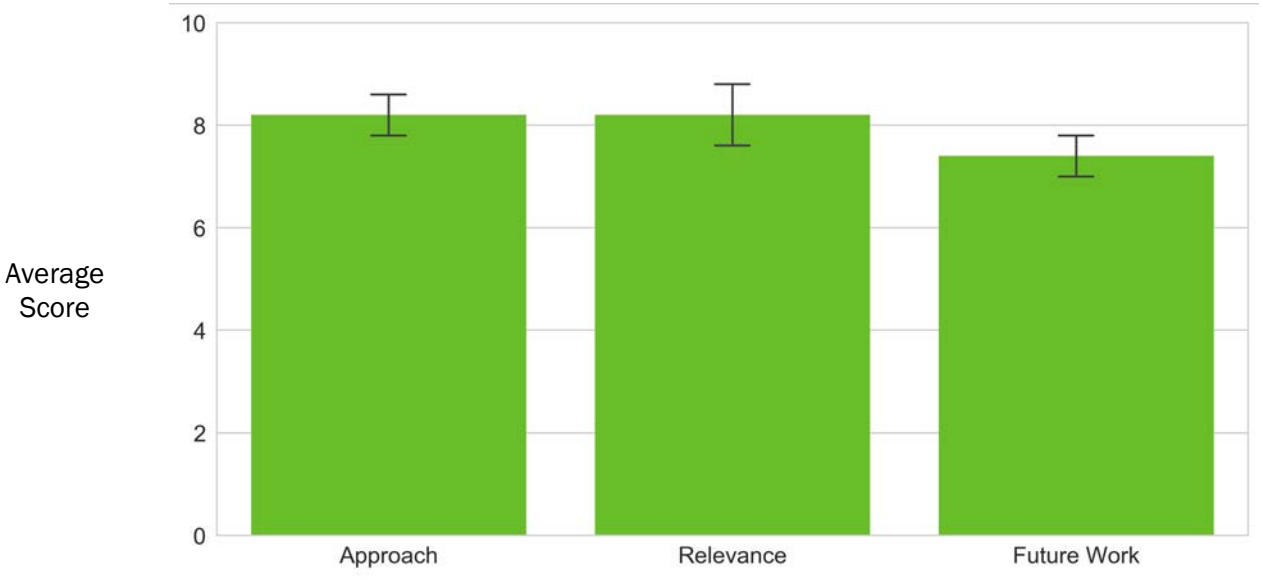
WBS:	2.3.1.704
CID:	NL0033626
Principal Investigator:	Dr. Andrew Sutton
Period of Performance:	7/1/2018–6/30/2020
Total DOE Funding:	$667,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$667,000
DOE Funding FY19:	$0
Project Status:	New

Surfactants are the key active ingredient in cleaning products, with long lists of additional builder ingredients added to boost function while maintaining product safety and shelf life. These builder chemicals increase product cost and volume and biodegrade poorly. Sironix Renewables has invented a new class of surfactants, called Oleo-Furan Surfactants (OFS), which eliminate the need for these additional chemicals, reducing volume and resulting in a product that biodegrades readily. Our OFS link the function of bio-based furan building blocks with natural oils to produce multifunctional and eco-friendly cleaning products. Our technology gives improved performance, and by eliminating builder chemicals, we reduce the volume (and therefore packaging) by 30%. This reduces overall energy consumption while producing a more environmentally friendly product.

The proposed joint research project with Sironix Renewables is designed to leverage the catalytic reaction engineering, catalyst development, and furan chemistry resources of the ChemCatBio consortium with the

Weighted Project Score: 8.0

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



I One standard deviation of reviewers' scores

surfactants platform of Sironix Renewables to accelerate the DOE-invented and DOE Small Business Innovation Research-funded technology toward market commercialization. Technical goals include process improvements to achieve efficient scale-up of existing surfactants and the development of a new class of furan-based structures to address an emerging market need for nonionic surfactants.

OVERALL IMPRESSIONS

- The project seems like a strong and successful collaboration. The link to the LANL performers is clear and perceived as a benefit to the industrial partner. Significant progress has been made on the project. Future work on the project is well delineated in time and metric milestones. Additional details on scarcely mentioned aspects of future work would have strengthened the case for expansion of the project into new areas involving computational and catalyst characterization.

- The furan coupling approach/play into the surfactant market seems like a viable pathway with high margins. Work is being done on optimizing an industrial problem that impacts commercial margins directly when progress is made on the project. Current lab setup looks reasonable with the batch reactor configuration. There is a good approach to demonstrate yield improvements over the current state-of-the-art copper-chromium mixed oxide-based catalyst under same conditions and even optimized conditions. The chemistry is sound and reliable to reproduce under the observed operating conditions. It appears that there are even more opportunities to reduce space time even more and go out further with time on stream (TOS) with an hydrodeoxygenation (HDO) catalyst operating at 99% conversion. Partial HDO seems like it will be tricky to scale even though lower pressures of 150 psi are used. Process safety hazard analysis should start early. Feed composition currently has 3 wt % of reactant in the feed, so increasing the concentration in future work to keep equipment sizing modest could be a near-term goal. The project team should continue to benchmark with commercial catalyst materials in parallel and develop a technology milestone chart to visually see progress. There has been good progress achieved in this work thus far.

- This is a really interesting technology that may have a fairly short-term path to market, in that it specifically targets performance-advantaged bioproducts. This is perhaps due to the nature of the DFA program, but it is challenging for an external reviewer to comment on progress as technical details are relatively sparse. I had some concerns about the ways that stability and selectivity are being assessed. They may not be appropriately benchmarked, and it may give a false impression as to the origin of enhanced selectivity and/or stability.

- The initial catalyst development for both the carbon-carbon coupling and HDO of the intermediate appear to be quite successful. Additional process intensification would be achieved if both reactions could be conducted simultaneously (though no explanation was given for why this might work), and if the process could be demonstrated to work in continuous mode.

- The collaboration with Sironix Renewables has a clear short-term commercial target. The production of nonionic surfactants is a good approach to adding value to biomass-derived furans. The product is an example of a bioadvantaged chemical. A new surfactant was discovered by the LANL group. There has been good progress in a short period and has already transferred materials to Sironix Renewables, LANL's industrial partner. The project is very likely to produce a commercial product.

- This is a new technology to accelerate and develop an emergent market of new surfactants.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the opportunity to present our current results on this successful CRADA with Sironix Renewables. Our collaboration to this point has been extremely productive and we acknowledge the reviewer’s comments regarding the need to fully investigate our catalysts in terms of recyclability, stability, and effective lifetimes. Our initial efforts for the nine months of the project presented at peer

review were focused on developing alternative catalysts to those currently employed to increase overall yield and selectivity to the desired product, a task which was achieved and successfully transitioned from batch to continuous flow reactors. As we refine and optimize the reaction conditions, we are excited to probe the extent and limits of our catalyst performance in order to fully support the commercialization efforts of Sironix Renewables, which will include a TEA of a fully refined process.

DIRECT CATALYTIC CONVERSION OF CELLULOSICS

National Renewable Energy Laboratory

PROJECT DESCRIPTION

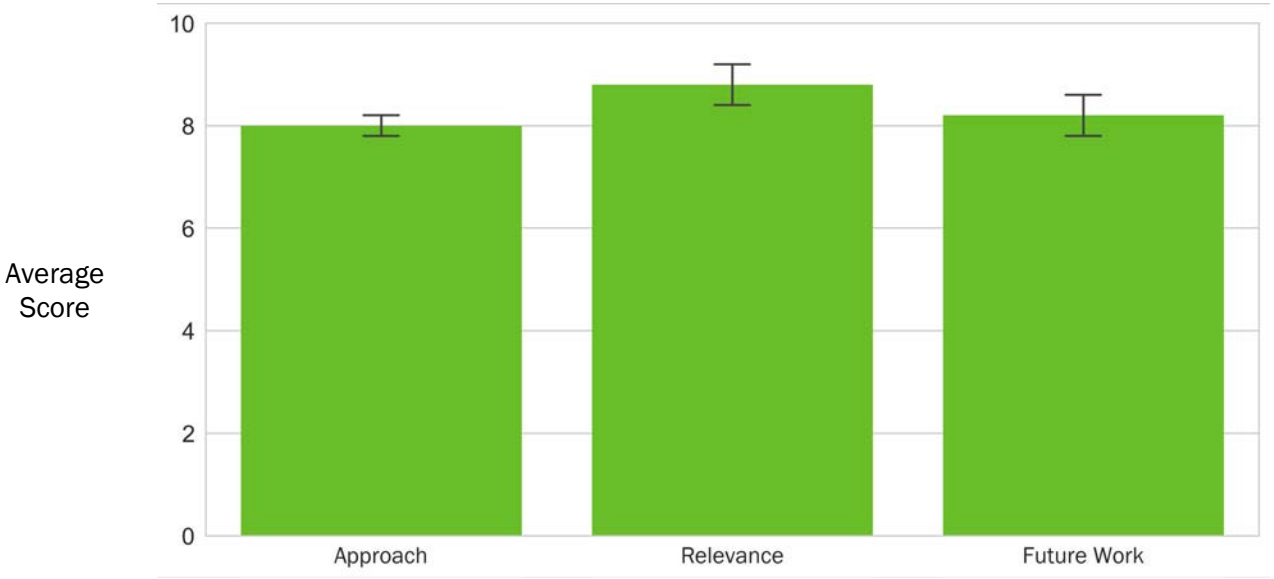
The Direct Catalytic Conversion of Cellulosics (DC3) project is set out to (1) develop a semicontinuous solvolysis and chemo-catalytic process to upgrade cellulosics residuals from woody biomass and (2) evaluate the resulting mixed oxygenate products for fuel applications. The abundancy of delignified cellulosics from the pulp and paper industry, as well as a byproduct from a lignin-first biorefining process, offers the opportunity to valorize an inexpensive feedstock to performance-advantaged fuels. While enzymatic hydrolysis is a leading and highly selective approach for cellulosics depolymerization, it can be economically challenged by recalcitrant feedstocks that require high enzyme loadings. As such, direct solvolysis with chemo-catalytic conversion is a promising alternative for delignified woody feedstocks.

WBS:	2.3.4.503
CID:	NL0034402
Principal Investigator:	Dr. Derek Vardon
Period of Performance:	10/1/2018–10/1/2020
Total DOE Funding:	$200,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$200,000
Project Status:	New

DC3 aims to develop a dual-bed semicontinuous design with the capability to separate biomass feed and catalyst to overcome the inherent challenges associated with the current state-of-the art batch processes. These challenges include: (1) problematic separation of feed and catalyst, (2) challenging scale-up considerations, and (3) convoluted reaction network for solvolysis and monomer conversion. In addition, DC3 has the advantage of being able to utilize the same initial biomass, reactor system, and solvent system employed for biomass delignification during lignin first. Following lignin removal, DC3 can convert the cellulosic residuals from lignin first to C2–C6 aliphatic alcohols for fuel applications.

Weighted Project Score: 8.3

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



I One standard deviation of reviewers' scores

DC3 is a new start seed project within ChemCatBio that will leverage the consortia's catalytic process development capabilities. Collaborators from the enabling capabilities include the ACSC task, as well as the Catalyst Cost Model Development task. In addition, DC3 will interface closely with lignin first to coordinate on feedstock and solvent selection, as well as the Co-Optima consortia to leverage the latest fuel property prediction and characterization tools.

DC3 will achieve its first phase objectives by (1) synthesizing, characterizing, and testing various multifunctional mixed metal-oxide catalyst designs and correlating their properties to product distribution; (2) outfitting a high-temperature, high-pressure dual-bed semicontinuous reactor for testing downselected catalysts; and (3) evaluating the fuel properties of oxygenated products and tuning catalyst and process variables to improve target product yields.

Preliminary data obtained in the first 25% of the project will lay the foundation for future work. In FY 2019 and FY 2020, research efforts will focus on (1) preparing delignified biomass as the feedstock for DC3; (2) establishing analytical methods for the complex solid, liquid, and gas product mixtures; (3) benchmarking in-house catalyst design against commercial formulations and evaluating the effects of catalyst properties on product distribution; (4) commissioning a high-temperature, high-pressure dual-bed semicontinuous reactor to test reactivity and stability of downselected catalysts; (5) assessing the mixed oxygenate product fuel properties; and (6) integrating the process with preliminary TEA in conjunction with lignin first. Milestones are crafted to measure progress towards success outcomes with risk analysis and go-no-go decisions to refine options.

In summary, DC3 employs a science- and engineering-driven approach with a collaborative team to enable a pathway to advantaged oxygenated fuels from residual cellulosic biomass.

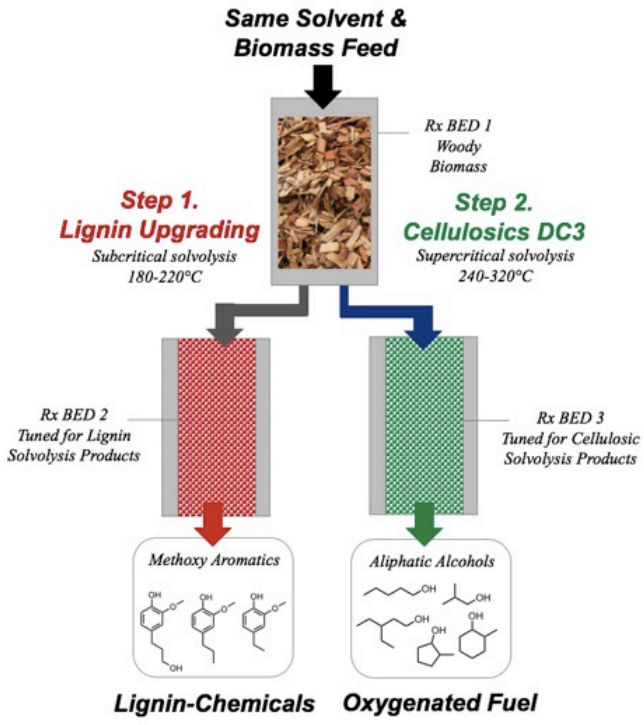


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Overall, a very thoughtful project which clearly defined goals, approaches, and future directions of the seed effort. Makes a clear connection to the characterization efforts of ChemCatBio but could provide stronger connections to other ChemCatBio capabilities. The integration with the solvolysis portion of the processing could have been further delineated, as only catalyst development may not lead to an effective semicontinuous process.

- This project is in the early stages, but it has a very straightforward, clear pathway to success with the proper support team, tools, and knowledge-leveraging resources throughout ChemCatBio.

- TEA has made it clear that biomass upgrading is unlikely to be economical without lignin valorization, and lignin-first approaches have emerged in response. They seem more amenable to lignin upgrading than conventional lignin removal by, for example, Kraft pulping, and so should have an impact on valorization and possibly be more economical. This project is aimed at devising technologies to upgrade the residual carbohydrate fraction, in particular, converting them into monooxygenates by solvolysis and (probably) hydrotreating. Academic partners already working in this area appropriately inform this project. I like the interface with the Co-Optima project to determine what type of upgrading will provide the best biofuel/engine design.

- Direct catalytic conversion of cellulose couples a lignin-first separation with continuous direct cellulose conversion. It provides another potential route to renewable fuels and chemicals. This is an early-stage low-TRL project that evaluates an emerging approach that is receiving increasing attention in the literature. There are several groups that have evaluated organosolv and subcritical water separations coupled with fermentation of the obtained cellulose. Any direct catalyst conversion process could replace fermentation in these processes. The mixed aliphatic alcohol products are not a drop-in fuel and will require a follow up to ensure their utility. This would likely fall under the Co-Optima program, as discussed in the presentation.

- Seed project from the Catalytic Upgrading of Biochemical Intermediates effort and coordinated with lignin first.

- The conversion of dissolved cellulosics left over from lignin-first processing is a superb example of utilizing all the carbon in biomass feed. The research plan is thought out in detail and is very involved—so much so that the adequacy of the budget is in question.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate that the reviewers of the DC3 project found value in our approach to convert a residual waste stream from lignin-first processing. Per the reviewers' suggestions, DC3 will continue to focus on transitioning to semicontinuous processing in close coordination with lignin valorization efforts to ensure feedstock and process consistency with harmonized economic analysis. In addition, future efforts will focus on the biomass solvolysis step, as we agree this is as important as the catalytic upgrading step. Interactions with the Co-Optima team will help de-risk the novel oxygenates as a fuel. The DC3 team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

CONSORTIUM FOR COMPUTATIONAL PHYSICS AND CHEMISTRY

Oak Ridge National Laboratory

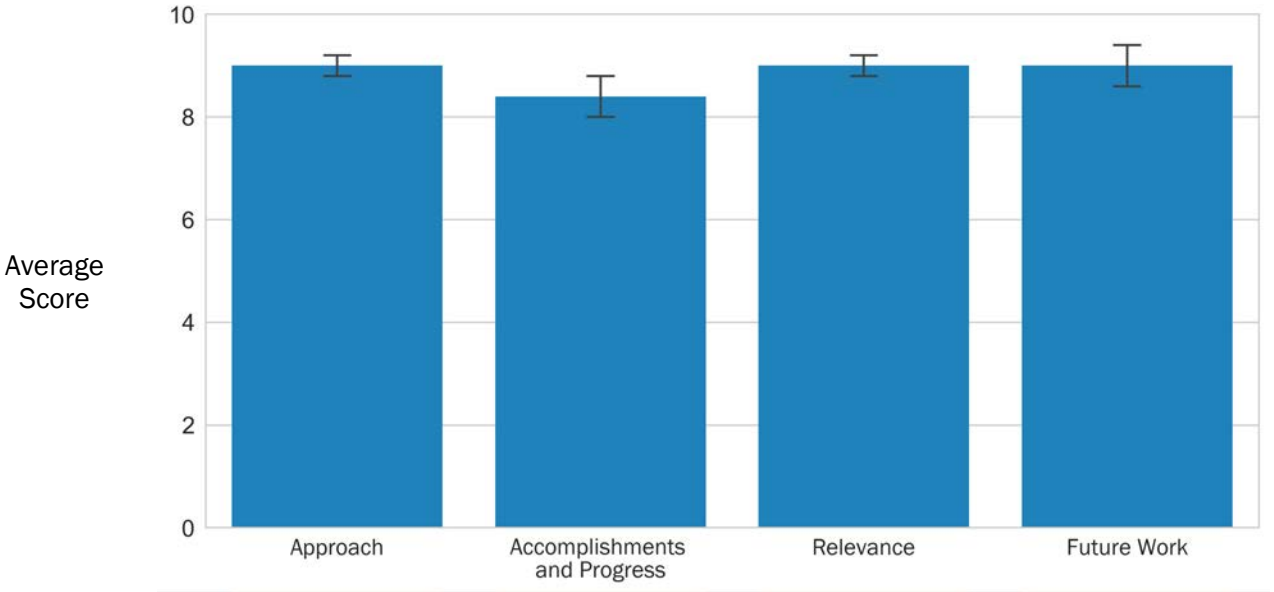
PROJECT DESCRIPTION

WBS:	2.5.1.301
CID:	NL0025890
Principal Investigator:	Dr. James E. Parks II
Period of Performance:	10/1/2015–9/30/2021
Total DOE Funding:	$12,854,800
DOE Funding FY16:	$3,144,000
DOE Funding FY17:	$3,150,000
DOE Funding FY18:	$3,280,400
DOE Funding FY19:	$3,280,400
Project Status:	Ongoing

The ChemCatBio-enabling project Consortium for Computational Physics and Chemistry (CCPC-CCB) accelerates progress in catalytic conversion R&D through theoretical simulation of surface chemistry reactions to enable ChemCatBio experimental teams to achieve the BETO targets for each conversion technology (e.g., goal of $2/GGE fuel for CFP). Furthermore, the CCPC-CCB enables verification of core BETO pathways via modeling of conversion reactions and critical transport phenomena at meso and process scales. Overall, the CCPC-CCB verifies scalability and translation of biocomplex surface science technologies to biomass-to-fuel product conversion processes at scales relevant to the bioenergy industry. Our mission is to utilize core computational capabilities across the DOE national laboratory system to enable and accelerate the development of new materials and optimize process scale-up to advance the bioenergy economy. The CCPC-CCB is a well-developed and actively functioning consortium that combines synergistic technical capabilities across five core national labs (ORNL, ANL, NREL, PNNL, and the National Energy Technology Lab) and critical collaborating partners to advance bioenergy research rapidly and cost effectively. The consortium began in FY 2013 by request of BETO Director Jonathan Male to develop a cohesive plan and structure for modeling activities in the conversion program. The specific technical focus and scope change as needed based on needs identified by collaborating BETO experimental projects and feedback provided by

Weighted Project Score: 8.8

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



I One standard deviation of reviewers' scores

industry through an advisory panel and periodic program peer reviews. As such, the CCPC-CCB represents a flexible and rapid response team of computational expertise to enable success toward critical BETO objectives. The enabling aspect is a core tenet of the project, and close collaboration with partner experimental projects is essential to success. The CCPC-CCB provides a culture to promote the necessary technical exchange and collaboration, which is key to achieving the project objectives.

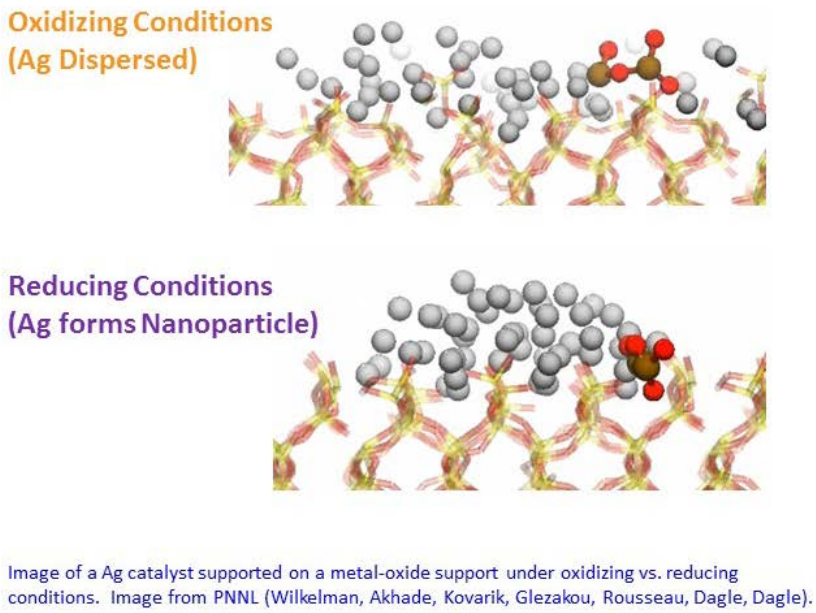


Photo courtesy of Oak Ridge National Laboratory

OVERALL IMPRESSIONS

- A well organized, expansive center-level effort, which did an excellent job of demonstrating its pervasive value throughout ChemCatBio. Tends to lean a little more toward the basic science side than most ChemCatBio projects, but this has advantages. The center strives to continue to increase level of systems complexity in new proposed projects, which can still lead to significant technology impact while also contributing to basic science.

- CCPC is a strong organization with a good foundational direction. Experimental validation will always continue to be the key to computational programs, building both the researchers and process design engineer's confidence as a reasonable agreement is reached at all scales. This consortium is equipped with all the right resources.

- CCPC was the first consortium-type project and is still a role model for demonstrating the potential impact of the approach on many different projects centered at multiple labs. The organization and management of the project are major factors in its success. It shares its findings and methods both within and outside BETO projects. The approaches taken by the CCPC team are the scientifically sound applications of mathematical models to problems that arise from biomass conversion technologies. They have established two goals for the project involving catalyst selection and scaling function for one technology. Establishing these types of general goals as a metric for the consortium project enables a more objective evaluation. However, the work of the consortium is much more expansive and impacts many different projects.

- This is a very impressive effort that covers many scales of catalyst/reactor performance. It will be interesting to see continued outputs from this work going into the evolving data hub. I think machine-learning algorithms might be a great fit for these multiscale reactor models as they can lump much of the model complexity and avoid much of the effort in parameterization and model solution, but still allow meaningful predictions about reactor performance.

- The operation of the CCPC is what all the enabling capability projects might aspire to. What a solid, helpful, impactful consortium.

- The goal of providing a computational toolset developed by CCPC and facilitating the modeling of biomass industrial technologies from atomic to process scales, thereby reducing the cost, time, and risk in commercializing bioenergy technologies, is certainly an important cross-cutting capability. It's a very large effort with a large outreach that is also involved with other BETO consortia (especially the relevant Bioprocessing Separations Consortium). It involves many national labs and has evolved throughout the years. It tends to lean a little more toward the basic science side than most ChemCatBio projects, but this has advantages. In addition, the group is encouraged to pursue partnerships with the existing basic science programs. The approach is comprehensive and involves many scales, and the group is commended for investing in the kinetic work, which is absolutely necessary for this effort. CCPC strives to continue to increase level of systems complexity in new proposed projects which can still lead to significant technology impact while also contributing to basic science.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Regarding feedback in specific areas, we agree that the data hub and associated machine-learning tools offer interesting opportunities for modeling. We intend to further support the data hub and will seek opportunities for machine-learning applications. However, we intend to be cautious with machine learning to ensure that our modeling outcomes have a tangible science-based underpinning, which is critical to the accuracy of our results.

- We agree completely that experimental validation is a critical aspect of our efforts. We have benefited greatly from validation data supplied by our experimental colleagues, and we intend to grow the interactions with experimentalists as we move forward. Specifically, we seek to jointly define critical experiments that will yield specific model parameter data critical to accurate model predictions.

- Thank you for the reinforcing guidance to (1) leverage the basic science programs and (2) continue to define and apply kinetics. Our liaison approach of defining a specific person to track key partnerships, such as with the basic science catalysis program, is relatively new but has provided benefits to date, and we will continue that approach to strengthen our awareness and connections to the basic energy science programs. Our kinetics efforts are relatively new as well but are critical to bridging ChemCatBio catalysis successes to larger scales. We will continue kinetics development in close collaboration with our experimental colleagues.

- The CCPC appreciates the numerous positive feedback comments on our project’s approach, organization, accomplishments, relevance, and future work. We appreciate the compliment on the wide range of scales we are addressing, and we consider our multiscale approach to be critical to success. We also thank the reviewers for the compliments on the impacts demonstrated across many projects in the BETO program.

CATALYST COST MODEL DEVELOPMENT

National Renewable Energy Laboratory

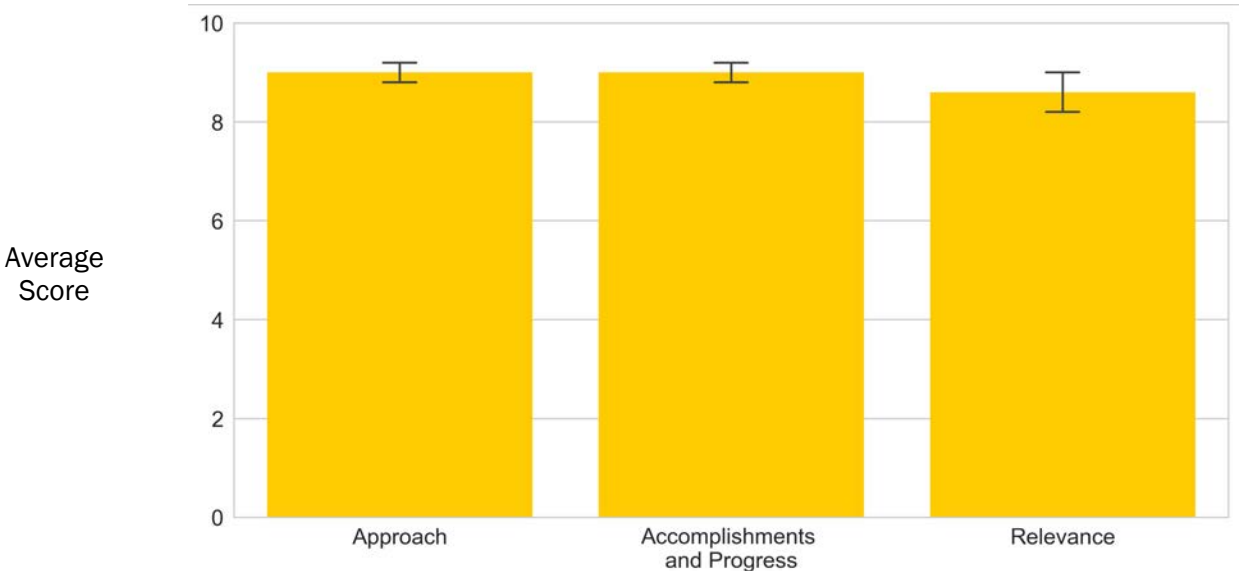
PROJECT DESCRIPTION

WBS:	2.5.4.301
CID:	NL0030154
Principal Investigator:	Dr. Fred Baddour
Period of Performance:	10/1/2015–9/30/2018
Total DOE Funding:	$900,000
DOE Funding FY16:	$300,000
DOE Funding FY17:	$300,000
DOE Funding FY18:	$300,000
DOE Funding FY19:	$0
Project Status:	Sunsetting

The goal of the joint NREL-PNNL Catalyst Cost Model (CCM) project was to develop a free and publicly available catalyst cost estimation tool that enables rapid and informed cost-based decisions in early-stage research and commercialization of catalysts. This goal was successfully realized in October 2018 with the release of the complete web- and spreadsheet-based CatCost™ tool, online at catcost.chemcatbio.org. CatCost is a first-of-its-kind, publicly available tool for determining the costs of precommercial catalysts that employs state-of-the-art estimation methods coupled with an intuitive user-interface and comprehensive visualizations. CatCost dramatically simplifies the process of assembling cost estimates for precommercial catalysts, enabling synthetic chemists and process design engineers alike to prepare rigorous early-stage economic assessments for the production of catalytic materials. This information enables researchers to (1) focus R&D efforts on areas of greatest cost, (2) make informed decisions based on combined performance and cost data, and (3) guide catalyst synthesis early in development. CatCost was industrially reviewed throughout its three-year development to ensure the accuracy and relevance of the integrated estimation methods and tailor the user interface based on expert feedback. This presentation will highlight the cost estimation methods developed and integrated in FY 2017 and FY 2018, the methodologies for considering spent catalyst value, and demonstrate use cases in which CatCost has been successfully deployed to give insight to the value proposition of catalysts being developed within BETO's catalysis portfolio.

Weighted Project Score: 8.9

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



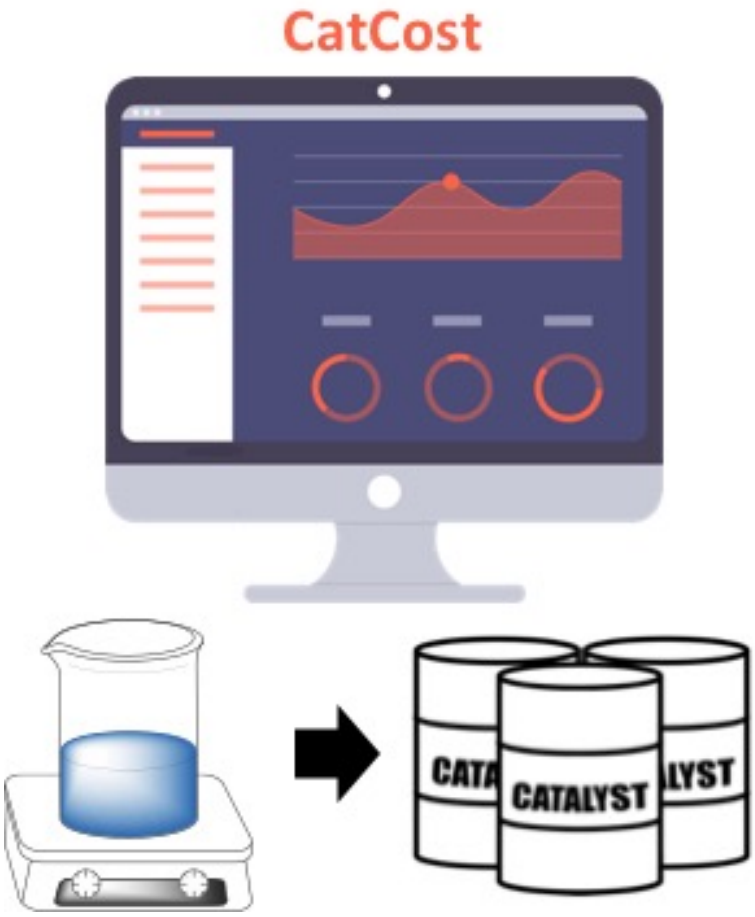


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- The concept of a catalyst cost estimation tool for R&D professionals designing and characterizing new catalytic materials that show technical promise is invaluable. Often, the engineering design basis has to make many assumptions by using the most similar commercial catalyst in order to provide a reasonable estimate for the novel catalyst. With catalyst costs making up close to 4%–20% of the MFSP for some bioenergy pathways, an estimation tool to help design engineers avoid a "show-stopping" commercial factor when moving the project along to greater scales and higher risk is essential. Now with this tool, researchers can make resource priorities at the R&D and front-end loading (FEL)-0 conceptual design phases for projects.

- The catalyst cost-estimating tool is an extremely useful tool for biomass conversion and all chemical processes. The project team has done a remarkable job of collecting the data and rolling it into a usable model. They have produced a usable user interface that is freely accessible to the public. They have included appropriate safeguards to protect internal and external user data because the spreadsheet input and outputs are only stored on the user's computer. Reclamation costs for the catalysts are included. However, the recycling costs do not reflect the consequences of U.S. Environmental Protection Agency regulations, which limit the storage, recycling, and disposal of smaller quantities of catalyst. Also, the market dynamics of metal prices are not adjusted for the new demand added by the catalyst manufacture.

- This is a very nice complementary effort to general catalysis research in the field. It allows those working in a range of fields from material design to scale-up to account, at least partially, for catalyst cost. It's a huge outcome to provide a user-friendly tool to the community, and this group has been very active in improving awareness and educating potential users. Overall, to be commended. There may be slight concerns over deployment and whether a nonexpert can use the tool to generate a meaningful cost, particularly for a more complex catalyst, but the project leads have taken some measures to ensure the robustness of the tool.

- Public availability of a catalyst cost-estimation tool is a service to the field and helps provide more accurate TEA of a particular process. The impact of the work is diminished to the extent that catalyst cost is usually a small percentage of capital and operating costs. What works: Appears to be an accurate method to evaluate costs for precommercial and novel catalysts. What doesn't work: Can't necessarily address nonstandard methods of synthesis.

- The project has successfully developed an excellent tool for both ChemCatBio and the greater catalysis community. It has already shown direct impact on the consortium and will be a valuable tool for researchers and educational efforts moving forward. Some level of continued oversight should ensure the tool evolves to meet the needs of ChemCatBio and other users. It is only focused on catalyst cost, which averages about 10% of total process cost, including process costs to produce the catalyst, which somehow limits the impact. It would be interesting to see mechanisms of incorporating new synthetic methods in the tool. BETO should be encouraged to keep some funding for the maintenance and improvement of the tool. It is especially important to get input from the advanced synthesis effort.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's feedback and hope that the tool will prove to be valuable in helping researchers prioritize resources at early R&D stages.

- We appreciate the feedback about the utility of the tool and agree that there are some limitations regarding waste handling and market dynamics. We agree that there are a number of external influences that may affect catalyst price and have sought to include these types of boundary conditions into the documentation to make users aware of the potential impact of market and policy factors on catalyst manufacture.

- We thank the reviewer for their insight and agree that there is always a tradeoff between accuracy and complexity. The CatCost tool has been released in two versions with this in mind, with a more visually oriented online interface and a companion spreadsheet that is more flexible and customizable.

- We agree with the reviewer that there are some limitations to the tool regarding nonstandard synthesis methods, but we have included some process templates for synthetic methods that may fall into this category (e.g., millifluidic nanoparticle synthesis). We concur that increasing the types of synthetic methods and templates that are included in the tool will increase the value and reach of the tool.

- We appreciate the reviewer's feedback and hope that we can continue to expand the tool to include additional synthesis methods and manufacturing techniques to be better aligned with the advanced synthesis efforts that are ongoing within the ChemCatBio consortium.

ADVANCED CATALYST SYNTHESIS AND CHARACTERIZATION

National Renewable Energy Laboratory

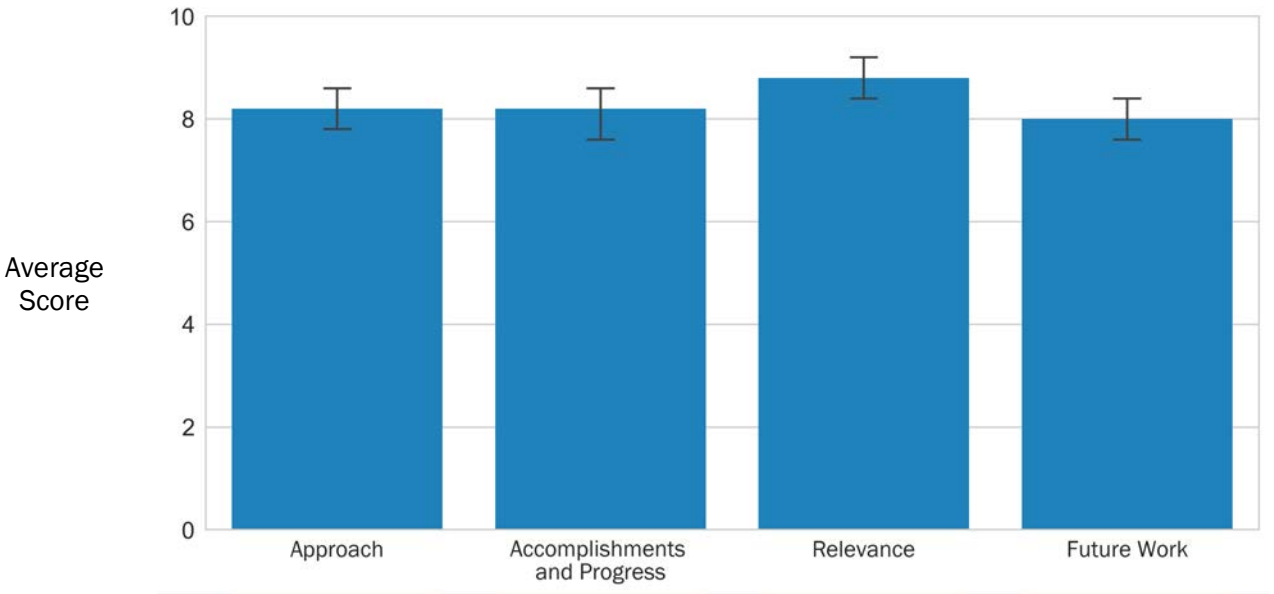
PROJECT DESCRIPTION

WBS:	2.5.4.304
CID:	NL0032282
Principal Investigator:	Dr. Susan Habas
Period of Performance:	10/1/2017–9/30/2019
Total DOE Funding:	$4,427,500
DOE Funding FY16:	$0
DOE Funding FY17:	$1,492,500
DOE Funding FY18:	$1,342,500
DOE Funding FY19:	$1,592,500
Project Status:	Ongoing

The ACSC project provides fundamental insight into critical research challenges leading to actionable recommendations for ChemCatBio catalysis projects by leveraging world-class synthesis and characterization capabilities across multiple DOE national laboratories. The ACSC was based on a collaboration between ANL and NREL, in which X-ray absorption spectroscopy (XAS) studies performed by ANL at the Advanced Photon Source (APS) user facility coupled with experimental work at NREL identified the active sites responsible for the enhanced performance of a copper-modified zeolite catalyst for the conversion of dimethyl ether to hydrocarbons. This highly successful collaboration identified a need for access to advanced characterization for all ChemCatBio catalysis projects. As the ACSC, this collaborative effort was expanded to encompass (1) *in situ* and operando spectroscopic techniques for bulk and surface structural and chemical characterization, including XAS at ANL, Raman spectroscopy at NREL, and neutron scattering at the Spallation Neutron Source at ORNL; (2) *in situ* and operando spatially resolved imaging and characterization, including sub-ångström resolution electron microscopy and spectroscopy at the Center for Nanophase Materials Sciences at ORNL; and (3) a dedicated synthetic effort focused on developing next-generation catalysts through innovative synthetic routes, including solution synthesis methods for highly controlled nanostructures at NREL and metal organic frameworks at Sandia National Laboratories (SNL). As a

Weighted Project Score: 8.3

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



I One standard deviation of reviewers' scores

ChemCatBio-enabling technology, the ACSC works closely with the CCPC and the Catalyst Deactivation Mitigation for Biomass Conversion project, with cost insight from the CatCost tool, to (1) identify active site structures in working catalysts, (2) inform computational models to predict structures with enhanced performance, and (3) deliver cost-effective next-generation catalysts that exceed performance targets. The ACSC portfolio of capabilities is reevaluated annually to ensure that we are meeting the evolving needs of the ChemCatBio catalysis projects as well as tackling overarching research challenges to enable rapid response to new conversion technologies. Since the start of the project, the ACSC has collaborated with all of the ChemCatBio catalysis projects to provide fundamental insight leading to actionable recommendations for critical research challenges, supported the 2022 engineering-scale CFP verification by enabling improvements to catalyst performance that minimize the loss of carbon, and directly interacted with industry through the nearly 50% of ChemCatBio DFA projects that are leveraging ACSC capabilities and expertise. The ACSC has also facilitated the complete catalyst and process development cycle for the dimethyl ether to hydrocarbons pathway, leading to next-generation catalysts with increased dehydrogenation activity. The end of the three-year goal is to rationally design bimetallic zeolite catalyst formulations with tailored dehydrogenation-hydrogenation activity to enable products with targeted fuel properties. The capabilities and expertise developed for this effort will be leveraged to develop next-generation metal-modified zeolite catalysts with increased C3–C6 olefin selectivity during the conversion of ethanol to distillates, and to assess the accelerated catalyst and process development cycle with the goal of enabling demonstrated performance enhancements in half the time.

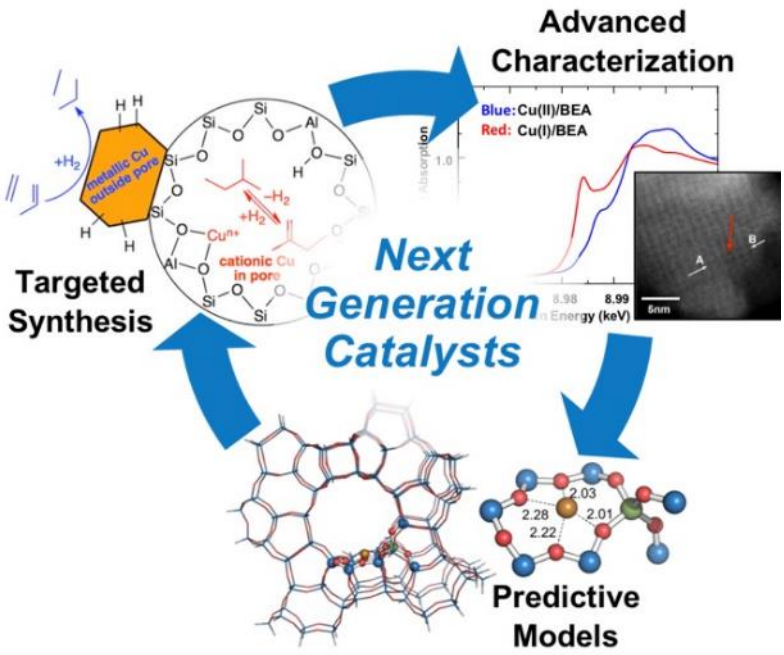


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- Overall, a well-integrated activity that strengthens the entire ChemCatBio project portfolio. The expertise of the group complements the needs of the ChemCatBio projects. The value has been demonstrated in past and existing projects. The future projects ask clear questions, which the current characterization efforts assist in answering. The attempt to remain responsive to the needs of the

ChemCatBio portfolio by introducing new techniques is very important but should continue to be evaluated so the right tools are used in the appropriate settings.

- The ACSC is another solid, good technical story coming out of ChemCatBio with money well invested and the scientific discovery return on investment very important. The ACSC is a well-managed project knowing where their targets, challenges, and milestones lie. They should be applauded by ChemCatBio for their ability to work together across labs as a unified organization that will most likely change the trajectory of the biofuels industry. Their work is impressive, and they understand that they must create actionable recommendations that also allow for practical implementation.

- The ACSC project can impact most of the process development work supported by BETO. The characterization portion of the project has clearly impacted a number of BETO projects and has helped several bioeconomy startups. The synthesis portion is less evolved and has not yet had a major impact. However, it is difficult to show the clear benefits of fundamental research in this area in the short term. It is a high-risk, high-reward project. Most new catalysts are not successful. The work done by the ACSC team is similar to that conducted as part of R&D at leading commercial and government catalyst and development labs throughout the world. There is wide agreement that this work is worthwhile. What makes the ACSC team unique is the focus of the BETO mission and integration into the BETO project teams. One area in which the project is lacking is in the ability to prepare industrial-style formed catalysts. The BETO team relies on outside industry groups to provide this expertise and to prepare the volumes of these types of materials required for testing.

- This is a nice foundational effort that really goes toward enabling all other upgrading research within the various DOE-supported consortia. Susan Habas gave an excellent presentation. It is really difficult to make sense of catalyst performance without an accompanying effort in controlled synthesis and characterization. I like the nice effort toward characterizing materials under reaction conditions and/or complex media (to the extent that the capabilities will allow). Our conventional approach has been to study the reactor performance of a material under steady-state conditions, where the structure of the material is almost certainly different from the synthesized material. This effort goes toward addressing that discrepancy.

- The ACSC project is vital to the entirety of ChemCatBio and meshes nicely with CatCost and CCPC. One area which might be added to the portfolio is a controlled deposition of metal precursors onto catalyst supports (as opposed to solution synthesis of nanoparticles [NPs] followed by deposition). This suite of methods did not appear in the presentation.

- The goal of providing fundamental insight leading to actionable recommendations for critical research challenges by leveraging world-class synthesis and characterization capabilities across multiple DOE national laboratories is certainly a core need for all the projects within the consortium. Integration with the ChemCatBio Data Hub seems to be working really well and the researchers are encouraged to continue this effort. The attempt to remain responsive to the needs of the ChemCatBio portfolio by introducing new techniques is very important but should continue to be evaluated so the right tools are used in the appropriate settings. For instance, neutron efforts should be evaluated to make sure it is suitable for the work being emphasized in this project, as well as have a good justification for inclusion of MOF synthesis work. Also, the synthesis portion of the project was downplayed relative to characterization efforts and should be better highlighted in the future.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for the positive feedback regarding the value of the ACSC project to the ChemCatBio catalysis projects and fully agree that it is important to remain responsive to the needs of these projects and to continue to create actionable recommendations to support the catalysis portfolio.

- We agree that the characterization component of the ACSC has been impactful and was well highlighted during the review, and we will make similar efforts to highlight the synthesis capabilities similarly in the future. The synthesis platform has been critical to advancing the state of technology for a number of catalysis projects. For example, within the IDL project, the synthesis of model catalysts with defined active sites was essential to enabling the identification of the active site for dehydrogenation by operando characterization. Realization of the next-generation catalysts, identified by the CCPC, relied on targeted synthesis methods to controllably incorporate dehydrogenation and hydrogenation active sites. We are addressing the absence of technical catalyst synthesis capabilities by engaging with the Engineering of Catalyst Scale-Up project that started in FY 2019.
- As part of the review, we sought to highlight what we believe are the unique capabilities of the ACSC, including advanced synthesis methodologies. However, the controlled deposition of metal precursors and impregnation-based methods are core components of our catalyst synthesis capabilities and have been instrumental in the development of model catalysts and next-generation materials for the IDL and CFP projects.
- We are encouraged by the reviewer's thoughts on introducing new capabilities into the ACSC project and we will continue to evaluate the suitability of the techniques for the catalysis projects. The neutron scattering characterization and MOF synthesis efforts will be subject to a go-no-go decision point to assess their ability to meet the needs of the consortium, as will all future efforts.

CATALYST DEACTIVATION MITIGATION FOR BIOMASS CONVERSION

Pacific Northwest National Laboratory

PROJECT DESCRIPTION

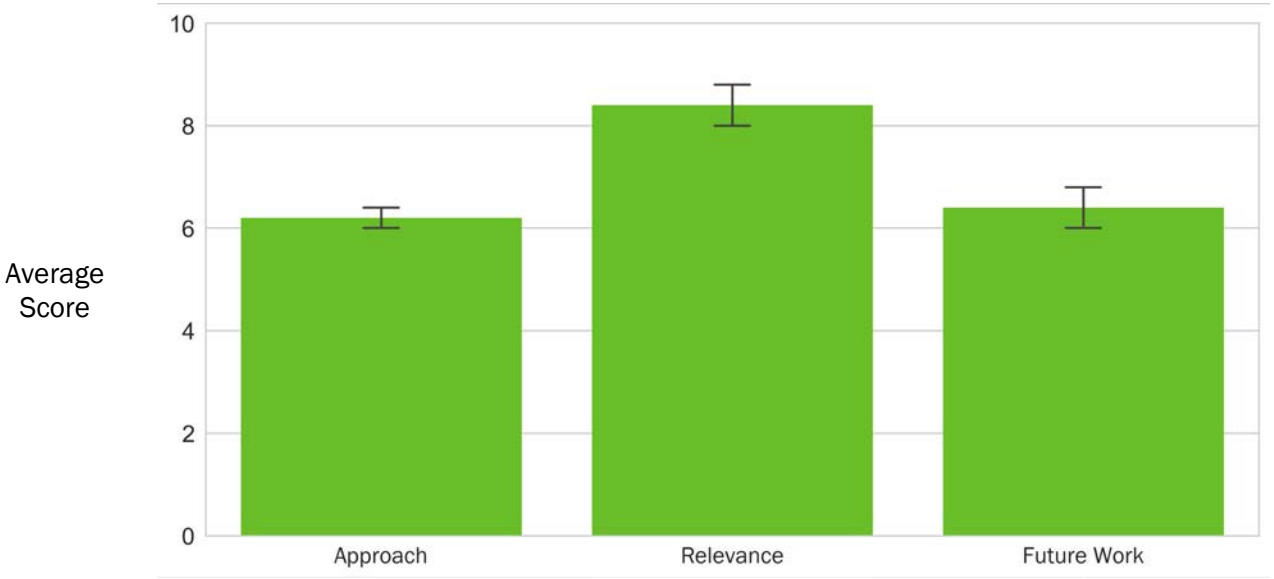
This project is a new "enabling" capability of ChemCatBio for addressing catalyst deactivation issues associated with catalytic conversion of biomass materials. Industrial catalyst lifetimes are on the order of years, while catalysts being developed under ChemCatBio may not see times on stream beyond 500 hours while in early-stage R&D. As an enabling capability, this project serves as an R&D team specialized in correlating catalyst deactivation with characteristics of biomass-derived process streams, identifying catalyst deactivation mechanism, and developing solutions for improved catalyst lifetime, stability, and regeneration.

WBS:	2.5.4.501
CID:	NL0034446
Principal Investigator:	Dr. Huamin Wang
Period of Performance:	10/1/2018–10/1/2021
Total DOE Funding:	$300,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$300,000
Project Status:	New

The concept for this project is based on a systemic need within ChemCatBio to address catalyst deactivation issues. Some unique qualities of biomass materials (e.g., high oxygen content, high moisture content, highly reactive functional groups) bring significant issues to catalyst longevity, which is an overarching challenge for ChemCatBio technologies. Previous successes addressing this challenges include (1) improvement of sulfided catalyst lifetimes for fast pyrolysis bio-oil hydrotreating (extended operation time from approximately 90 hours to 1,400 hours); (2) improvement of reduced metal catalyst for bio-oil hydrogenation (extended lifetime from approximately 150 to 800 hours); and (3) improvement of zeolite catalyst for aqueous phase dehydration of alcohols (over five times improvement of lifetime).

Weighted Project Score: 6.8

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



I One standard deviation of reviewers' scores

This project will achieve greater success by (1) coordinated and formal collaboration with ChemCatBio catalysis projects; (2) systematic approaches to accelerated deactivation evaluation, deactivation mechanism identification, and development of catalyst regeneration protocols; and (3) documenting, publishing, and communicating summaries of the connections established between characteristics of biomass-derived feedstocks and catalyst deactivation for guiding more rational catalyst and process designs. This project will provide needed information on catalyst deactivation and mitigation to catalysis R&D communities. The Catalyst Deactivation Mitigation project directly addresses the catalysis barrier of improving catalyst lifetime and ChemCatBio's goal of accelerating catalyst development and technology readiness for industrial application.

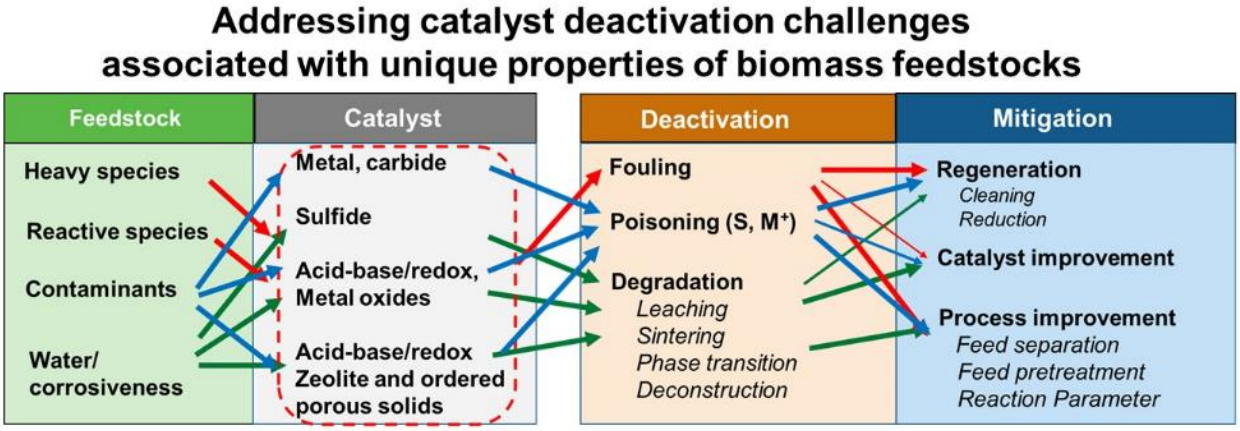


Photo courtesy of Pacific Northwest National Laboratory

OVERALL IMPRESSIONS

- This overarching project, along with the theory program, can be a broad but impactful component of ChemCatBio. The initial systems of investigation are "low-hanging fruit" that have been studied in related systems. However, impact can certainly still result in these studies across all the ChemCatBio portfolio. Management of this component seems in order and will be critical moving forward, as the diverse catalysis-related portfolio may be a challenge to home in on specific challenges for maximum impact rather than spread the project too thin.

- This project has the potential of becoming an entire center of excellence focused on deactivation of catalysts in bioenergy applications. This will require many researchers and possibly much more when the time is right. More industrial partners, especially catalyst OEMs, should be involved in this work. The approach of elucidating the various modes of deactivation, controlling rates, and then establishing accelerated deactivation methods is quite plausible. This project has a huge task and requires many more resources and partners.

- Overall, this is an important project that aims to address catalyst stability in a variety of biomass-upgrading technologies. It would be helpful to see more specifics about the important modes of deactivation in a specific technology, how they will be investigated, how they will be mitigated, etc. The slide deck would benefit from decreasing redundancy; several figures appear repeatedly and did not seem to add substantially to the discussion.

- Catalyst deactivation is a critical reason for the poor economics of a variety of different proposed biomass conversion processes. Highlighting this problem both in terms of finding ways to assess the long-term deactivation rate and design catalysts with longer useful lives may help develop robust cost-effective processes. The project needs to focus on identifying clear targets and approaches. It would have

benefited from a better discussion of the hypothesis involving catalyst deactivation being studied and the approaches. The impact of the project on BETO projects needs to be more clearly demonstrated.

- The goal of the project—to improve catalyst stability (lifetime) for ChemCatBio catalysis projects through understanding catalyst deactivation and developing mitigation approaches—is surely relevant for the core work of the consortium. This reviewer had more concerns about the presentation being too general rather than the overall idea of the project being faulty. It would be interesting to see more solid and articulated ideas on how to provide stability on the more complicated systems being studied in this consortium, such as the multifunctional systems.

- The correlations, mitigation strategies, and documentation to be produced are potentially valuable. It seemed like more homework could have been done by the authors of the proposed work to identify the needs of the consortium, instead of making one of the tasks to find out what the needs are.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their support of the relevance and potential impact of this new enabling project to the overall program and the fundamental importance of understanding and mitigating catalyst deactivation to the ChemCatBio and scientific community.

- We agree that addressing deactivation is a broad and impactful component of ChemCatBio. As an enabling project, one important objective is to support ChemCatBio core catalysis projects, and this project should target the most impactful process and not "reinvent the wheel." We will work with two multifunction catalysts, Pt/TiO_2 catalyst for CFP and Ag/ZrO_2-SiO_2 for ethanol conversion. Both processes are unique and recently developed within ChemCatBio for their specific application, and their deactivation and mitigation still require extensive research to extend/verify their lifetime. The study of the two different multifunctional catalysts for different reactions, including simple alcohol or complicate pyrolysis vapor, will not only improve the individual catalytic process, but also have a bigger impact by providing insights and approaches for addressing catalyst deactivation issues for similar processes.

- We agree with the importance of having catalyst developers being involved. Modification of catalysts is one approach to address deactivation, and this project will provide an understanding to guide catalyst modification. We will specifically focus on catalyst regeneration to enhance lifetime. We will get input from the industry by subcontracting with an industrial consultant and meeting with an industrial advisory board. We will further identify industrial collaborators and access their inputs.

- We developed the specifics about the hypothesis for modes of deactivation, the approach to investigate and mitigate, and the targets with the core team for the two specific catalytic processes. Based on their current experimental results and understanding of activity-function relationship, we hypothesized a possible deactivation mechanism and mitigation approach. The goal is to conduct an analysis of the working catalysts and specify a hypothesis on the deactivation mechanism and verify through controlled experiments or accelerated aging. Based on the determined deactivation mechanism, the mitigation approach will be developed.

- We discussed extensively with the ChemCatBio catalysis teams to identify the need. We will continue to communicate with them to ensure the most impactful needs to be included. The ChemCatBio catalysis teams include various labs and research areas, and will also have an adjustment of scopes and focus areas, especially in FY 2020, for starting a new three-year project period. We will include the task to ensure a good connection and relevance with the core catalysis projects.

CHEMCATBIO DFAS: COMPREHENSIVE CHARACTERIZATION OF MIXED-METAL OXIDE CATALYSTS WITH GEVO

National Renewable Energy Laboratory

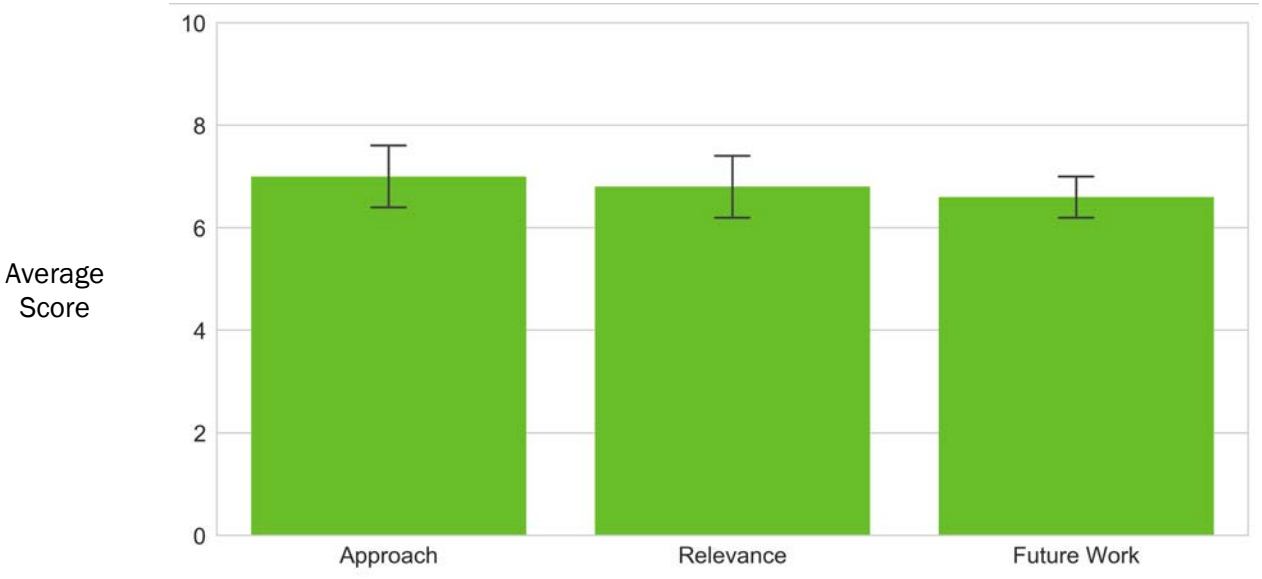
PROJECT DESCRIPTION

Gevo has developed mixed-metal oxide MMO catalysts to selectively convert biomass-derived C2–C6 oxygenates to olefins and then hydrocarbon fuels to meet DOE 2022 fuel targets. Selective conversion of ethanol to isobutylene with mixed-metal oxide catalysts requires low ethanol feeds to maintain performance. Increasing the feed results in rapid catalyst deactivation. Gevo has increased catalyst stability by adding additional metal oxides. However, variations in performance based on the level and type of additive and catalytic conditions have been observed. This project will use advanced catalyst characterization capabilities and expertise available through the ChemCatBio ACSC project to gain insight into key catalyst features and deactivation modes with the goal of tailoring catalyst composition to improve performance.

WBS:	2.5.4.700
CID:	NL0033614
Principal Investigator:	Dr. Susan Habas
Period of Performance:	4/1/2018–12/31/2019
Total DOE Funding:	$125,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$125,000
DOE Funding FY19:	$0
Project Status:	New

Weighted Project Score: 6.8

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



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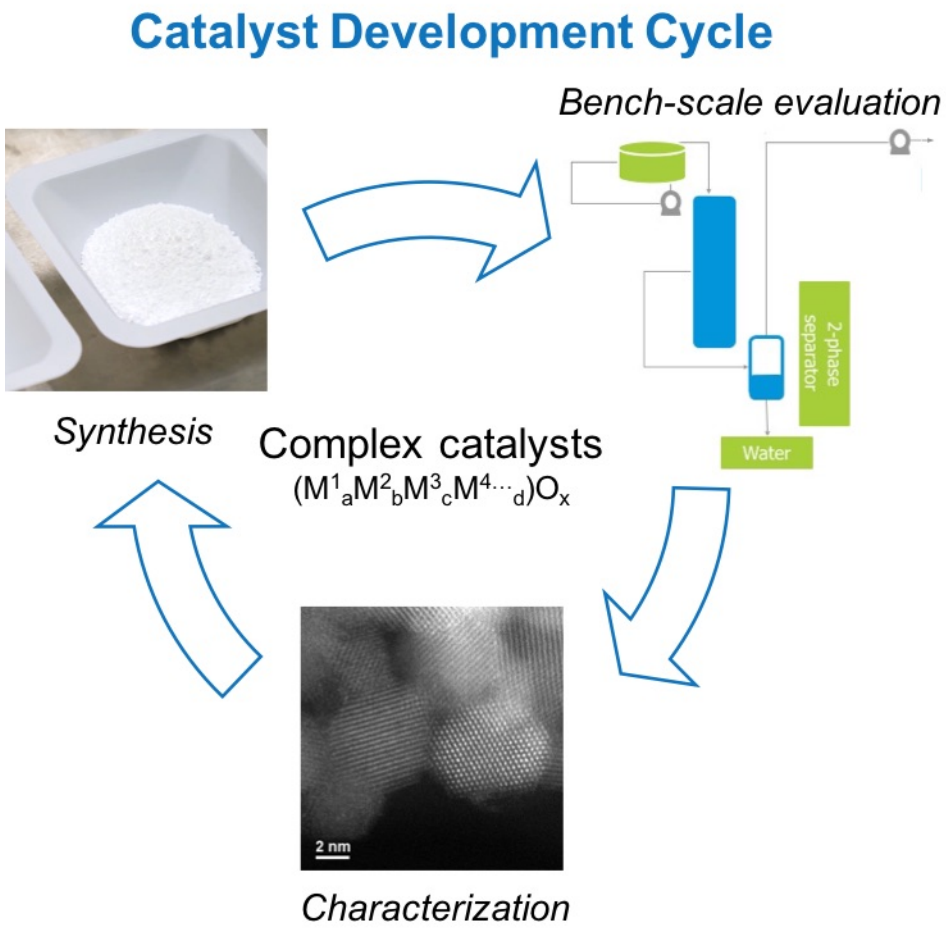


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- This is an early-stage project that fits into BETO's strategy model for working with industrial partners on novel catalytic materials that can be launched in a few years. These types of projects are good to keep in the technology pipeline.
- The direct-funded NREL/Gevo characterization of mixed-metal oxide catalysts provided useful data that would aid Gevo's commercial development. This type of limited, highly focused progress is a good example of how the national labs can help improve the economics of biofuel production. While the impact of this program will be somewhat limited due to its failure to enable a major new product route, it will have an incremental benefit on the cost of ethanol. The mixed-metal catalysts identified could be licensed to other ethanol producers. The technology could also be extended to other light oxygenate streams. The benefits to BETO include developing expertise at analyzing commercial catalysts, proving the consortium can impact industry, building relationships with key players in the bioeconomy, and developing joint intellectual property.
- This is a project that allows Gevo to leverage the expertise of the ACSC. Overall, this seems like a good way to answer questions that Gevo would be otherwise unable to address. Comments raised the issue that characterization revealed deactivation modes, but it did not necessarily provide guidance on how to address them with new synthesis and application strategies.

- The collective team appears to lack the expertise with which to infer from the characterization—which revealed that deactivation was correlated to phase segregation of the mixed-metal oxide—what steps could be taken to stabilize the mixed-metal oxide. One wonders if the CCPC could help out here.

- This mid-cycle DFA effectively outlines how the capabilities of ChemCatBio are leveraged to assist in mixed-metal oxide catalyst development in collaboration with Gevo. The intellectual contribution of the ChemCatBio performers is vital to the project and the clear benefit to ChemCatBio is evident, given expanded expertise gained in synthesis and characterization of the complex catalysts. This new knowledge may well assist efforts in complex catalyst development described in other projects within ChemCatBio. Characterization work demonstrating a structure-performance relationship is clear, but catalyst design goals and stability are yet to be demonstrated.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate the reviewer's positive feedback on the role of novel catalyst development work in collaboration with industrial partners.

- We agree with the reviewer that the highly focused scope of the Gevo project can help to aid Gevo's commercial development. Towards this goal, the project has focused on enhancing the commercial viability of catalysts for both the ethanol-to-olefins process and a new process around fusel oil conversion.

- We agree that it has been helpful for Gevo to be able to leverage the capabilities and expertise of the ChemCatBio consortium, and as such, we have been able to provide them with insight into catalyst deactivation modes. Catalyst development at Gevo based on the insight provided by advanced characterization and corresponding guidance is ongoing.

- With the goal of providing guidance to Gevo around catalyst development based on insights gained from advanced characterization, we have made sure that the team includes catalyst synthesis and characterization experts as well as catalysis researchers from relevant ChemCatBio catalysis projects. We regret our inability to communicate fully the planned catalyst modifications due to intellectual property concerns. However, we agree that collaboration with the CCPC could be useful and opportunities to collaborate will be evaluated.

- We thank the reviewer for highlighting the synergy between industry and ChemCatBio within this project. We agree that the catalyst design and stability goals have yet to be demonstrated, as these are the focus of upcoming efforts in this project.

CHEMCATBIO DFAS: ADVANCED CHARACTERIZATIONS TO ACCELERATE COMMERCIAL CATALYST DEVELOPMENT WITH VERTIMASS

Oak Ridge National Laboratory

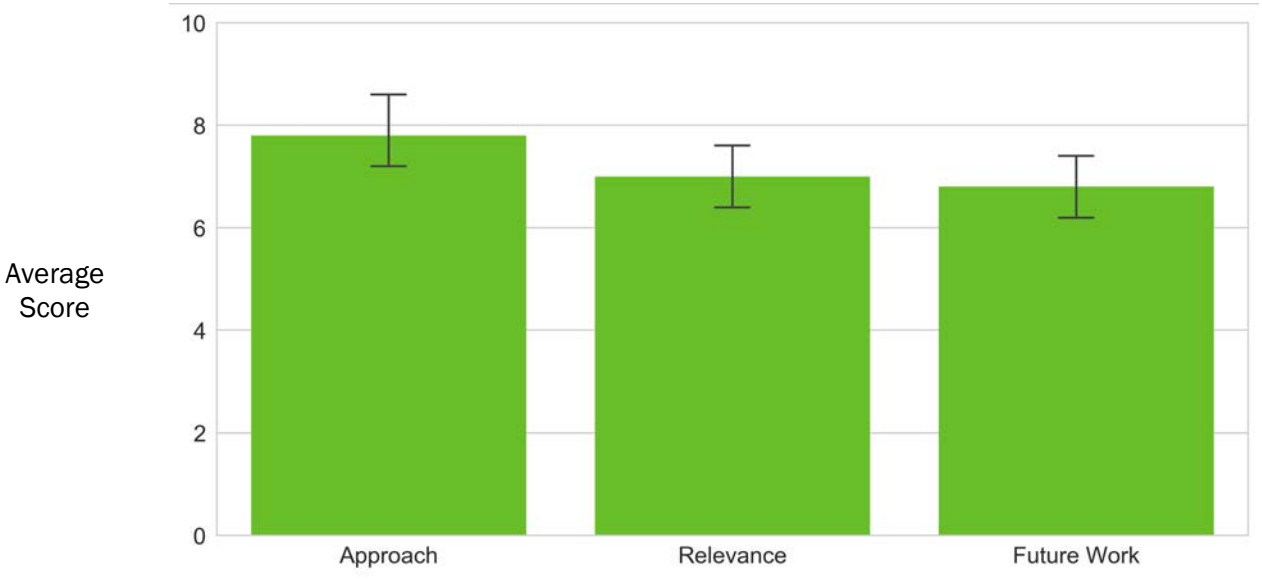
PROJECT DESCRIPTION

The goal of this project is to provide advanced catalyst characterizations to accelerate Vertimass LLC ethanol upgrading commercial catalyst development. Vertimass has a worldwide exclusive license for catalytic technology originally developed by ORNL in 2014 that converts ethanol into hydrocarbons over metal-modified zeolite catalysts. Vertimass is now taking the next critical step in scaling up to commercialize this technology by moving from pilot-scale catalysts to commercial catalysts. There is a critical need in the extensive catalyst characterizations to correlate the structure to catalyst performance, and to further provide critical information during successful catalyst commercialization and reformulation. In this project, we will utilize ORNL, ANL, and NREL's unique catalyst characterization capabilities and experienced staffs to bridge both catalyst synthesis production and catalyst testing at pilot scale (two types of industry partners: a catalyst producer and process engineering company), which will provide valuable catalyst characterization information to accelerate the commercial catalyst development. The characterization information will provide key data to mitigate risk on moving to commercial catalysts, save time and money for both catalyst and process development, and to optimize

WBS:	2.5.4.703
CID:	NL0033618
Principal Investigator:	Dr. Zhenglong Li
Period of Performance:	4/9/2018–9/30/2020
Total DOE Funding:	$325,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$325,000
DOE Funding FY19:	$0
Project Status:	New

Weighted Project Score: 7.3

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



I One standard deviation of reviewers' scores

formulation to improve catalyst performance. More importantly, the lessons learned in this proposed work will have a broader impact on the biofuels and bioproducts industry by providing suggestions to avoid unnecessary catalyst development failures and accelerate their commercialization. More specifically, both fresh and used catalysts will be analyzed to examine the structural and compositional changes after ethanol-upgrading reactions. ORNL, ANL, and NREL will provide the following characterizations to understand these catalysts: (1) ORNL will apply scanning transmission electron microscopy (STEM), X-ray 3D tomography, acid sites measurements, thermogravimetric analysis, physisorption, X-ray diffraction, and elemental composition analysis to analyze the metal distributions, coking, and catalyst structural and compositional changes after the reaction; (2) ANL will utilize *in situ* operando X-ray absorption spectroscopy to understand the metal distributions and oxidation states for both fresh and used catalysts; (3) NREL will use solid-state ^{27}Al nuclear magnetic resonance spectroscopy to examine the changes of aluminum. In the beginning three quarters, this project has provided valuable catalyst structural information to correlate with catalyst performance in the pilot-scale operation. We also developed a correlation between catalyst changes and the water vapor concentration. We will continue to characterize both the fresh and used commercial catalysts to understand the difference between pilot and commercial catalysts.

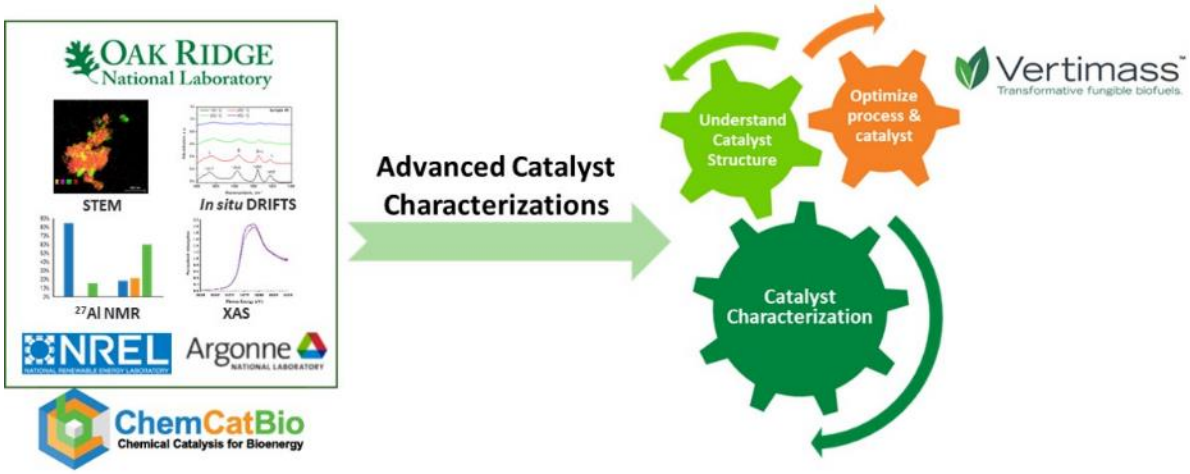


Photo courtesy of Oak Ridge National Laboratory

OVERALL IMPRESSIONS

- This project allows Vertimass to leverage national lab tools and expertise to identify modes of deactivation in their catalysts. It was not completely clear that the project is effectively leveraging prior knowledge from partner Clariant. The presentation did not establish a clear path forward for addressing challenges in future work.
- This project has straightforward goals. Smaller industrial organizations often don't have the characterization tools to do this work, so the efforts of ChemCatBio are commendable to help this effort. The communication plan is appreciated showing how frequently and openly the project members will meet. This is important strategy and should be continued. This type of work takes quite a bit of coordination. There was a lot of effort put into the characterization effort in this work using really advanced methods like extended X-ray absorption fine structure, STEM-energy-dispersive spectroscopy and Al-nuclear magnetic resonance (solid state). These are not inexpensive analytical methods and take significant professional resources to maintain, so a careful project plan must be executed to conserve resources. Other members in the CRADA should get involved in this early work. For instance, it would be useful for Clariant to assist from an industrial perspective on the catalyst characterization activities with one of their quality-control labs. All catalyst manufacturers have quality-control labs offering minimal characterization techniques. It may also be useful to see some overlap in the characterization activities between ChemCatBio and Clariant on some parameters to make sure the reproducibility is reasonable. In general, project stewardship using an official, professional project manager taking on major roles to keep tasks moving and hold targets accountable, also serving as conduit with other third-

party vendors, may be a good strategy for this work. The project team should provide quality assurance specifications on the final catalyst material on behalf of Vertimass to Clariant.

- The ORNL/Vertimass project to characterize their ethanol conversion process provided data that was used to develop improved formulations and operating conditions. The ORNL relationship with Vertimass is a great example of how a national lab can work with a startup to push forward new technology. The production of hydrocarbons from alcohols is one of the most promising routes to biomass-derived fuels. The cost of production is the main limiting factor but leveraging development by using the national labs provides support for this development process. However, this type of catalyst development could have been accomplished by Vertimass' commercial partner Clariant without the help of the lab.
- The project seeks to leverage catalyst development for ethanol upgrading, leveraging the expertise of ChemCatBio performers for catalyst characterization. In general, the partnership shows clear value for the company but not so much for the lab/consortium. It is vital these projects are not ultimately merely service relationships. ChemCatBio is uniquely positioned to participate in the project. A higher level of detail regarding the scientific questions studied and approaches was needed to evaluate the project more effectively.
- This is a relatively simple project on catalyst characterization in which a nicely complementary suite of techniques has been assembled. The interpretation of the characterization data is not well presented and calls into question the ability to further refine the catalyst.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that it's useful to leverage the knowledge from Clariant regarding catalyst scale-up. Due to limited presentation time, we didn't cover the role of Clariant clearly. Vertimass has a separate service contract with Clariant to obtain commercial samples. Clariant is not directly involved in this DFA's R&D work. We do have a clear path forward to address challenges in the future work, including characterization of both fresh and spent commercial samples to understand catalyst changes (if any) during ethanol upgrading.
- We agree that some level of interactions with Clariant will benefit the whole project. The ChemCatBio team is planning to discuss this topic with Vertimass and will try to make a reasonable plan within the scope of the project and in light of intellectual property protection.
- We agree that it's helpful to involve Clariant in some typical scale-up characterizations from an industrial perspective. Meanwhile it's critical for ChemCatBio to be heavily involved. ORNL originally developed the new catalyst and has a broad depth of knowledge about the catalyst structures and performance. It's very important to leverage that knowledge to accelerate the understanding of pilot-scale catalysts and commercial catalysts. ChemCatBio provides unique characterizations (e.g., extended X-ray absorption fine structure, advanced STEM) to help Vertimass understand the catalysts. It's critical to keep the involvement of ChemCatBio to accelerate the catalyst development for Vertimass. This is consistent with the reviewer's comment that ChemCatBio is uniquely positioned to participate in the project.
- Ethanol upgrading represents a revolutionary bioenergy technology to produce fungible hydrocarbon fuels and bioproducts from ethanol, one of the largest biofuels produced in the United States. Leveraging ChemCatBio capabilities to accelerate this type of technology development will help to achieve BETO's mission. It also helps to meet the BETO's goal to enable sustainable, nationwide production of biofuels that are compatible with today's transportation infrastructure.
- Not all the interpretations were presented in this short presentation. The characterization information already provides useful insights to Vertimass to help understand catalyst changes under different conditions. We feel confident that we will be able to further help Vertimass with the next level of catalyst development.

CHEMCATBIO DFAS: ENHANCED CATALYST DURABILITY AND SULFUR TOLERANCE BY ATOMIC LAYER DEPOSITION WITH ALD NANOSOLUTIONS AND JOHNSON MATTHEY

National Renewable Energy Laboratory

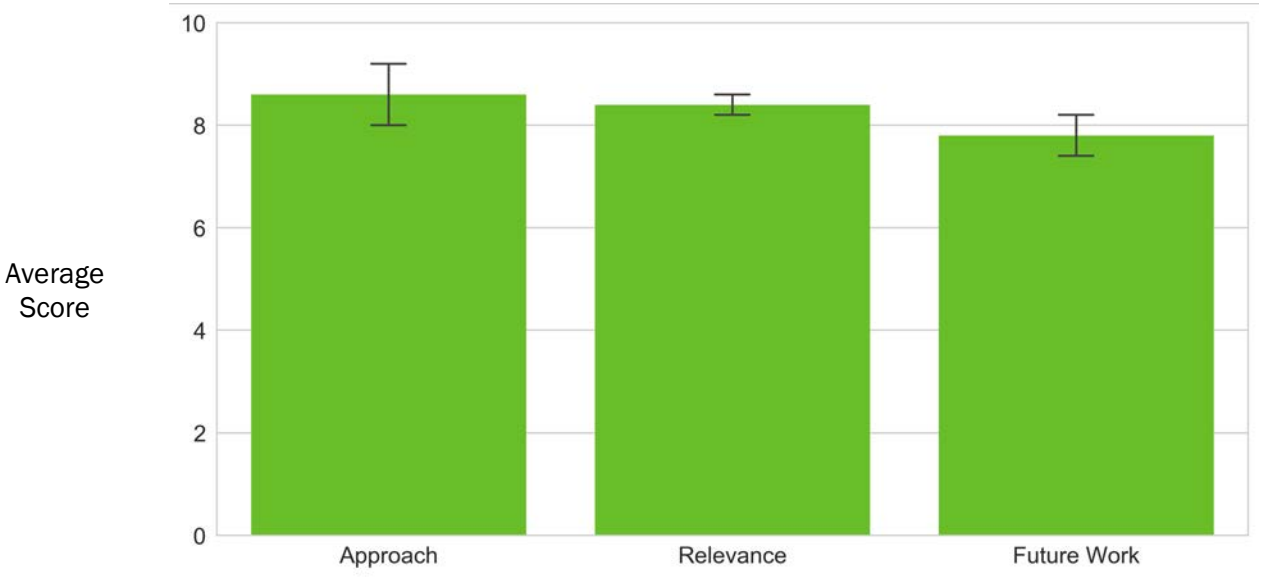
PROJECT DESCRIPTION

One of the multiyear program goals of ChemCatBio is to accelerate the development of catalysts and related technologies for the commercialization of biomass-derived fuels and chemicals. Biomass processing often requires challenging environments that conventional catalyst materials cannot withstand, leading to catalyst deactivation by leaching, organic fouling, and poisoning. These modes of deactivation result in reduced catalyst lifetime productivity due to the requirement for frequent catalyst regenerations, or, more severely, irreversible catalyst deactivation. The development of a new class of catalytic materials that can address these challenges is critical for the progression of the bioeconomy. Atomic layer deposition (ALD) is a method for improving the durability of catalysts by depositing an atomically thin protective metal oxide coating that still retains access to catalyst active metal sites. This project seeks to develop and advance the industry relevance of ALD catalyst coatings to improve durability and enhance biogenic sulfur tolerance of supported metal catalysts.

WBS:	2.5.4.706
CID:	NL0033623
Principal Investigator:	Dr. Derek Vardon
Period of Performance:	4/1/2018–9/30/2020
Total DOE Funding:	$536,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$536,000
DOE Funding FY19:	$0
Project Status:	New

Weighted Project Score: 8.3

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



I One standard deviation of reviewers' scores

Internally, the NREL project team is composed of technical experts in bench-scale ALD coatings, experimental catalyst testing, characterization, computational modeling, and TEA. Our team includes industry partners ALD NanoSolutions and Johnson Matthey, who are world leaders in ALD manufacturing and large-scale catalytic materials production, respectively. Leveraging the unique capabilities of each partner, the objective of this project is to achieve the goal of improved understanding and accelerated commercialization of ALD for next-generation catalytic materials.

Our project team will achieve this goal by:

- Developing novel ALD-coated catalyst materials to increase durability during muconic acid hydrogenation and catalyst regeneration in the presence of sulfur impurities
- Incorporating computational modeling to address ALD impacts based on a first-principle basis
- Utilizing laboratory-scale findings to inform a final ALD coating formulation for scalable synthesis
- Updating existing ALD manufacturing and process TEA for refined sensitivity analysis at scale.

During the initial stages of this project, we have made progress towards enhanced catalyst stability using targeted ALD coating strategies. We have demonstrated catalyst stability improvements against leaching and sulfur poisoning during the hydrogenation of muconic acid—an emerging biochemical intermediate—to adipic acid. Furthermore, we have shown dramatically enhanced thermal stability of our materials as compared to a conventional, uncoated catalyst. Using data gathered through reaction testing and application of advanced characterization techniques, we have gained materials insights used to inform continued ALD coating refinement by our industrial partners.

Planned activities for the continuation of this project include (1) utilizing computational modeling to inform relationships between ALD coatings and sulfur tolerance, (2) scaled synthesis of ALD-coated materials for validation, and (3) further refining preliminary cost models for ALD manufacturing and bio-based adipic acid production at scale. Collectively, these efforts are progressing the development and commercialization of robust ALD coatings for lowering the cost of biomass conversion through enhanced catalyst lifetime productivity in harsh reaction environments.

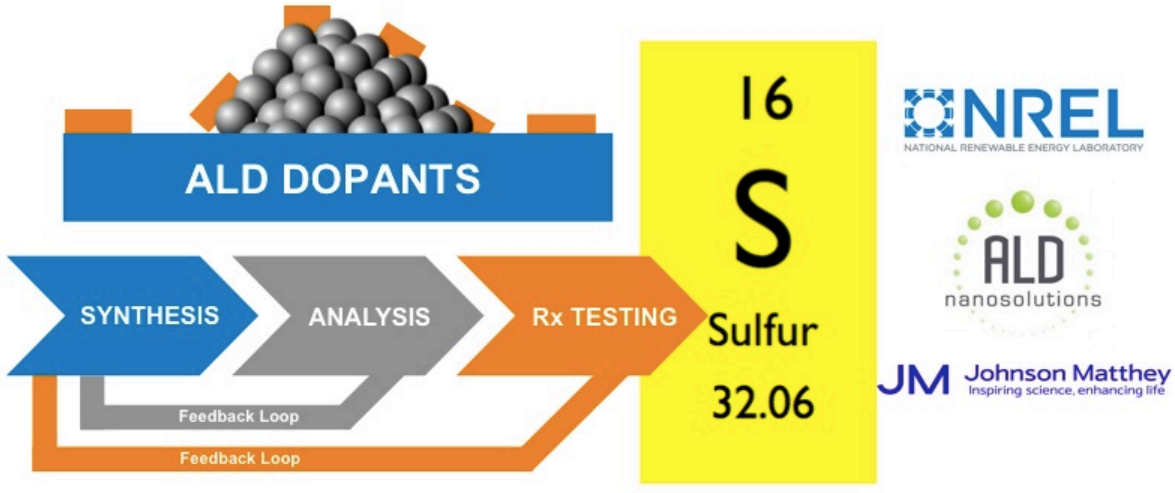


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- In general, a well-integrated effort with clear connection of the resources of ChemCatBio enhancing the partnership in a unique way. Results indicate targets are achievable while also providing some general understanding of catalyst function that may be translatable to other systems and potential technologies. Organized management with clear and achievable milestones suggests continued success for the project in the future.

- Catalyst stability is always a challenge, and biomass-upgrading technologies face some unique challenges, particularly in liquid media and when upgrading crude feedstocks. ALD provides a nice way to stabilize metal nanoparticles against various deactivation modes, and so this project could have a significant benefit to process economics.

- This project had a well-organized presentation and story. This project has a good start at reaching the end-of-project objectives, especially in the area of critical partnerships.

- ALD has been shown to produce unique catalytic materials with superior performance; however, it has not been used commercially because of perceptions that it is difficult and expensive. Developing a cost-effective way to produce a catalyst with controlled structure by atomic deposition has long been the goal because it is believed that this approach can yield unique performance. This project is an industry and national lab collaboration aimed at determining how this can be done practically. It leverages the developments in the commercial application ALD to the production of sensors and electronic products. It couples the nanoparticle and atomic deposition skills, testing and computational skills of the national labs with industrial catalyst suppliers. NREL characterization capabilities provide critical information for adjusting the preparation procedures. The project would not be possible without the direct funded project team that brought together capabilities from a government lab, ALD NanoSolutions, ForgeNano, and Johnson Matthey.

- Initial work on a small-scale batch of sample shows promising results for NP stability and reactivity durability, though sulfur resistance is yet to be tested. No details are provided on the means for scale-up; this will be critical for the method to be translated to industry.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate that the reviewers of the DFA ALD found value in our approach to address catalyst deactivation through improved material design. Per the reviewers' suggestions, the DFA ALD project team will continue to leverage the private-public partnership to address major cost and scaling barriers for catalyst stabilization by ALD. In addition, future efforts will specifically address scale-up concerns as downselected materials are identified in the project. Ongoing sulfur tolerance testing will inform which ALD coatings are of most interest based on process cost considerations. The DFA ALD team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

CHEMCATBIO DFAS: CATALYST DEVELOPMENT FOR SELECTIVE ELECTROCHEMICAL REDUCTION OF CO_2 TO HIGH-VALUE CHEMICAL PRECURSORS WITH OPUS 12

National Renewable Energy Laboratory

PROJECT DESCRIPTION

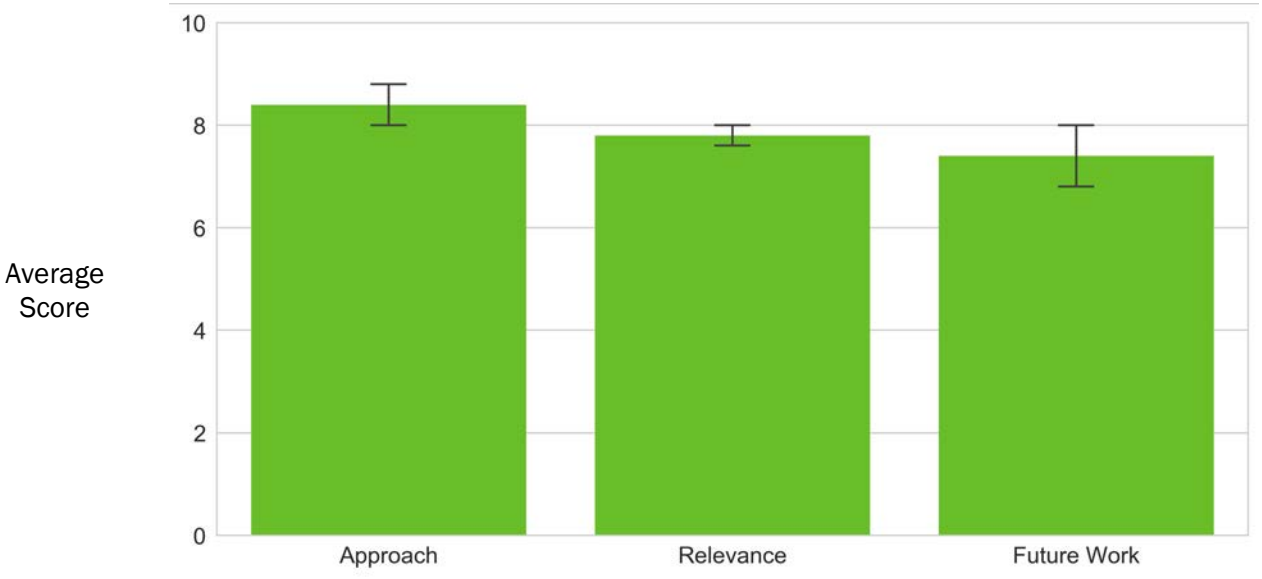
Cost-effective electrochemical reduction of CO_2 (ECO2R) is considered one of the holy grails of green chemistry. ECO2R combines just three inputs: CO_2, water, and electricity, and converts them into cost-competitive fuels and chemicals. However, widespread commercial fuel and chemical production via ECO2R is limited due to the lack of a suitable reactor design and catalysts with high selectivity to the desired products. This technology has the potential to convert CO_2 into a range of molecules that would benefit the biofuels and bioproducts industry. Within the bioenergy industry, over 4.5 million metric tons per year of CO_2 are generated from existing domestic biorefineries. Utilization of this domestically produced CO_2 to make fuels and chemical products has the potential to create a multibillion-dollar market.

WBS:	2.5.4.707
CID:	NL0033625
Principal Investigator:	Dr. Fred Baddour
Period of Performance:	1/1/2018–12/31/2019
Total DOE Funding:	$250,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$250,000
DOE Funding FY19:	$0
Project Status:	New

The core innovation developed by Opus 12 is a reactor design that enables ECO2R in a polymer electrolyte membrane (PEM) electrolyzer. A novel polymer blend and CO_2-reducing transition metal NP catalysts on carbon in the cathode layer transform a PEM water electrolyzer into a PEM CO_2 electrolyzer. The goal of this

Weighted Project Score: 8.0

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



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project is to gain a fundamental understanding of the impact of metal NPs and carbon support physical properties on electrochemical CO_2 reduction performance. Leveraging the synthesis and characterization expertise developed within the ChemCatBio consortium through the ACSC project and the advanced PEM diagnostics developed by the Hydrogen and Fuel Cells group at NREL, this project seeks to generate insight that enables the development of customizable reactors that can convert CO_2 with high selectivity to CO, CH_4, or C2+ products for the specific needs of customer segments within the biofuels and bioproducts industry.

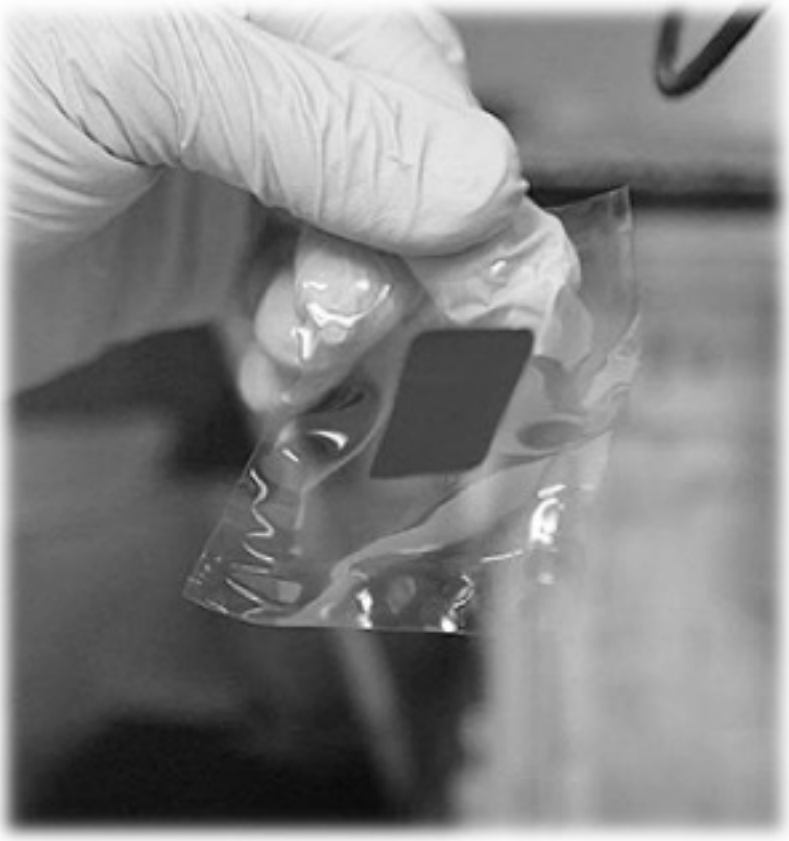


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- This targeted project seems to have a logical partnership between the performers. Results appear promising, both in catalyst development and performance. While scant on some details that could be valuable in assessing fully the current and future trajectory of the project, the NREL portion provides a unique expertise in catalyst synthesis and characterization that is clearly valued by the industrial partner.

- This program has a great long-term future with a potential for many breakthrough design optimizations that can reach commercial application swiftly. The overall spend of the project is quite reasonable for the commercialization story being told from the partnership. Funding should continue for this work, especially with the TEA/LCA efforts. The opportunity to develop large-scale electrochemical units for the future integrated biorefinery is critical and needed for the bioenergy industry. The project team should continue to be more transparent about technical barriers to solicit support across BETO with the cross-cutting efforts and CCPC.

- This is an interesting and important effort geared toward electrochemical upgrading of CO_2; however, the level of detail was somewhat light. This may be due to nondisclosure agreement requirements from the commercial partner, but it is a difficult to assess the project without full technical details.
- It is not clear how the second-generation catalyst will be improved over the first-generation catalyst. The products of the reaction are not specified, nor is there a TEA to justify the expense of running the cell.
- The ability to convert CO_2 to fuel and chemicals would be a major boon to the fight against global warming. Electrochemical catalysis is one of the more promising approaches because it would allow the conversion of renewable electricity available from a variety of sources into an easy-to-store high energy density liquid fuel. Demonstrating improved performance and determining the potential costs are critical for the continued development of the technology.
- The topic is the investigation of catalysts for electrocatalytic CO_2 reduction. This targeted project seems to have a logical partnership between the performers. Results appear promising, both in catalyst development and performance. While scant on some details which could be valuable in fully assessing the current and future trajectory of the project, the NREL portion provides a unique expertise in catalyst synthesis and characterization that is clearly valued by the industrial partner. Opus 12 in return provides the lab feedback of the performance of the materials. There is a clear advantage of obtaining some expertise on electrocatalytic CO_2 reduction for the consortium.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewer for their positive feedback and regret our inability to communicate fully the results due to intellectual property concerns.
- We appreciate the reviewer's feedback that this type of collaborative effort is necessary to address many of the economic and technical barriers of highest priority to BETO. We agree that increasing the transparency around this type of effort may assist in achieving these targets and expanding opportunities to collaborate across ChemCatBio.
- We have targeted established methods to modify the first-generation materials related to increasing current density and catalyst lifetime for Opus 12's targeted products. The current scope of the collaborative project has focused on catalyst development and characterization at NREL and evaluation at Opus 12 with the economics surrounding the process are ongoing at Opus 12.
- We agree with the reviewer on the promise of electrochemical catalysis and the value in demonstrating performance and understanding the economics of deployment of this technology.
- We appreciate the reviewer's insight and agree that there is an advantage to expanding the expertise in electrocatalytic CO_2 reduction for the ChemCatBio consortium as a whole.

CHEMCATBIO DATA HUB

National Renewable Energy Laboratory

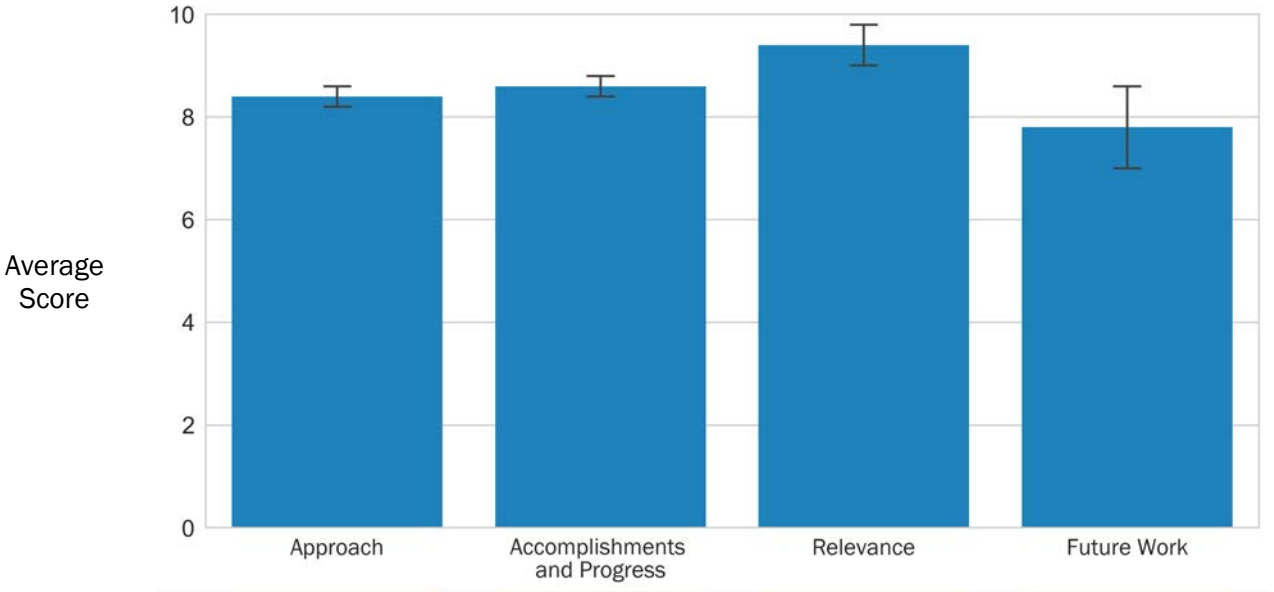
PROJECT DESCRIPTION

WBS:	2.6.2.500
CID:	NL0033706
Principal Investigator:	Dr. Carrie Farberow
Period of Performance:	11/1/2017–9/30/2020
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 goal of this project is to accelerate the catalyst and process development cycle by establishing the ChemCatBio Data Hub for (1) centralized and secure data storage, sharing, and analysis and (2) development and application of publicly available advanced analytics tools to provide predictive capabilities for catalyst research and development. Toward the first goal, a secure data repository for storage and sharing of data amongst project team members has been constructed, and a data release process for knowledge dissemination through sharing of data with the public has been established. Alongside the repository, this project develops and releases plug-ins for ease of data upload, search, filter, and visualization while allowing data to be easily and quickly mined and processed into formats that provide key actionable information to researchers. The design and development of data tools in this project are achieved through (1) continuous input from ChemCatBio researchers ensuring that deliverables are responsive to researcher needs and (2) close collaboration with the other DOE Energy Material Network consortia to avoid redundancy and address common and complementary data analysis needs efficiently. With the data repository in place, based on researcher feedback obtained through the FY 2018 go-no-go, the focus of this project has now shifted heavily toward the development of transformational tools to enable predictive capabilities in catalyst research and development. Specifically, the ChemCatBio Data Hub project aims to develop a pathway-independent catalyst design engine, which will be a publicly available tool

Weighted Project Score: 8.6

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



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for application by both ChemCatBio researchers and the bioenergy industry. The catalyst design engine tool would consider the critical tradeoff between predicted performance and material costs to accelerate the design of optimized catalyst formulations for the production of a diversity of end products from biomass and waste resources.

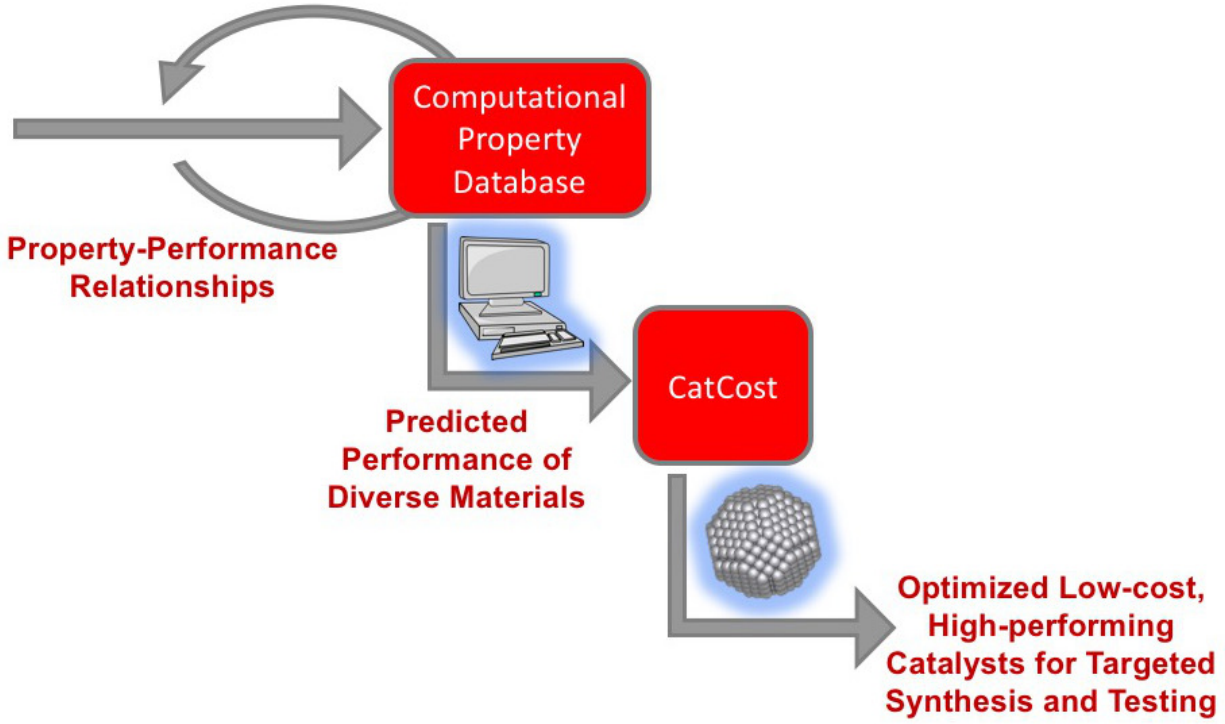

Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- The ChemCatBio Data Hub is an important component of ChemCatBio. No real issues with the presented objectives, structure, and future goals. The researcher-centric approach is great to ensure maximum use and potential impact. Performers should continue to strive to implement new concepts to better manage and use data in innovative ways.

- This is an exciting project for ChemCatBio, and resources should be dedicated to make sure it continues to upgrade in functionality year after year. The catalyst design engine will be a major innovation. ORNL has a long and documented history of successful software application launches, and they should be engaged at some point in the future before the next few version releases. There is a story in cost savings and efficiency that must be told at some point. This metric should be established as a measure of success, as well as usage and any other business-process streamlining benefits like the sample management tool.

- This is a very timely effort that seeks to centralize data and make it accessible to project partners to streamline collaboration. I think we see considerable duplication of efforts in catalysis research, and I like the effort that has gone into providing unique sample identifiers that code data about specific materials, etc. I would love to be able to log into this type of a repository and view, for example, binding energies, vibrational spectra, reaction mechanisms, etc., so I think this can provide a very powerful impact for the greater catalysis community. The PIs may need to take additional precautions in providing extremely user-friendly tools to a public audience. The tools will ultimately be crafted to be easy to use; however, the methods they depend on are actually sophisticated and require detailed knowledge. There is some concern that an uninformed user might generate bogus outputs and give them undue weight

because they are generated by a tool that has been vetted by experts. I used the example of Gaussian software in our discussions about this project; it is extremely easy to use and so it often gets misused.

- The ChemCatBio Data Hub is an enabler of the consortium project and provides public access to BETO project information that can be used to advance biofuel development. This is increasingly important as BETO and the national labs move to a more collaborative and consortium-oriented approach to research. A single gateway to the publicly shared computational tools is particularly useful. The approach taken by the project of integrating user feedback throughout the process is appropriate. In the past, the need for multistage review has delayed the release of reports and information to the research community. This needs to be balanced with the need for accuracy and control of proprietary information. The ChemCatBio Data Hub project should be expanded to allow the inclusion of more tools and perhaps data from outside sources; this would require some additional curating. It would be good to continue to support this project in the future to maintain and expand the database.
- The group should strive to implement a clear mechanism to require/maintain data storage. Data storage and data tools are very distinct efforts, and both are important.
- The group is also encouraged to have a mechanism to receive feedback from users to measure their success. Also, performers should continue to strive to implement new concepts to better manage and use data in innovative ways (machine learning/advanced data mining). Another missing objective is use of the data for benchmarking purposes.
- The ChemCatBio Data Hub is the easy-access bank vault and safety net of the ChemCatBio consortium. Data storage, manipulation, and retrieval is a very necessary, if not glamorous, role to have. It will be interesting to see how the catalyst development engine pans out.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The ChemCatBio Data Hub project thanks the reviewers for support for the project goals and insightful feedback. The team will work throughout the coming year to implement the recommendations. The reviewers identified the need to establish a metric for measuring project success in terms of cost savings or process efficiency. This project's FY 2019 annual milestone requires comparison of a conventional data analysis workflow with a workflow enabled by tools developed to demonstrate a 50% reduction in time used to share, store, or analyze data. Thus, we agree that demonstrating achievement through similar quantitative metrics should remain a criterion for project success. As noted by the reviewers, misuse of tools developed is a concern that warrants careful consideration. Public release of any tool will be accompanied by a publication and documentation to advertise tool features, define assumptions, and provide clear guidance on application. While we acknowledge we cannot eradicate misuse or misinterpretation, we firmly believe the value of the transformational tools envisioned necessitates continued development and deployment despite this concern. Ultimately, it is the responsibility of the user to follow best practices in research toward tool application. We agree with the reviewers' point that extensive and diverse data are needed for predictive tools. Current efforts toward developing a computational catalyst property database are not limited to data generated within ChemCatBio; greater than 95% of the data in the database to date are published data generated by external organizations. In the future, should the project scope enable development of similar public databases of experimental data, processes to incorporate data from external organizations will be included. Similarly, we agree that it is desirable to utilize the databases developed for benchmarking, and while it was not discussed in detail, this is within the scope of current goals. The reviewers recommended engaging experts to plan a software release. We agree and have initiated discussions with the NREL technology transfer team and will proceed with leveraging software development expertise at the other national labs. Lastly, the reviewers' suggestion to establish a clear mechanism for user feedback is well taken and will be integrated in FY 2020 milestones.