ADVANCED DEVELOPMENT AND OPTIMIZATION: ANALYSIS AND MODELING

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Advanced Development and Optimization (ADO): Analysis and Modeling 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 from March 4–7, 2019, at the Hilton Denver City Center in Denver, Colorado. A total of 10 projects were reviewed in the ADO: Analysis and Modeling session by five external experts from industry, academia, and other government agencies.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $8,092,031 (fiscal year [FY] 2016–FY 2019 obligations), which represents approximately 0.90% of the BETO portfolio reviewed during the 2019 Peer Review. During the Project Peer Review meeting, the principal investigator (PI) for each project was given 30 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 Peer 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 ADO: Analysis and Modeling 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. Siva Sivasubramanian as the ADO: Analysis and Modeling Technology Area review lead, with contractor support from Mr. Remy Biron and Mr. Joshua Messner (Allegheny Science & Technology). In this capacity, Dr. Sivasubramanian was responsible for all aspects of review planning and implementation.

ADO: ANALYSIS AND MODELING OVERVIEW

ADO conducts integrated systems research up to and including the engineering scale. ADO efforts focus on understanding the relationships between and within unit operations and discovering research-and-development (R&D) gaps for further technology development. In support of BETO’s goals to reduce minimum fuel selling price and achieve other BETO programmatic milestones, ADO identifies and leverages potential biofuel pathways to hydrocarbon fuels developed in the Feedstock Supply and Logistics (FSL), Advanced Algal Systems, or Conversion R&D programs. This includes developing testing protocols and performing the necessary verification testing. Results of verification testing, shared across BETO, inform future R&D priorities.

The Analysis and Modeling session reviewed projects that interact with experimental work and challenges anticipated to exist at the large scale or across bioenergy industries and markets. The resulting analytical and modeling products can be used to refine research and engineering strategies or to investigate product properties and how that might impact existing and future infrastructure and markets.

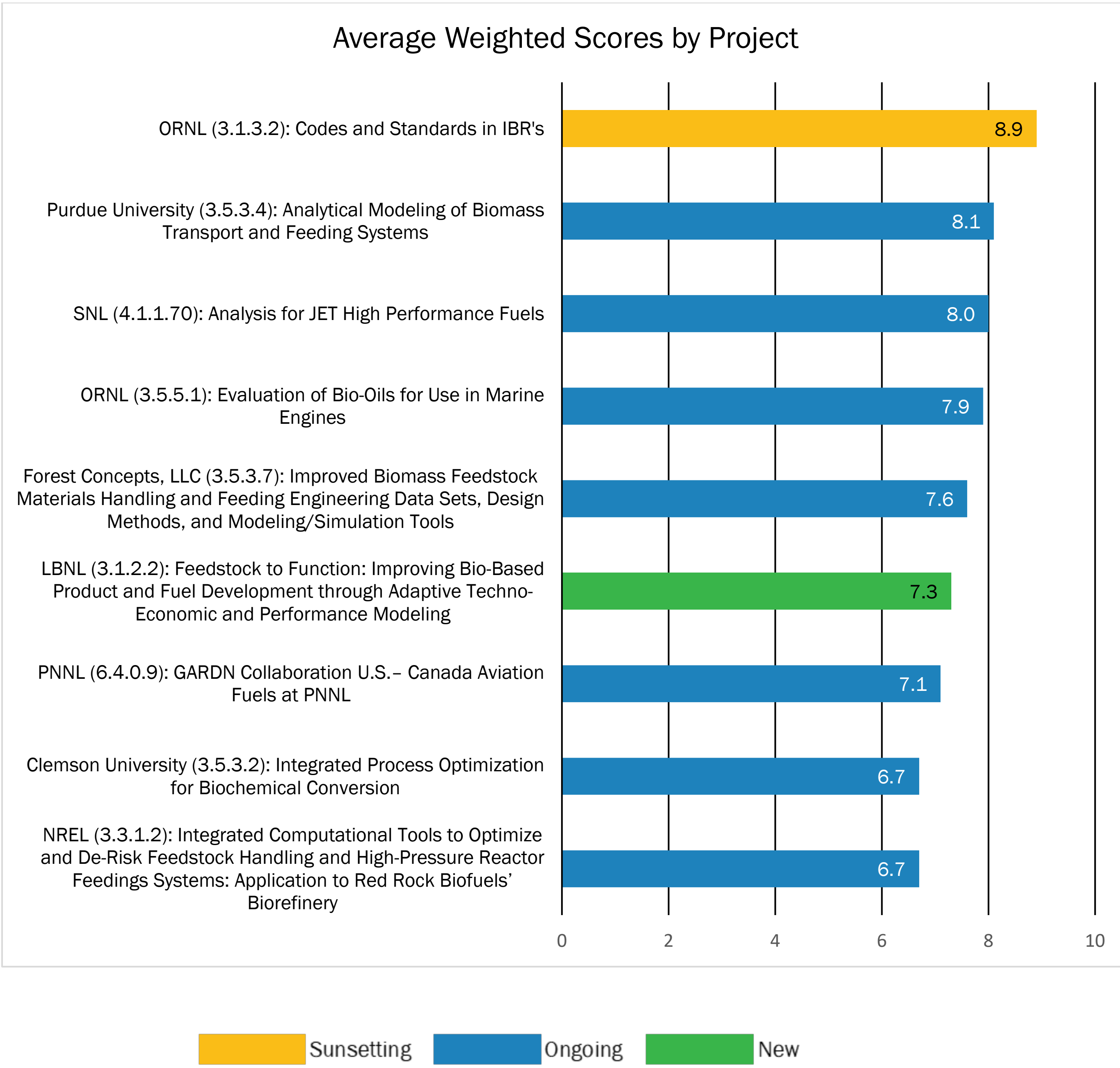
ADO: ANALYSIS AND MODELING REVIEW PANEL

The following external experts served as reviewers for the ADO: Analysis and Modeling Technology Area during the 2019 Project Peer Review.

Name	Affiliation
Lucca Zullo*	VerdeNero, LLC
Mike Fatigati	Taylor Energy
Daniel Lane	Saille Consulting, LLC
Mark Warner	Warner Advisors, LLC
Raghubir Gupta	Susteon Inc.

* Lead reviewer

TECHNOLOGY AREA SCORE RESULTS



ADO: ANALYSIS AND MODELING REVIEW PANEL SUMMARY REPORT

Prepared by the Advanced Development and Optimization: Analysis and Modeling Review

In general, developing broad, general-purpose industrial modeling tools, or modeling complex phenomena with broad applicability to industrial processes, is a prime target for government-funded research. The BETO portfolio in this area is quite broad, spanning from empirical studies to extremely fundamental ones using *ab initio* and first-principle methods and including the development of validation tools and specific applications of the emerging field of machine learning. This varied portfolio appears balanced across such a broad spectrum.

The review panel found that all projects are supportive, at least qualitatively, of BETO goals as expressed in the BETO *Multi-Year Plan* (MYP). There was consensus, however, that at times the link to the quantitative goals of the BETO MYP was either weak or somewhat forced. This is not necessarily a negative review.

Many projects are at an early or fundamental stage, and although they provide a positive benefit to the industry, the benefit might be challenging to evaluate as a specific contribution to the goal of $3/gasoline gallon equivalent.

We also had consensus that the presentation format and time limits were not conducive to properly communicating the value and status of the projects. In particular, the format of the presentations consumes too much space in boilerplate information regarding the project budget, timeline, and other programmatic information that could probably be presented as a session summary by the BETO program director before the PIs' presentations.

The PIs' answers to the reviewer comments made it clear that much relevant information was omitted because of space and time constraints. Some of this information was critical to provide a fair and informed assessment of the projects. Not surprisingly, the reviewers found that the techno-economic analysis (TEA) was one of the weakest parts on most projects. Given the broad potential impact, this was not considered a particularly significant weakness. Instead, the panel identified deficiencies with industrial practitioners' participation and validation methods as more substantial weaknesses needing more immediate correction.

IMPACT

We noted three main themes in the portfolio of research. All have a significant impact, although the immediacy of their effects on the industry is different.

The first is that of empirical or semiempirical studies. These have a straightforward and often clearly quantifiable impact. Among them, we found that the Oak Ridge National Laboratory (ORNL) study on fire propagation in biomass storage facilities is of particular relevance because it led to immediate but straightforward and actionable solutions to a real problem affecting industry safety. Also from ORNL, the work on evaluating the use of bio-oils in marine engines was particularly well received. The industry has always struggled to find a viable and straightforward pathway for the exploitation of pyrolysis oil, and this analysis lays an original and impactful approach that provides clear possible economic viability without much of the complexity associated with upgrading to fuels for road applications. A commercially viable pathway to deploy bio-oils is exceptionally significant.

Second, the more fundamental first-principle mathematical modeling applied to the analysis of performance and design of biomass feeding systems was well represented in different projects. Given the known impact that biomass handling has on a biorefinery's ability to reach its design goal, this is significant research with clear implications. Nonetheless, the panel felt that the impact, though qualitatively apparent, is not immediately quantifiable.

Third, some projects are dealing with still unresolved fundamental issues. There is agreement on the promise of the discrete element method (DEM) as a technique to approximate the complex behavior of biomass particles, but significant work is needed to fully assess the correct predictive envelope of the method and provide fully validated results.

The qualitative impact of modeling exercises is challenging to evaluate without appropriate validation data and techniques; thus, the panel was appreciative of the Forest Concepts, LLC project aiming to develop a quantitative method to measure flow properties in biomass and felt that much more work and emphasis in this area is needed.

The use of multiple nested or parallel modeling techniques—such as DEM, computational fluid dynamics (CFD), and the finite element method (FEM)—to address the entire slate of equipment and processes used in biomass handling are pragmatic approaches to achieving an adequate level of fidelity but add considerable complexity. In other industries, these modeling techniques are mature but remain the domain of specialists. These techniques often support the development and design of new equipment but are used sparingly in operations given the level of expertise and computer resources used.

As these programs evolve, we encourage more direct involvement with equipment manufacturers and the development of simpler, higher-level derived modeling tools that could be used more extensively by practitioners, as outlined in the Clemson University project on Integrated Process Optimization for Biochemical Conversion. We believe this type of layered approach and the direct involvement of equipment manufacturers significantly improves the impact of these projects. Also, although we welcome the direct participation of biorefinery operators and the development of the modeling tools in the context of their operation, we hope that the general lessons learned can be transferred to the broader industrial community and not remain confined to specific operations.

The panel was extremely intrigued by projects using *ab initio* chemical simulation and machine learning to scope molecules of interest with functionality for biofuel applications. We understand that these are relatively early-stage projects, and in the case of machine learning, the leveraged technology is still relatively immature. We believe these approaches and projects have substantial potential, and we encourage their continuation. Validation data and extension of the predictive envelope remain key metrics to expand to address more practical applications.

As discussed earlier, the direct impact to the BETO MYP, though clear to all, is not particularly easy to quantify. We felt that these tools could provide powerful screening. Although there is no substitute for the direct evaluation of a molecule for suitability to a task, these tools can help weed out unsuitable ones and lead to more effective, faster, and economically efficient development.

INNOVATION

The review panel did not find a lack of innovation in the portfolio. The exploration of relatively new computational methods such as machine learning and the creative use of DEM to simulate biomass flow are innovative and examples of integrating maturing technologies into a more sophisticated analytical framework.

As mentioned, data validation remains a relatively weak area of this portfolio. Given its importance and complexity, we believe this is a significant innovation opportunity, as demonstrated by the Forest Concepts project. As the portfolio evolves and expands, we encourage BETO to devote resources to more projects explicitly addressing gaps in data validation.

The use of distributed parameter modeling (DEM, CFD, FEM) techniques can achieve its full potential when applied to designing new biomass handling equipment and not only to optimizing existing ones, which is the most significant focus today. This goal requires a substantial leap in data validation techniques, as clearly understood by the PIs.

The use of molecular modeling tools—whether based on machine learning or *ab initio* calculations—to develop screening tools is also innovative and of great interest. We hope that as the work progresses, these tools are more directly integrated into the conceptual framework of a biorefinery by the introduction of links to the synthesis route and type of biomass feedstock.

SYNERGIES

Modeling efforts are synergistic because modeling is not a solution to a problem; it is a tool. Several projects model biomass flow using a combination of DEM, CFD, and FEM techniques and higher-level metamodels that are synergistic, and lessons—especially in the selection of tools and the approximation used—can and should be shared among projects and programmatic areas.

Screening tools aimed at molecular properties have clear possible synergies with other BETO programs—in particular consortia such the Co-Optimization of Fuels & Engines (Co-Optima)—although these possible or actual synergies were not always explicitly mentioned. The scope for synergies is substantive and not ignored by the PIs.

The modeling of fire in a biomass storage facility and the exploration of bio-oils as marine fuels are very focused projects, yet the PIs demonstrated extensive and broad capabilities that are relevant to many other aspects of the BETO program, and we hope BETO can leverage these capabilities in other areas.

The panel agreed that the TEA of the impact of these projects was wanting, and more detail would have been desirable. In some cases, such details were absent because of the limiting format of the presentations. The panel appreciates the difficulties in expressing a quantitative economic value for some projects at the current state of development, and this should prompt a more general discussion of appropriate TEA metrics, especially in the very early stages of these projects.

Further, we discussed whether some financial metrics used by BETO are the most appropriate. Nonetheless, we expect at least a qualitative and aspirational statement of the potential economic impact. Because individual projects fit into larger, more complex projects and development goals, such a statement becomes a critical assessment of the synergistic project value.

FOCUS

The projects in this programmatic area focus on addressing well-defined problems in BETO's larger programmatic area and are well aligned within the MYP. The panel was somewhat concerned with the possibility of projects losing internal focus either because of pushing the teams outside their sphere of competence or because of overambitious goals.

An example of the first problem is the project presented by Forest Concepts. The development of the measurement cell is an excellent effort and an example of innovative research both responsive to the BETO goals and capable of advancing the state of the art in this sector. The part of their project dealing with modeling, on the other hand, is less exciting and appeared to be included to fill perceived gaps in responsiveness to the funding opportunity announcement (FOA) rather than because it is essential. We believe that BETO could exploit the natural synergies existing in the program. BETO should then guide such a project to direct work where expertise is the strongest and foster collaboration with some other efforts among those who have higher expertise and can place an emphasis on modeling.

An example of a potentially overambitious effort is the National Renewable Energy Laboratory (NREL) project to model the feedstock handling and the high-pressure reactor of the Red Rock Biofuels biorefinery. We felt that attempting to model both the feedstock handling and the gasifier might be an overreach given the time and budget of the project and the acknowledged knowledge gap in several areas.

We found the screening tools using either machine learning or *ab initio* methods still too narrowly focused on a small set of physical properties and with a relatively weak link to the bioprocessing pathway and specific biomass types. These deficiencies in broader focus are nonetheless justified by the early stages of development and the complexity of the problem. They do not detract from the current value of the work but indicate needed future developments.

It should be clear that these problems are nonetheless minor and easily mitigated by guidance and coordination from BETO program directors. Such guidance is critical. The development of modeling tools and techniques is always fraught with risk when it comes to focus: on one hand, the work needs to be broad enough to serve a large audience and fulfill larger programmatic goals in solving shared problems; on the other hand, projects often need to be specific enough to provide a solution for one problem at hand and demonstrate that they can address real case studies.

TECHNOLOGY DEVELOPMENT PIPELINE

The panel found no substantial fault with the technology development pipeline, which strikes a balance between projects of immediate impact and the development of tools with a longer time horizon. We identify three themes:

1. Screening tools and systems for faster progress
2. Advanced modeling of biomass systems
3. Validation and measurement tools.

We believe this last area is particularly importance, and we hope to see in it more projects and with increased emphasis in the future. Within the broad strokes of this classification, we believe that the technology portfolio could be expanded. Without prejudice for modeling and optimization efforts carried within other programmatic areas, other technologies and consortia supported by BETO could benefit from the more systematic modeling and analysis approach presented in this technology area.

In the view of the panel, the project that was the least aligned in this portfolio was the project on the Green Aviation Research and Development Network (GARDN) U.S.-Canada Aviation Fuels at Pacific Northwest National Laboratory (PNNL) because it did not fit any clear technology pipeline. The project was not devoid of scientific merit nor was the panel concerned about its execution; it is an excellent example of international collaboration, which the panel considered very positive. The project did not provide any new insight or expand the scope of existing insights, however. The project ultimately stood alone without a clear objective to follow further down the path. In projects where new modeling approaches are being developed, BETO should ensure that they can maximize the impact on industry by ensuring complexity and computer resource demand do not become limiting factors. In these cases, metamodeling techniques—such as that proposed by the Clemson University project—appear to be a valuable approach.

Last, as machine learning and extensive data set analysis technologies continue to improve, we welcome and encourage continued and expanded investment in this area.

RECOMMENDATIONS

Our recommendations can be summarized as follows:

- The programmatic area is essential and needs to be continued and expanded.
- Modeling work should, in general, contain a stronger emphasis on data validation. Projects specifically focused on collecting needed experimental data—via new measurement techniques or instrumentation—should be included in the technology area.

- More industry and industrial practitioner input is necessary, including from equipment manufacturers, domain experts in the area of physical fuel properties, and others. In projects aiming to model specific sections of the biorefinery, the ultimate goal should be the design of new equipment, not only the optimization of existing ones.
- During the peer review, it would be beneficial to include an introduction by the program directors explicitly illustrating the logic behind the selection of the various projects, how BETO sees them fitting into the overall program, and, in the case of sunsetting projects, how the final results match initial expectations.
- The presentation format used by the PIs should have less boilerplate information. Such information could be presented as part of the proposed directors' overview. In general, the presentation format should allow for more relevant technical details to be included. It was a common occurrence for panel members to upgrade their initial assessment of the project based on the live presentation and questioning of the presenter.
- The area of tools for screening options, such as the selection of optimal molecules for a given performance, should be expanded because it is of great value and can take advantage of rapidly evolving areas of computer science such as machine learning. It should, however, more explicitly include links to biorefinery feedstock and routes. We believe that the value there is not that of predicting the best molecule or pathway but rather to support the early and rapid identification of bad ones.
- TEAs are often absent or marginal, reflecting the inadequacy of the standard metrics used by BETO for this area. Such deficiency needs to be corrected with the development of new and more flexible metrics.

ADO: ANALYSIS AND MODELING PROGRAMMATIC RESPONSE

INTRODUCTION/OVERVIEW

At BETO, we appreciate the participation of the review panel and the feedback received from both the review panelists and the steering committee during the Project Peer Review meeting in March 2019 and the Program Management Review meeting in July 2019, respectively.

The review panel classified the ADO Analysis and Modeling Technology Area portfolio of nine projects into three groups:

1. Empirical or semiempirical studies comprising codes and standards (ORNL) and evaluation of bio-oils (ORNL). The review panel highlighted that these projects have a straightforward and quantifiable impact by providing actionable solutions to the industry.

2. Fundamental first-principle mathematical modeling applied to the analysis of performance and design of biomass feeding systems projects consisting of Clemson University, Forest Concepts, Purdue University, and NREL. These projects focus on understanding operational challenges and help achieve reliable operations at design capacities. The reviewers noted that the impact of the research work in this area is significant with clear implications. In addition, they observed that the impact is qualitatively apparent, and because of the early nature of these projects, at present the immediate impact cannot be quantitatively ascertained.

3. *Ab initio* chemical simulation and machine-learning projects, including the projects from Lawrence Berkeley National Laboratory (LBNL) and Sandia National Laboratories. These projects address the identification of molecules with functionalities and relevant properties using computer-aided tools and techniques.

With respect to maximizing the impact of the ADO Technology Area, the program will consider the following actions:

- Validate mathematical models with relevant operating data to ensure high fidelity of these models

- Encourage industrial participation via a consortium such as the Feedstock-Conversion Interface Consortium (FCIC)

- Continue *ab initio* methods and machine-learning projects to realize their full potential

- Evaluate the importance of developing reduced-order (simplistic) mathematical models to enable wider adoption by stakeholders.

In terms of innovation, the panel provided the following suggestions:

- Integration of synthesis routes of molecules and types of biomass feedstocks using *ab initio* methods and machine learning should be pursued

- Expansion of modeling projects beyond optimization of existing equipment to new designs could help reach the full potential of this research and should be encouraged

- Development of improved data validation methodologies to ensure high fidelity of the mathematical models should be investigated.

The ADO program will implement the following actions:

- Pursue the idea of integrating synthesis routes of molecules with types of biomass feedstocks
- Consider the suggestion to expand the modeling projects to handle newer designs in addition to modeling the performance of existing equipment
- Emphasize improved validation techniques to ensure the accuracy of mathematical models.

The review panel observed that, given the similar nature of projects classified among the three groups mentioned previously, the projects are synergistic in nature and sharing lessons learned could be beneficial to current as well as future projects. In addition, the panel recommended that TEA metrics enabling critical assessment of synergistic values be considered. We will strongly encourage all our project participants to collaborate and share their learnings among themselves, as appropriate, and publish their results using proper channels for public dissemination.

The review panel commented that, in general, the ADO Analysis and Modeling portfolio of projects focuses on addressing problems and barriers of BETO's larger programmatic area and is well aligned with the MYP. The review panel cautioned the likelihood of some projects losing their internal focus because of the possibility of extending beyond their core competencies or being overambitious in their goals. We will provide the necessary guidance and assistance on an ongoing basis to ensure that the focus and objectives of these projects stay intact and are not lost. We appreciate the feedback of the review panel.

The review panel did not observe any substantial flaw with the technology development pipeline. They observed that the current portfolio strikes a balance between projects having an immediate impact on achieving the goals of BETO and those considering a longer-term viewpoint. The review panel suggested coordination with other program areas within BETO to garner greater benefits from systematic modeling and analysis approaches. In addition, the panel suggested the development of reduced-order models to increase the adoption of results obtained from modeling projects without requirements of increased computing resources to handle complex models. The ADO Technology Area, as needed, will coordinate with other programs in BETO to maximize the benefits resulting from modeling projects and analysis techniques. We agree that the development of reduced-order or simplistic models will be of great use to enable wider adoption, and this will be further evaluated with existing projects as well as identifying opportunities through additional funding mechanisms.

Recommendations

The review panel provided the following recommendations:

- The projects in the ADO Analysis and Modeling subprogram are essential and need to be continued and expanded
- Increase emphasis on improved validation procedures for the mathematical models
- Enhance participation and collaboration with industrial practitioners
- Revise the presentation template to better inform the value and status of each project
- Provide flexible TEA metrics for projects that are in early stages of development.

The ADO team will strive to increase industry participation through consortia activities such as the FCIC and impress upon the PIs the mathematical modeling projects to validate their models using relevant operating data to ensure high fidelity of these models. The ADO team will also coordinate with other programs in BETO to address the recommendation of revising the presentation template and development of flexible TEA metrics appropriate for early-stage projects.

Conclusions

We take this opportunity to thank all the members of the review panel for their thorough, insightful, and constructive review of the portfolio of projects presented in the ADO Analysis and Modeling session. The panel concluded that the primary strength can be attributed to a diverse portfolio of projects spanning from empirical studies to extremely fundamental ones using *ab initio* methods and including the development of validation tools. The review panel’s overall positive comments, performance rating of various projects, and identification of areas for improvement demonstrate that the ADO Technology Area is well managed and achieving the goals of BETO.

FEEDSTOCK TO FUNCTION: IMPROVING BIO-BASED PRODUCT AND FUEL DEVELOPMENT THROUGH ADAPTIVE TECHNO-ECONOMIC AND PERFORMANCE MODELING

Lawrence Berkeley National Laboratory

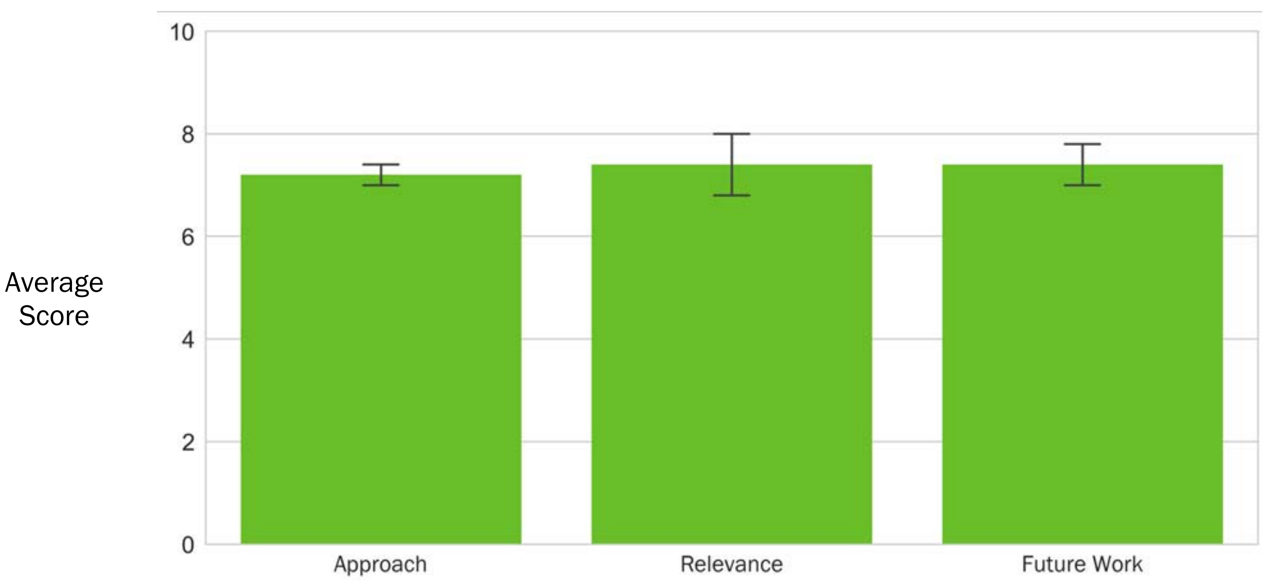
PROJECT DESCRIPTION

WBS:	3.1.2.2
CID:	NL0034839
Principal Investigator:	Dr. Vi Rapp
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$350,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$0
DOE Funding FY19:	$350,000
Project Status:	New

This project aims to develop the foundation for an adaptive computational tool that predicts bioproduct and biofuel properties for validation and certification and determines the cost, benefits, and risks of promising new and uncertified pathways and their blending effects. Many high-potential biofuel and bioproduct pathways are developed by mimicking the carbon number and chemical structures of commercially available products. Experimental property testing of these pathways is usually conducted years after initial bench-scale experiments are complete because of high experimental costs or high volume requirements; however, neglecting to conduct property testing early in the pathway development cycle can lead to investments spent on scaling up the production of bioproducts and biofuels that do not perform as expected.

Weighted Project Score: 7.3

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



One standard deviation of reviewers' scores

The comprehensive Feedstock to Function tool developed in this project will incorporate supervised machine learning to predict desired properties of high-potential bio-based molecules early on in technology validation and certification processes. Capabilities of the tool will be demonstrated and validated by predicting high-value properties of alternative jet fuel pathways. Coupled with a lightweight TEA and life-cycle assessment (LCA) model, this tool will enable bioproduct and biofuel developers and researchers to streamline bioproduct and biofuel scale-up, overcome experimentally and kinetically derived property bottlenecks, identify cost and emissions bottlenecks, and potentially de-risk investments needed to scale up fuel production for the technology certification process. Further, the Feedstock to Function tool could be a surrogate for high-throughput experimental property testing to derive insights on desired properties for individual or blended bio-based molecules and enable rapid evaluation.

FEEDSTOCK TO FUNCTION

Photo courtesy of Lawrence Berkeley National Laboratory

OVERALL IMPRESSIONS

- These sorts of online tools will offer industry tremendous opportunities to fine-tune efforts prior to much in the way of R&D expenditure.
- Focus on the development of the tool should really be on the ability to allow rapid “failure” of the potential project rather than only on the selection of molecules—the ability to eliminate options early on in the process will be critical to speeding up R&D efforts.
- I was initially skeptical about the project’s final ability to provide a significant improvement in the long adoption cycle of new biofuel molecules, but the quality of the presentation and the arguments made by

the presenter changed my mind. This is a worthwhile exercise in using rapidly advancing machine-learning technology to extract otherwise hidden information from large data sets.

- Although identifying possible suitable classes of molecules for an intended application might not help the adoption cycle considerably, identifying which molecules or class of molecules might not work could save considerable time spent on unproductive research and allow the researchers to focus earlier on targets that are more likely to deliver the desired performance.
- This modeling exercise can establish the framework not only for a predictive tool but also for a design tool for a new class of molecules amenable to novel production pathways.
- In general, this tool can provide learning for developing more general tools for physical property prediction and evaluation based on machine learning, and therefore its value might transcend.
- The TEA/greenhouse gas (GHG) part is currently the weakest.
- LBNL is developing a flexible, open-source tool to predict physical and chemical properties of high-potential molecules (fuels, fuel coproducts, and other bioproducts) derived from biomass and evaluate the cost, benefits, and risk of promising bio-based molecules or biofuels to enable faster, less expensive bioprocess optimization, certification, and scale-up.
- This project is in a novel area that has the potential to add value of focusing technical efforts in the early phase of process development.
- Early selection of potential products will reduce the development cycle time and cost.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the feedback. As we make progress with the tool, we will be sure to incorporate your recommendation to focus on the tool's ability to assist with "rapid failure" and screening of molecules to eliminate options early in the R&D process.
- Thank you for your comment. We are glad you value our project and property prediction of molecules. Regarding the TEA/GHG prediction, significant progress has been made on the development of this portion of the tool. We have completed the analysis of five jet fuel routes and established methods for allowing users to vary key input parameters and generate updated results in real time. Because the success of any biofuel pathway depends on its ability to (1) be economically competitive and (2) qualify for Renewable Fuel Standard categories/low-carbon fuel standard credits, the addition of the TEA/GHG module allows industry decision makers to quickly screen both end molecules and production pathways for viability.
- As a previous reviewer stated, this tool will offer industry tremendous opportunities to fine-tune efforts early on in the R&D process as well as to assess costs associated with production, the potential GHG footprint of different production routes, and the sensitivity of these key metrics to varying input parameters (e.g., biomass pretreatment method, product yield, on-site energy demand).

CODES AND STANDARDS IN INTEGRATED BIOREFINERIES

Oak Ridge National Laboratory

PROJECT DESCRIPTION

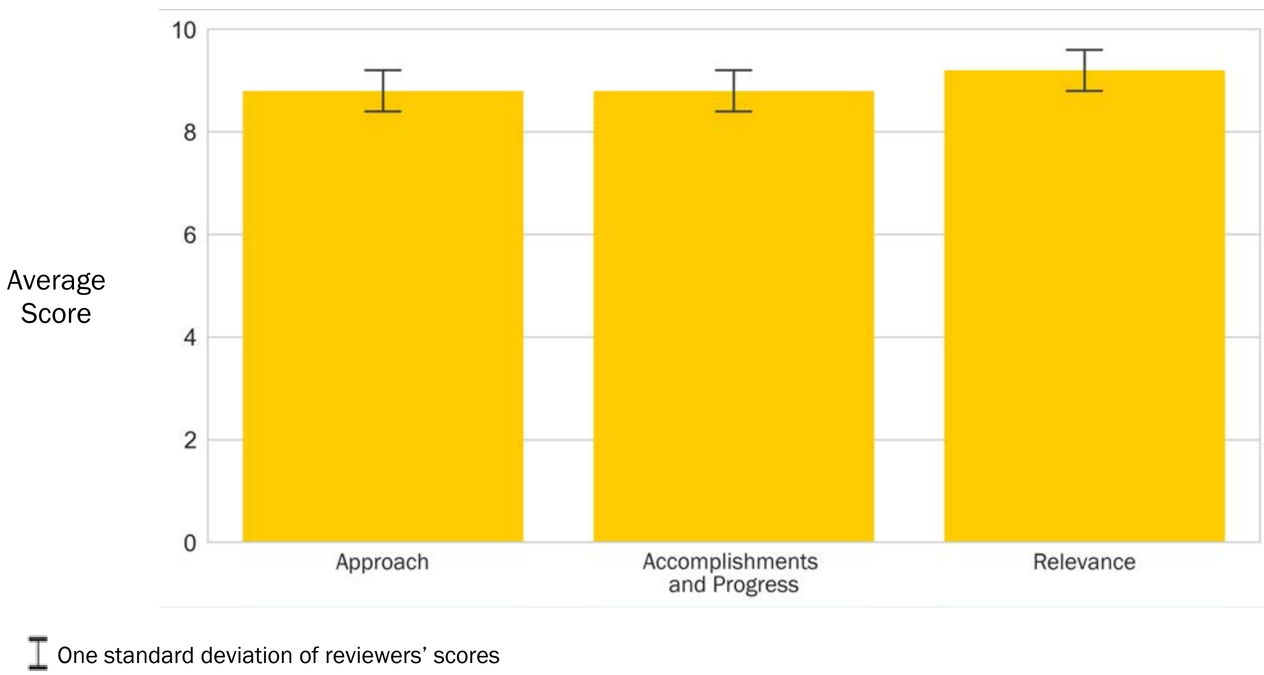
WBS:	3.1.3.2
CID:	NL0026705
Principal Investigator:	Dr. Erin Webb
Period of Performance:	10/1/2014–9/30/2019
Total DOE Funding:	$1,623,000
DOE Funding FY16:	$780,000
DOE Funding FY17:	$440,000
DOE Funding FY18:	$195,000
DOE Funding FY19:	$208,000
Project Status:	Sunsetting

Reports of recent fires in corn stover handling and storage areas have highlighted the increasing challenges of fire hazards (real and perceived) for commercial-scale biomass handling facilities. At the commercial scale, the volumes of feedstock required for a biorefinery exceed that of any existing biomass handling facilities, particularly for herbaceous biomass. The challenges of mitigating fire risk in such large-scale biomass handling and storage areas have not been fully addressed. A goal of this project is to engage industry in proactively addressing fire risks while not overburdening industry development. In previous research in this project (2014–2016), we worked with industry stakeholders to conduct biomass commodity classification tests at UL in Northbrook, Illinois, to determine how to classify corn stover and switchgrass bales in sprinkler design standards. We found that biomass bale fires tend to be more severe (faster growth, hotter) than expected and will require larger sprinklers than previously thought.

Industry stakeholders then asked us to investigate fire risk in biomass bale storage to identify storage strategies to reduce the probability and severity of these fires. Working with industry and rural firefighting stakeholders and engineers at UL, we developed corn stover bale stack fires to determine how fire grows and spreads within a stack of corn stover bales. Previous tests at UL were focused on fire in an individual bale, whereas these tests were designed to study fire spread through a stack of bales. We discovered that fire tends to grow and spread

Weighted Project Score: 8.9

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



along the vertical channels between columns of bales. We demonstrated in a series of small-scale stover fire tests conducted by UL and Iowa State University that if these vertical channels can be blocked, the fire growth and spread is dramatically slowed, giving responders a better chance to contain the fire. A new staggered stack design was developed to eliminate top-to-bottom vertical channels. Although this new staggered stack could increase costs by reducing the stacking efficiency, we hypothesize that the benefits of reducing the fire risk in stover bale storage yards will exceed the increased stacking costs.

Another benefit of the experiments conducted in this project has been an increased awareness of how dangerous large bale stack fires are to responders. Instability of bale stacks during a fire and rapid fire growth pose significant risks to firefighters. After observing fire tests conducted in this project, Nevada, Iowa, fire officials modified their response procedures to create a collapse zone around stacks on fire to protect firefighters from falling bales. They have already implemented these new procedures and applied them in May 2018 during a large lumber stack fire that posed similar threats (stack instability and quick fire growth).

In FY 2018–FY 2019, our goal is to disseminate the knowledge gained in this project to key stakeholder groups. We will submit a journal manuscript documenting the results of the corn stover stack fire tests to advance discussion of bale stack fires within the research community. We will also prepare and submit an article on lessons learned in improving the safety of firefighters responding to bale stack fires so that approaches being implemented in Nevada, Iowa, can be adopted in other biomass-growing regions. Finally, we will apply an existing corn stover logistics simulation model to evaluate tradeoffs between reduced fire risk and increased costs of implementing a staggered stacking design.

Photo courtesy of Oak Ridge National Laboratory

OVERALL IMPRESSIONS

- This is an outstanding project that has immediately applicable, real-world impact.

- The information needs to be disseminated broadly and quickly.
- Most people in the industry think of biomass fires (1) in the abstract or (2) in terms of wet smoldering; this work has the added benefit of demonstrating how much of an issue biomass fires can be and at the same time provides easily understandable, usable solutions.
- This is an excellent project on fire prevention. Fires are not caused by poor moisture in herbaceous biomass stockpiles but by arson and lightning.
- This is a well-guided empirical analysis of a real risk with clear economic consequences that leads to relatively simple and practical solutions for outdoor fires.
- It would be interesting to know how this cost compares to the standard practice and include a detailed assessment of fire risks, which appears to be large but is mostly defined in qualitative terms.
- This project is aimed at reducing the fire risk in biomass storage by developing strategies to slow the spread of unavoidable fires.
- This is a good example of enabling research that will help drive conformity and improve operation within the bioeconomy.
- An investigation into and determination of appropriate biomass handling standards is unrealistic for individual ventures to take on.
- Wide publication of these results and recognition is very important.
- The dissemination/implementation of the information developed in this project will be pertinent to reliable, dependable biofuels production.
- It is unfortunate that the team was not able to partner with the arsonists of past fires for early data collection regarding flame propagation, which results in duplicating efforts.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project team thanks the reviewers for their constructive and encouraging comments. We agree with the reviewers' suggestions that this information needs to be more broadly disseminated and that the costs of implementing fire risk mitigation approaches should be evaluated. We are working on that now in the latter half of FY 2019. We also agree with the reviewers that fire detection technologies should be implemented at biomass storage sites, and we will consider this approach in our cost simulations.
- A reviewer noted that reducing fire risk has impacts on safety that cannot be measured by cost alone. We could not agree more, and we are improving the safety of firefighters and surrounding communities, which is the most rewarding outcome of this project for us. We will take this advice and review other risk literature to develop additional metrics for our simulations of fire events in biomass supply chains.
- One reviewer asked how we can be confident that the new stacking approach will work at a large scale. The tests we conducted in this project were done with the largest stacks that we could safely set fire to. These stacks were designed to replicate a section of a commercial-scale stack, and we are confident that the tests were large enough for us to learn how fire moves through a stack of bales. We acknowledge that there will remain some uncertainty in how well this approach works at the industrial scale until a fire occurs in a larger stack using the new stacking design.

INTEGRATED COMPUTATIONAL TOOLS TO OPTIMIZE AND DE-RISK FEEDSTOCK HANDLING AND HIGH-PRESSURE REACTOR FEEDINGS SYSTEMS: APPLICATION TO RED ROCK BIOFUELS' BIOREFINERY

National Renewable Energy Laboratory

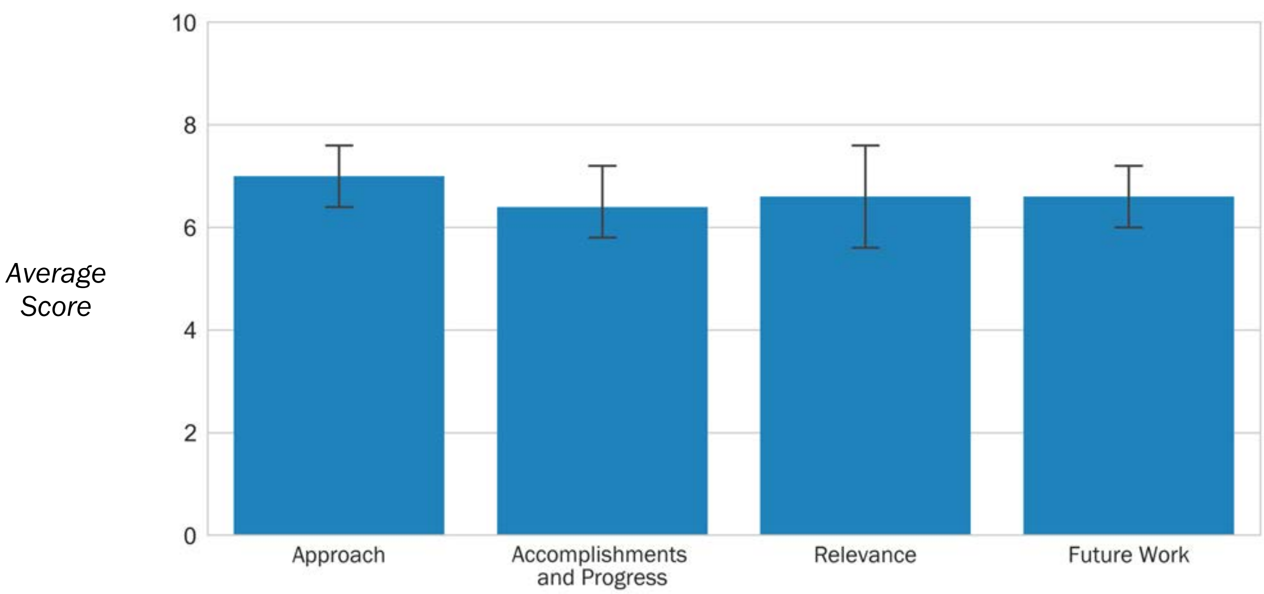
PROJECT DESCRIPTION

WBS:	3.3.1.2
CID:	EE0008253
Principal Investigator:	Dr. Jonathan Stickel
Period of Performance:	3/1/2018–2/28/2021
Total DOE Funding:	$1,799,999
Project Status:	Ongoing

Biomass feedstocks exhibit inherent heterogeneity and vastly different materials properties from common granular feedstocks, for which many solids handling unit operations were designed. These features have proven a significant impediment to the implementation of robust, continual biomass feeding systems for second-generation biorefineries. To address these challenges, we are developing integrated, experimentally validated simulations for several common feed handling and reactor feeding systems. We are building on previous investments of DOE that developed state-of-the-art modeling and simulation tools under the Consortium for Computational Physics and Chemistry, the FCIC, and other BETO-funded projects. We are leveraging and extending these tools to model the solids handling processes that constitute the front end of the Red Rock Biofuels (RRB) gasification and Fischer-Tropsch conversion process. This key partnership will facilitate experimental validation of the simulations as well as provide immediate impact whereby the resultant models will be used to optimize and de-risk commercial-scale deployment of the RRB process. Specifically, we are developing simulations for the feed hoppers, compression screw feeder, and conveyor pyrolyzer units employed in the RRB process. We will inform the parameterization of these models for feedstock-specific

Weighted Project Score: 6.7

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



One standard deviation of reviewers' scores

scenarios by multimodal characterization of the structure, physical properties, and flow behavior of various feedstocks. Once validated, this simulation toolkit will be generalized to aid in optimizing and de-risking other biomass conversion processes that use these common solids handling reactor feeding units. In addition, we will provide correlations that can be used to adjust optimal operating conditions based on feedstock parameters. We have a uniquely qualified team (a national laboratory, a university, and three corporations) to undertake the computational tasks and corresponding validation experiments. Completion of the project will constitute substantial progress toward understanding and overcoming the barriers associated with handling and feeding biomass, which will facilitate and de-risk the commercial-scale deployment of second-generation biorefineries.

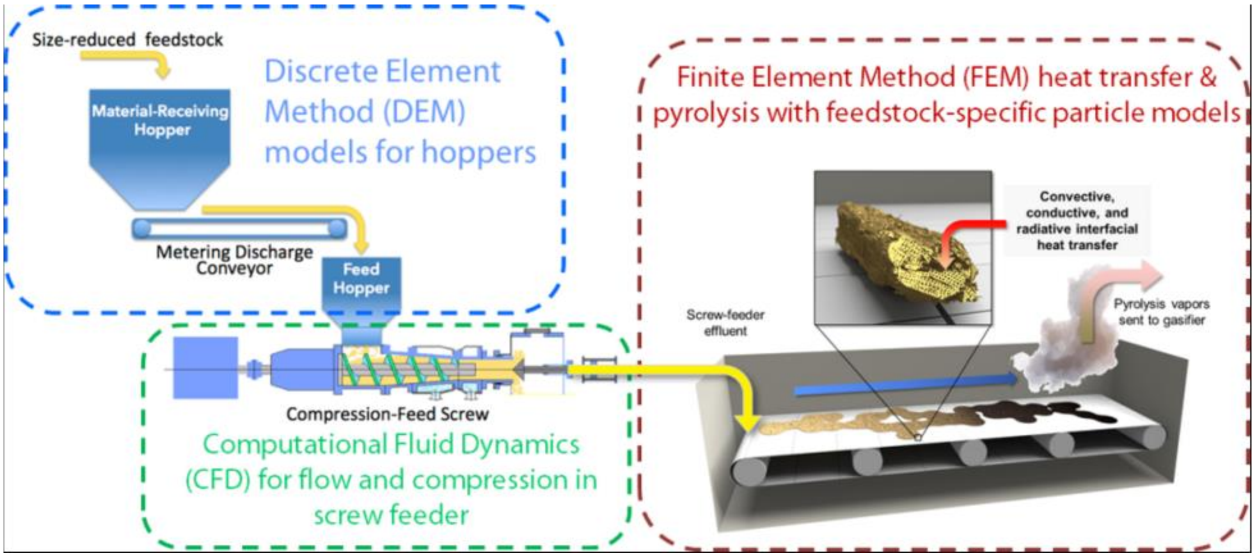


Photo courtesy of National Renewable Energy Laboratory

OVERALL IMPRESSIONS

- A fundamental question in this project is that it is trying to both address an industrial optimization problem while addressing the novel use of complex computational techniques across three different unit operations.
- As a scientific endeavor, this is quite challenging, and although the potential exists to optimize the reactor feed line and performance, the project is overambitious.
- Validation of the model with experimental data is not clear, and real assessment of economic value is missing at this point.
- There are nuggets of interest (e.g., the screw feeder), but the overall project is disjointed and lacking the ability to make a strong case for itself.
- In addition, the quality of the gasification modeling is somewhat limited.
- We would like to see direct involvement of equipment manufacturers.
- This project, led by NREL involving a multi-institutional team, is aimed at developing physics-based models for feed handling and feeding biomass solids to the RRB gasifier.
- This is an ambitious project with multiple challenges in modeling the physics and most importantly validating the model to be used for design/optimization of the RRB plant.

- This project is good enabling research to support general bioeconomy commercialization.
- The heavy reliance on one specific project and computational models could limit the broad applicability of the results.
- This project might reduce the time required to resolve problems of biomass feed handling and transport.
- This project addresses a real need to help de-risk feedstock handling challenges.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We agree that our project is challenging and ambitious, but we feel that the role of national laboratory projects is to address challenges of this magnitude. Although we will do our best to achieve the goals we proposed, there is always risk associated with scientific research. We expect to provide significant new methods and insights for feedstock feeding, even if we are not completely successful at using our models to optimize RRB's process. Experimental validation of the computational models is a key part of our work plan, and we apologize if that was not clear in the presentation. The equipment manufacturers Jenike & Johanson and Valmet are team members on this project. In addition, RRB has facilitated discussions between the team and TCG, the gasification-reactor vendor for RRB. Economic assessments performed by RRB have identified that reducing downtime associated with failures in the feeding system is critical to achieving economic targets; thus, success in this project will provide substantial economic benefit.
- Because of the constraints of the FOA, we need to focus our scope to the unit operations of one vendor and use one set of computational tools. This approach, by its nature, cannot be comprehensive; however, this project will connect nicely with other computational projects being funded by BETO.

INTEGRATED PROCESS OPTIMIZATION FOR BIOCHEMICAL CONVERSION

Clemson University

PROJECT DESCRIPTION

WBS:	3.5.3.2
CID:	EE0008255
Principal Investigator:	Dr. Sandra Eksioglu
Period of Performance:	4/1/2018–3/31/2021
Total DOE Funding:	$1,149,999
Project Status:	Ongoing

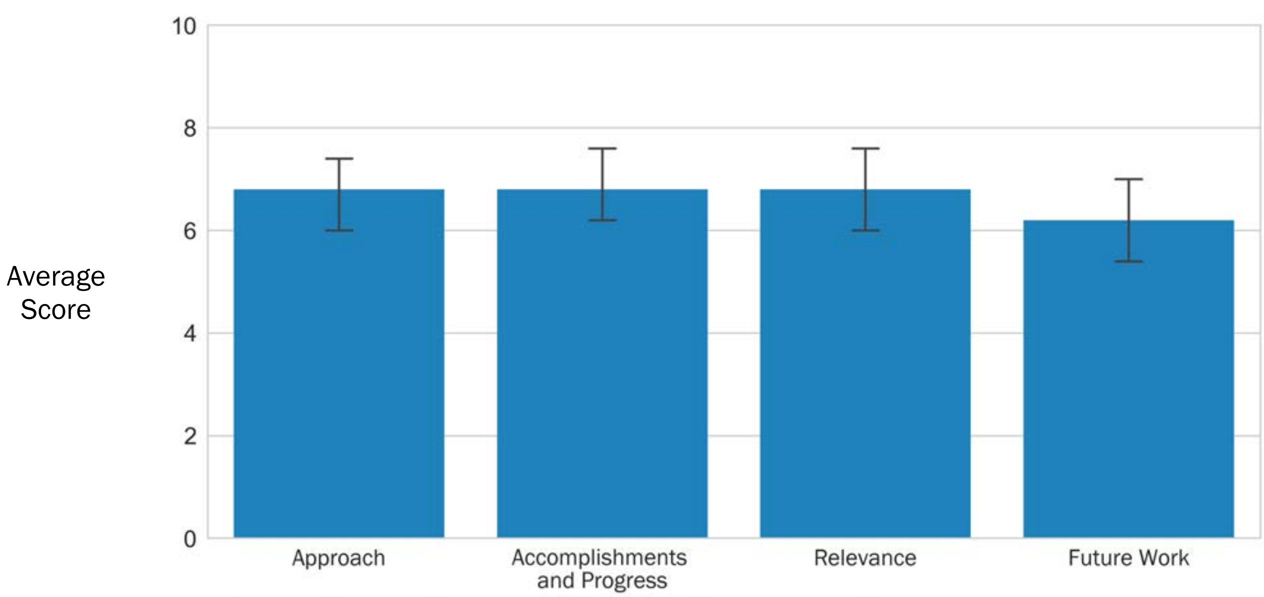
The main objective of this research project is to develop analytical tools to enable a biorefinery to identify an optimal integrated process design that ensures a reliable, cost-effective, sustainable, robust, and continuous feeding of biomass feedstocks to achieve the design throughput of the reactor.

This project will develop and integrate several analytical models that are expected to improve the performance of the proposed feeding system design (from biomass grinding to the pretreatment reactor throat design). The proposed feeding system design incorporates additional processes than current practices followed by the industry. These processes (fractional milling, high-moisture pelletization and cooling) positively impact the uniformity of the feedstock and improve the reactor's time onstream.

The analytical models proposed include DEM and mathematical optimization models. DEM models will provide functional relationships between biomass characteristics (such as particle size, shape, distribution, moisture) and biomass flowability and the failure mode of equipment. Modeling efforts also include the development of functional relationships that capture the effect of temperature and pressure on feedstock handling. We will incorporate these functions into mathematical models to optimize the performance of the

Weighted Project Score: 6.7

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



One standard deviation of reviewers' scores

proposed process. The optimization models will identify (1) optimal process parameters to ensure uniform particle sizes and uniform material flow with reduced fine particles; (2) optimal queue location and size to optimize costs, equipment use, and throughput; and (3) blendstocks that optimize costs and the reactor's performance in the face of biomass quality variations. Analytical results from the models will be validated at a process demonstration unit at one dry ton/hour for two weeks. This technology will be tested on corn stover, switchgrass, and miscanthus.

The analytical models will be integrated into an alpha version of a cloud-based decision-support system that will be available on the web free of charge. This decision-support system will serve as a training tool for bioenergy stakeholders (industry practitioners, government, academia, etc.).

This research is expected to deliver an optimized feeding system design. This system considers processes starting with biomass grinding, then the pretreatment and the reactor's throat. The system will deliver a consistent feedstock that meets biochemical conversion specifications as designed by NREL at one dry ton/hour for two weeks. We expect that the optimized system will maintain the reliability of the reactor to 90% for biomass with 10%–30% moisture levels and 5%–15% ash content. The optimized design will potentially result in tighter particle size distributions, reduced fines, reduced grinding energy consumption, improved flowability, etc.

Another outcome of this research is a decision-support system that will enable decision makers to undertake sound actions and impact stakeholders in the short, medium, and long terms.

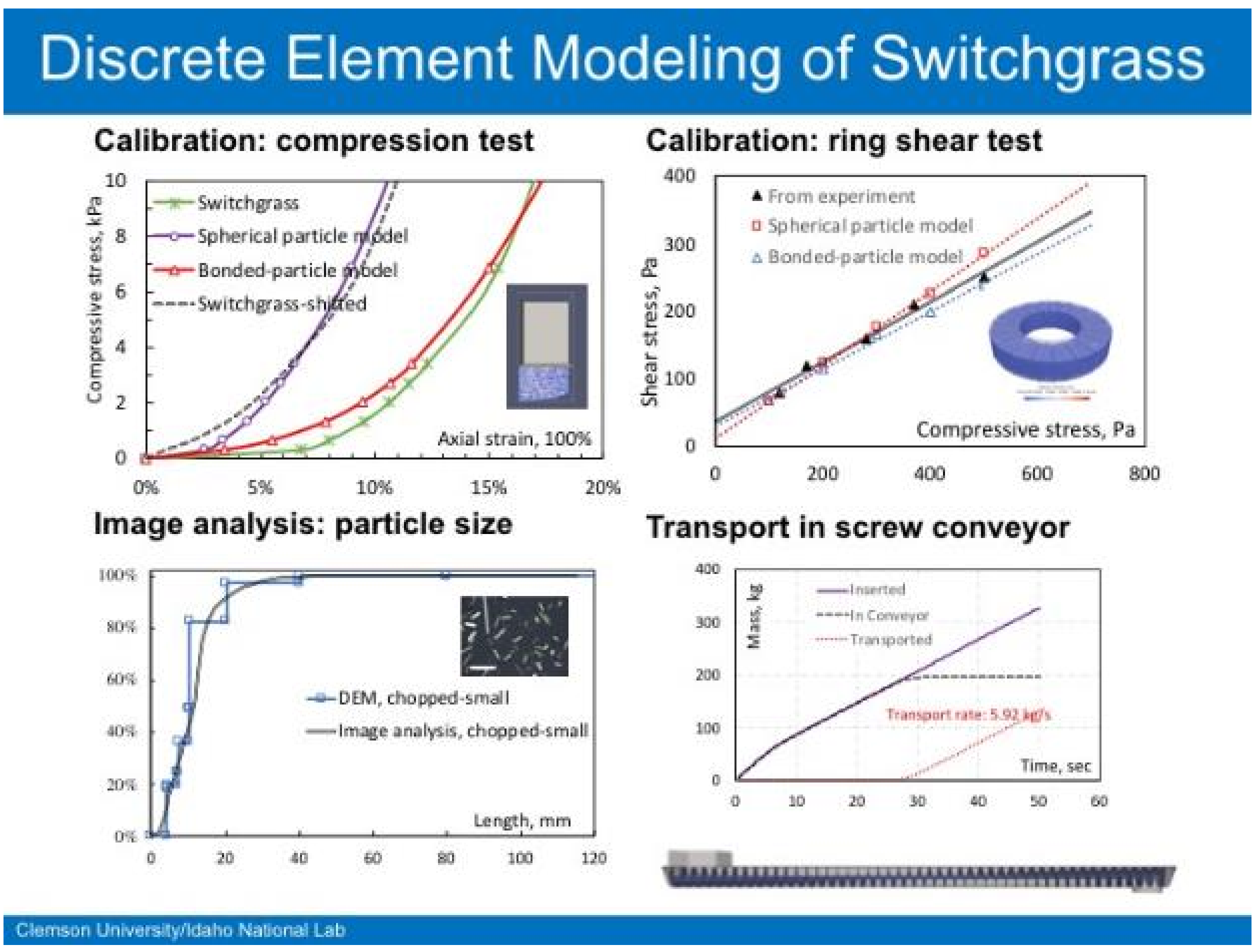


Photo courtesy of Clemson University

OVERALL IMPRESSIONS

- This project addresses a significant problem. The approach is intriguing—nested or hierarchical models—and promising; however, it has not yet sufficiently proven to be able to provide quantitatively correct results.
- The impact of some key process variables (e.g., moisture) is not yet explained explicitly, but the potential ability of using glued spheres to model the geometric complexity and size variability of biomass is extremely interesting.
- This is a complex tool, and it is not likely to be used on a routine basis for plant-level studies; however, it could become an excellent tool in the hands of designers of new handling equipment. Requirements from that audience should be included.
- The next phase of the project is critical to proving whether a practical toolkit for industry practitioners can be developed.
- The commercialization strategy is unclear. Equipment manufacturers appear as a prime audience but are missing from participation.
- This project aims at developing a DEM to optimize feeding to a biomass conversion reactor.
- The majority of the project work focuses on heavy-duty computer modeling with two-week testing at Idaho National Laboratory (INL) to get experimental data for model validation.
- This is a good example of basic research to support industry commercialization.
- The focus on the critical nature of assumptions and requirements for confirmation was clear.
- This is an intensive modeling approach to develop an optimized feedstock handling and supply system model with significant uncertainty regarding a pathway to market.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Although quantitatively correct results are challenging for any model, our DEM model efforts aim to provide quantitative relationships between biomass characteristics and equipment performance for planned processing equipment. The model has been calibrated for switchgrass and shown quantitative agreement with experimental data of compression and ring shear tests. Additional calibrations of other biomass materials are planned. The DEM models also need to be validated to provide quantitative accurate results of biomass handling and flow in different processing units. Such an effort is underway.
- Key process variables (e.g., moisture) are being considered in the DEM model through a new cohesion model. This will allow the modeling of moisture and fine content effect.
- The optimization team and the DEM modeling team are working closely together for the next phase to develop a framework for system-level optimization. The final product is intended to be more practical.
- Although we hope the models and the resulting tools will have broader applicability and commercial values, the current focus is still on model and capability development.

ANALYTICAL MODELING OF BIOMASS TRANSPORT AND FEEDING SYSTEMS

Purdue University

PROJECT DESCRIPTION

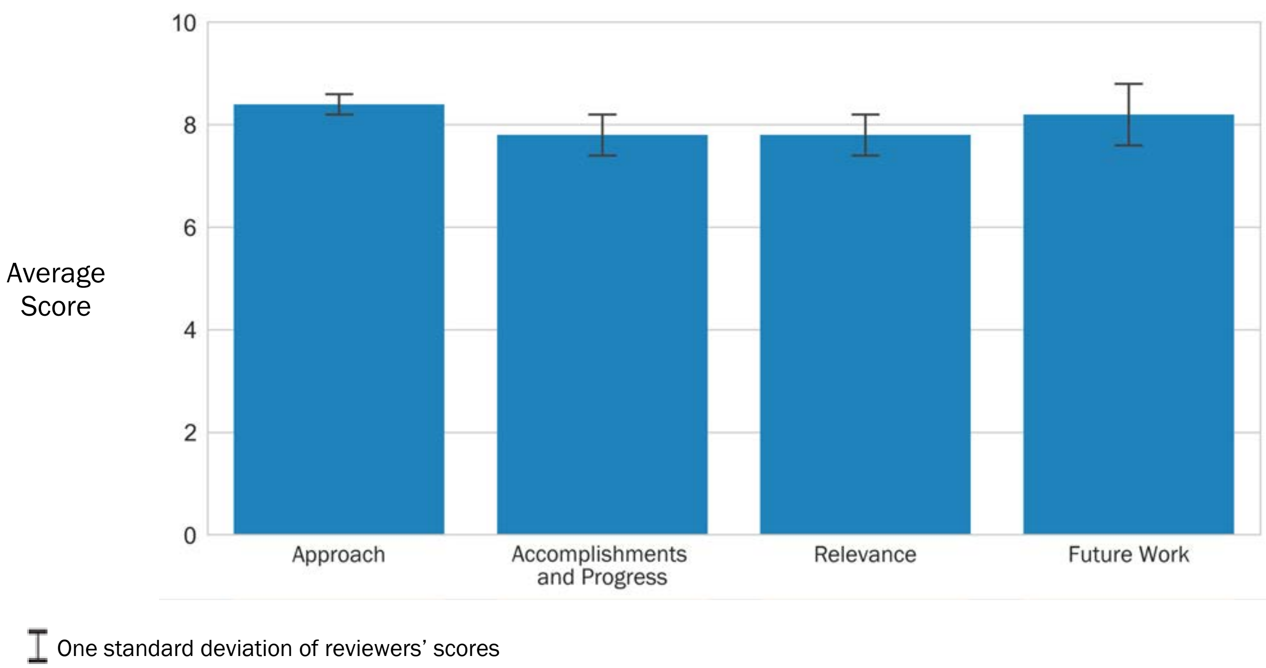
WBS:	3.5.3.4
CID:	EE0008256
Principal Investigator:	Dr. Michael Ladisch
Period of Performance:	3/1/2018–2/28/2021
Total DOE Funding:	$1,190,000
Project Status:	Ongoing

Major improvements in lignocellulose pretreatments and enzyme, microbial, and thermochemical catalysts, together with demonstrations of these technologies in reactor volumes ranging from 1–20 m^3 or larger, have proven to be key concepts in cellulose conversion. The BETO programs carried out in cooperation with industry have demonstrated pathways and process designs that decrease enzyme loadings; broaden substrate range; and enhance titer, rate, and yield using industrial microorganisms; however, the movement of lignocellulosic biomass solids between and within unit operations of a biorefinery remains a challenge because of the difficult material-handling characteristics of solid forms of biomass materials and aqueous slurries formed from these materials during pretreatment, hydrolysis, and fermentation.

Our team consists of Purdue University, INL, Argonne National Laboratory (ANL), Forest Concepts, and AdvanceBio. We are addressing the analytical modeling of corn stover in the forms encountered in a biorefinery: loose material, pellets, and slurries at high-solids loadings. Our goal is to develop strong and innovative computational and empirical models that rigorously represent the flow performance of biomass materials and enable a deep understanding of how particle and equipment characteristics impact biomass flow.

Weighted Project Score: 8.1

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



Ultimately, these models will be used to predict operational envelopes for stable feeding of biomass into a biorefinery reactor.

Dry solids feeding is being modeled using two computational techniques: DEM and FEM. These models will account for the effects of moisture, temperature, and pressure on feedstock handling and use measurements at conditions encountered when these materials are processed at temperatures between ambient and 200°C, pressures up to 20 bar, moistures ranging from 15%–85%, and solids loadings of 150 to more than 300 g/L as defined by conditions in the biorefinery. LCA and TEA, carried out in cooperation with ANL, will provide metrics for how process changes impact GHG reduction and costs.

The resulting models, together with experimental verification in INL's Process Development Unit, will be applied to predict optimal control points and to simulate process variability for continuous feeding into a biorefinery reactor. Key to model development is the measurement of properties at conditions that are encountered in the plant. These measurements are being carried out at Purdue University and in the INL laboratory as well as pilot equipment including pressure vessels. Specialized rheometry systems for measuring flow properties, imaging methods, and NREL's laboratory analytical procedures for particle characterization are providing measured parameters necessary for the modeling research. The near-term impact of this work will come from validated models that predict flow behavior during feeding, define critical operating ranges, and provide a quantitative basis for new equipment designs that will help to alleviate the operational reliability issues experienced by the DOE-supported pioneer biorefineries.

OVERALL IMPRESSIONS

- This is an excellent project with specific and measurable results that will have impact on industry.
- The inclusion of stover slurry rheology characterization (and potential modeling?) is outstanding and needs to be shared widely with industry because this is an area that causes problems with scaling processes across industry.
- Overall, this project outlines a clear use of a powerful analytical tool to provide a predictive framework to increase the reliability and amount of biomass throughput in a biorefinery. The oral presentation managed to eliminate some doubt about the wisdom of considering pelletized biomass.
- The conveyor analysis is the most interesting part because it is of general interest and useful to processors that might use other devices (e.g., stirred tanks), which might be used for liquefaction as an alternative to the proposed screw reactor. The use of a screw reactor for liquefaction is intriguing—mainly because it might work at much higher dissolved solids percentages than conventional methods. It is likely—although not a given—that the tradeoff is more mechanical complexity and increased operating and capital cost.
- I would like to see as future work some level of comparison with other approaches to liquefaction. This could be at a relatively high level but should be enough to provide a practitioner confidence in further pursuing the proposed liquefaction approach.
- Explicit involvement of equipment manufacturers would be desirable to increase awareness and use of these models.
- This project addresses the development of engineering solutions to alleviate biomass feeding problems in reliable biorefinery operation.
- This project has an excellent balance of computational modeling and experimental testing with a very strong project team.
- This project has the potential to produce good background research and is well managed.

- Limiting the project to corn stover and an unusual process configuration somewhat constrains the ultimate applicability of the results.
- This program appears to be more about the development of a model for the sake of model development than the actual development of a robust feedstock supply system.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for these comments. We plan to share results with industry through presentations and papers.
- Two approaches are under consideration for the liquefaction: (1) liquefaction with maleic acid in the screw reactor and (2) batch liquefaction with enzymes. Both are being modeled. Additionally, the equipment manufacturer is a partner on the project, and it is worth noting that the INL system was reverse engineered from larger equipment for ease of scale-up of results.
- Modeling is directed to corn stover because this is the primary herbaceous feedstock used by the pioneer biorefineries. Regarding process configuration, both batch (enzymatic) and continuous (screw reactor with maleic acid) are considered. We expect that the modeling approach can be used for other materials, but that would need to be verified in a future project.
- The focus of this project is on developing a modeling approach that will give guidance on how to feed corn stover more robustly. The models are expected to predict which material properties and operating conditions will result in acceptable screw torques and material bulk densities.

IMPROVED BIOMASS FEEDSTOCK MATERIALS HANDLING AND FEEDING ENGINEERING DATA SETS, DESIGN METHODS, AND MODELING/SIMULATION TOOLS

Forest Concepts, LLC

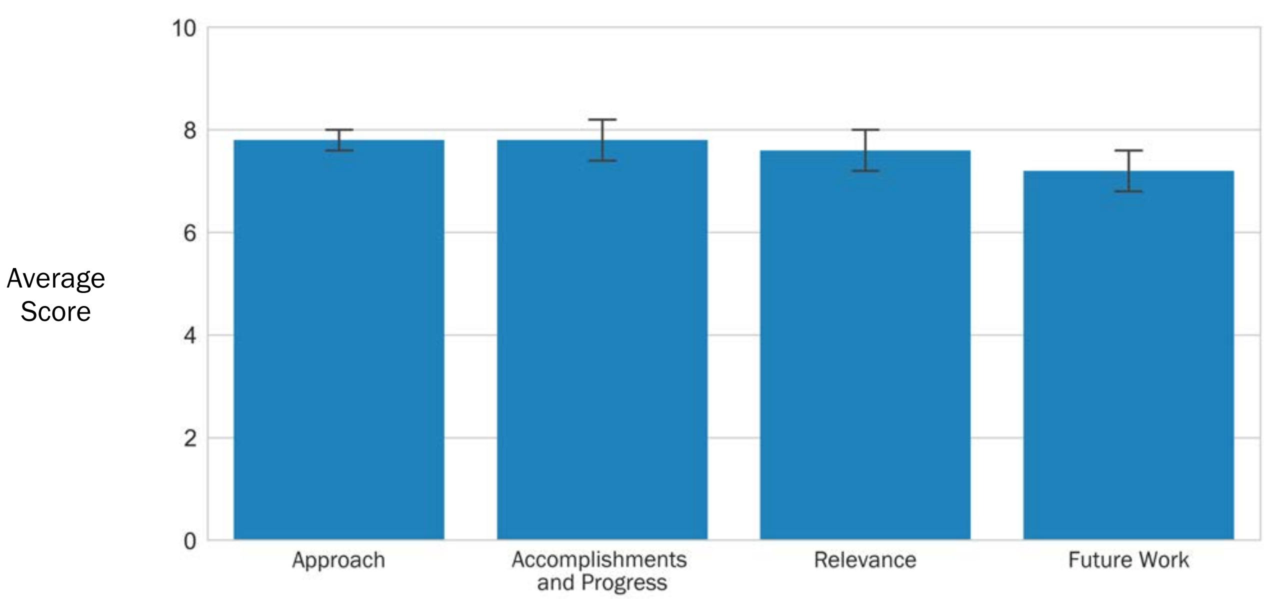
PROJECT DESCRIPTION

WBS:	3.5.3.7
CID:	EE0008254
Principal Investigator:	Dr. James Dooley
Period of Performance:	6/1/2018–1/31/2021
Total DOE Funding:	$1,479,033
Project Status:	Ongoing

The overarching objective of this project is to contribute to the design and operation of reliable, cost-effective, continuous feeding of biomass feedstocks into a reactor of an integrated biorefinery. The overarching goal comprises two sub-goals: (1) develop and validate a comprehensive computational model to predict mechanical and rheological behavior of biomass flow to enable the systematic and reliable design of a biomass handling/conveying system; and (2) engineer and improve laboratory protocols and equipment to generate property-driven response curves for specific biomass feedstock species and formats accounting for their dependence on biomass physical properties, including particle size distribution, true density, bulk density, and moisture content, as well as external mechanical properties, including temperature and pressure. The project team includes Forest Concepts, Pennsylvania State University, and Amaron Energy. Forest Concepts leads the design and construction of new laboratory methods and equipment. Penn State leads the development and adaptation of bulk flow models to the problem of biomass materials and equipment. Amaron Energy provides a case study site for validation of project outcomes. New equipment to be developed includes a 250-mm cubical triaxial tester (CTT) to provide biomass mechanical property data, a 300-mm wall friction tester to quantify the

Weighted Project Score: 7.6

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



One standard deviation of reviewers' scores

interaction of biomass with materials of construction, a large gas pycnometer to quantify biomass particle density, and other laboratory devices to ensure simulations are populated with biomass-specific data. Biomass materials used in the project include milled wood chips and corn stover.

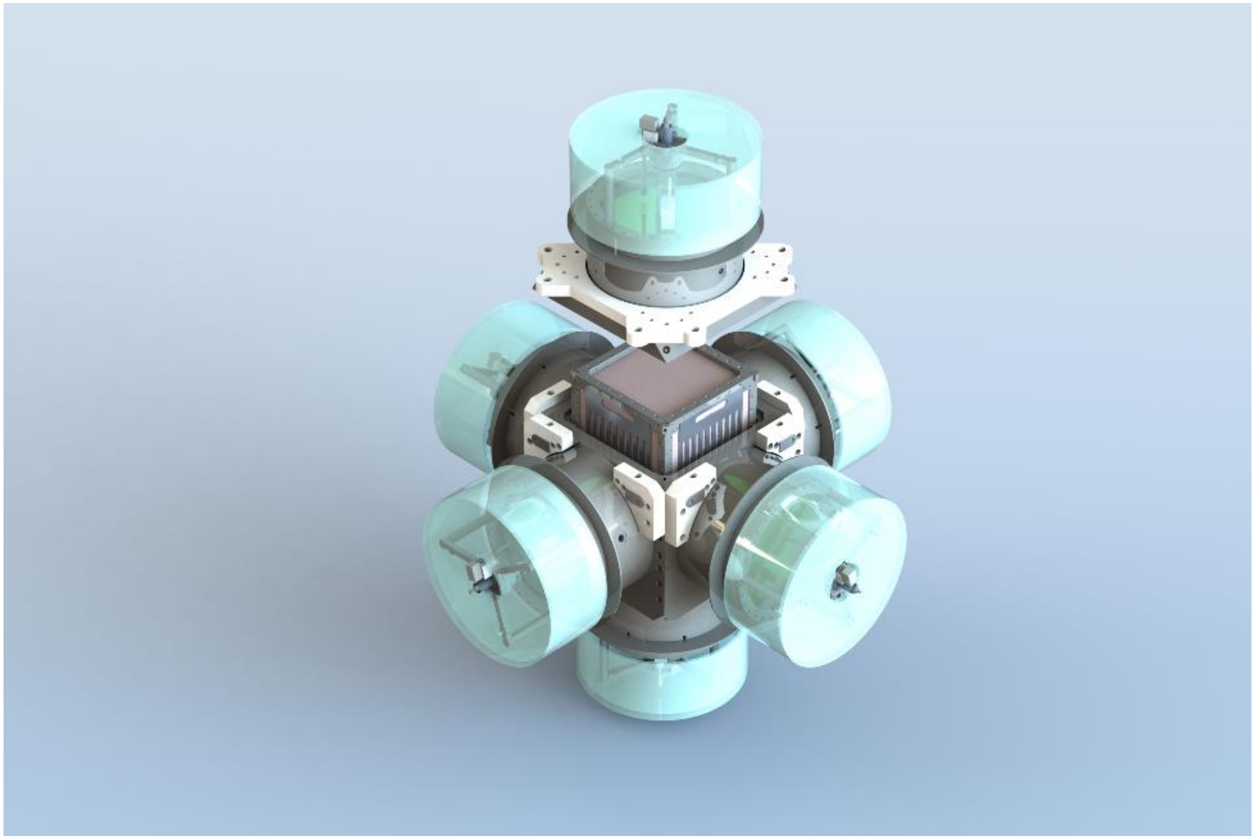


Photo courtesy of Forest Concepts, LLC

OVERALL IMPRESSIONS

- This project has significant potential for physical property measurement of large particle biomass. A focus on the correlation of results from the developed technology to results from the "original," smaller technology should be of primary importance because this will be critical to the application of the measurements in an area where the smaller technology has been dominant in the past.
- This work is commendable because it is driven by a vendor that has correctly identified the need to improve the ability of measuring bulk flow properties of biomass material and proposed the development of an enhanced laboratory device (CTT) to carry out such measurements.
- The results are validated using a flow model of a hopper. This is a very valuable effort that might have impact beyond the scope of this project because it can help define a general approach to experimentally measure the flowability of bulk biomass.
- The project would benefit from a better explanation of the scientific basis and a more descriptive treatment of how measurements from the CTT inform flow simulations.
- I strongly recommend participation of vendors and equipment manufacturers in the modeling exercise.

- This project is aimed at developing a measurement technique to better understand biomass particle flow in biomass feed systems.
- The development of a CTT is planned to alleviate the limitations of the current system developed by Penn State.
- This is a well-focused project with a good mix of hands-on industry experience and well-qualified academic staff with a thoughtful approach to addressing biomass handling issues.
- This project appears well defined and managed.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Statistically valid experiments with matched sets of biomass material will be used to correlate the output of the new large CTT with existing systems at Penn State University, which is planned for early in Budget Period 2.

EVALUATION OF BIO-OILS FOR USE IN MARINE ENGINES

Oak Ridge National Laboratory

PROJECT DESCRIPTION

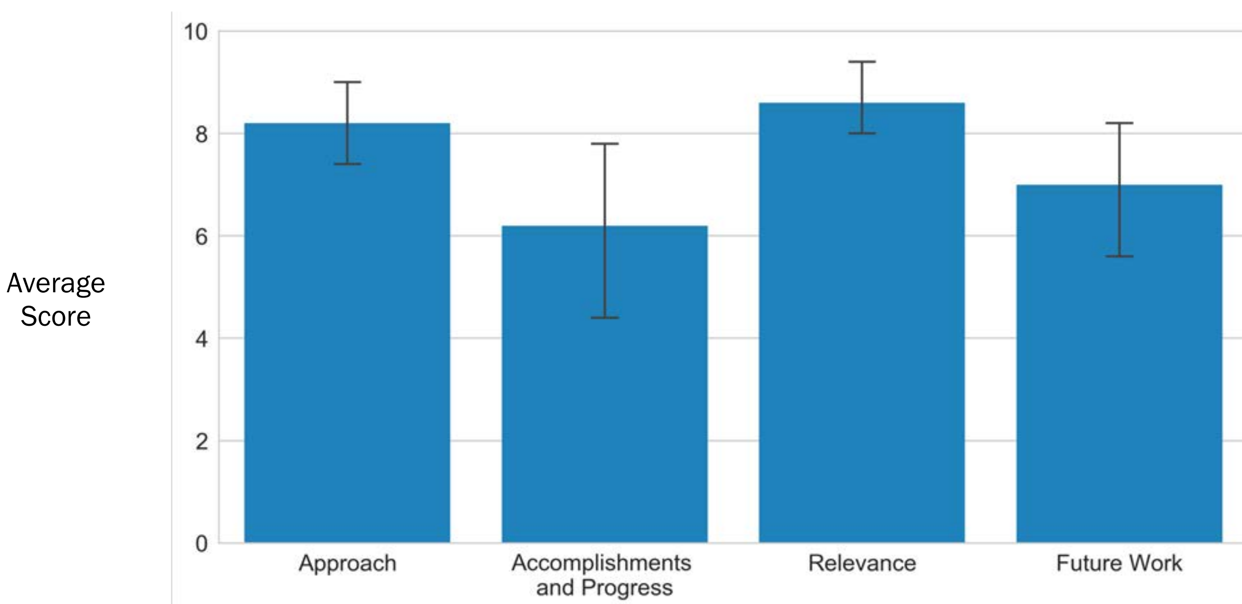
WBS:	3.5.5.1
CID:	NL0033568
Principal Investigator:	Dr. Michael Kass
Period of Performance:	10/1/2017–9/30/2020
Total DOE Funding:	$200,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$200,000
DOE Funding FY19:	$0
Project Status:	Ongoing

This project is in the second year of a multiyear effort to determine the feasibility and impact of biofuels (especially bio-intermediates) as viable fuel candidates for marine engines. The engines used to power cargo vessels, cruise liners, and many service vessels are fueled with a residuum heavy fuel oil (HFO). This low-quality fuel is highly viscous and contains high levels of sulfur (~3.5 vol %) and appreciable levels of water and sludge. Before it can be burned in the engine, the HFO must be heated to reduce the viscosity to enable proper flow characteristics. This fuel must also be processed onboard to remove the entrained water and sludge. When burned, HFO produces high levels of sulfur and particulate emissions. In fact, the sulfur emissions from one ship are equivalent to those produced from 50 million cars in one year. The level of HFO used in one year by marine ships is roughly equivalent to the sum of diesel used on highways in the United States.

The International Maritime Organization has set aggressive emission targets to reduce fuel sulfur content from 3.5% to 0.5% in 2020. Likewise, in the United States, the California Air Resources Board and other state agencies have regulations limiting the sulfur content of fuel used in coastal regions to 0.5%. This requirement will force ship operators to either operate on more expensive fuels, such as low-sulfur HFO, liquified natural

Weighted Project Score: 7.9

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



One standard deviation of reviewers' scores

gas, or distillate fuels; or, they can incorporate expensive emissions-control systems. Low-cost biofuels, especially bio-intermediates, are potential low-sulfur alternative fuels. The bound oxygen is also a known pathway to particulate matter reduction, and their inherently low viscosity means that less energy is required to achieve proper flow characteristics, thereby improving overall efficiency. This effort addresses several key technical barriers associated with and expanding a renewable resource to improve energy independence.

The general research plan is to (1) determine the feasibility of bio-intermediates as blends with HFO and (2) assess the impact of bio-intermediates on ship fuel systems and engine performance. Initial empirical studies have focused on obtaining rheological (flow) properties of HFO and its blends with bio-intermediates. A fast-pyrolysis bio-oil derived from softwood was obtained and blended with HFO to assess and confirm miscibility. These blends remained miscible even when heated. Viscosity measurements were also performed on bio-intermediate HFO blends. A key (and unexpected) finding was that the addition of 5% bio-oil dramatically reduced the viscosity of HFO at ambient temperature. Polymerization of bio-oil HFO blends was not observed. These results are highly encouraging. The research team also begun compiling literature on relevant bio-oil combustion in engines, and a determination of the combustion characteristics of bio-oil HFO blends will begin in the current quarterly period. Future work is planned to determine the compatibility of bio-intermediates with fuel handling systems and to conduct engine-based experimentation to determine combustion characteristics and the emissions profile.

Photo courtesy of Oak Ridge National Laboratory

OVERALL IMPRESSIONS

- This is an outstanding concept and approach with a clear identification of a critical need (low-sulfur fuels, no progress toward supply), and shortcuts are needed to further process bio-oils and can lead to the rapid commercialization of specific technologies once desired properties are identified.
- There is high potential for global impact if major risks can be assessed and addressed.
- This could finally be a practical application of bio-oils that is not hampered by exceedingly high upgrading costs.

- A clearer definition of the suitable bio-oil—a description that has been used for a vast variety of somewhat different liquids obtained from biomass—would be very useful. That, in turn, could help with more focus on the TEA, which is missing.
- This is a high-impact project of great interest and excellent effort.
- This project is aimed at determining the technical feasibility of using bio-oils (raw or slightly processed/stabilized) in marine engines.
- Marine engines currently use HFO, and bio-oil could be a great replacement considering upcoming sulfur regulations.
- This project is targeted at finding potential ways to blend bio-based oils into marine fuel, which is a major source of worldwide pollution.
- The work is generating key data to perform an empirical screen.
- This is a logical extension of the use of bio-oils and biocrude, which appear to be underused at present.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for supporting feedback. This effort has been focused on the technical feasibility aspect of bio-intermediates as a marine fuel. As we progress, we will continue to evaluate issues related to supply, including infrastructure needs and scale-up.
- Determination of a suitable bio-oil will be important. It is our thought that the marine application will be suitable for a broad range of bio-oils. Our initial studies have focused on softwood-derived bio-oils, and we plan on assessing their compatibility as a function of properties, such as water content, oxygenates, total acid number (TAN), and other variables. Our plan is to define the boundaries associated with water and chemistry that are suitable. A result would be a determination of suitable bio-oil properties.
- Yes, this is an accurate assessment of the project goals.
- Yes, the research team's immediate focus is on assessing the impact and compatibility of bio-oil with HFO. Early studies have emphasized miscibility and viscosity, and we are extending these to include compatibility (i.e., corrosivity) and lubricity.
- Yes, our study appears to be the first to look at blends of bio-intermediates with HFO for engine use. In our literature search, we were only able to find a study that looked at blends for burner applications. Unfortunately, that source did not evaluate the properties we are interested in.

ANALYSIS FOR JET HIGH-PERFORMANCE FUELS

Sandia National Laboratories

PROJECT DESCRIPTION

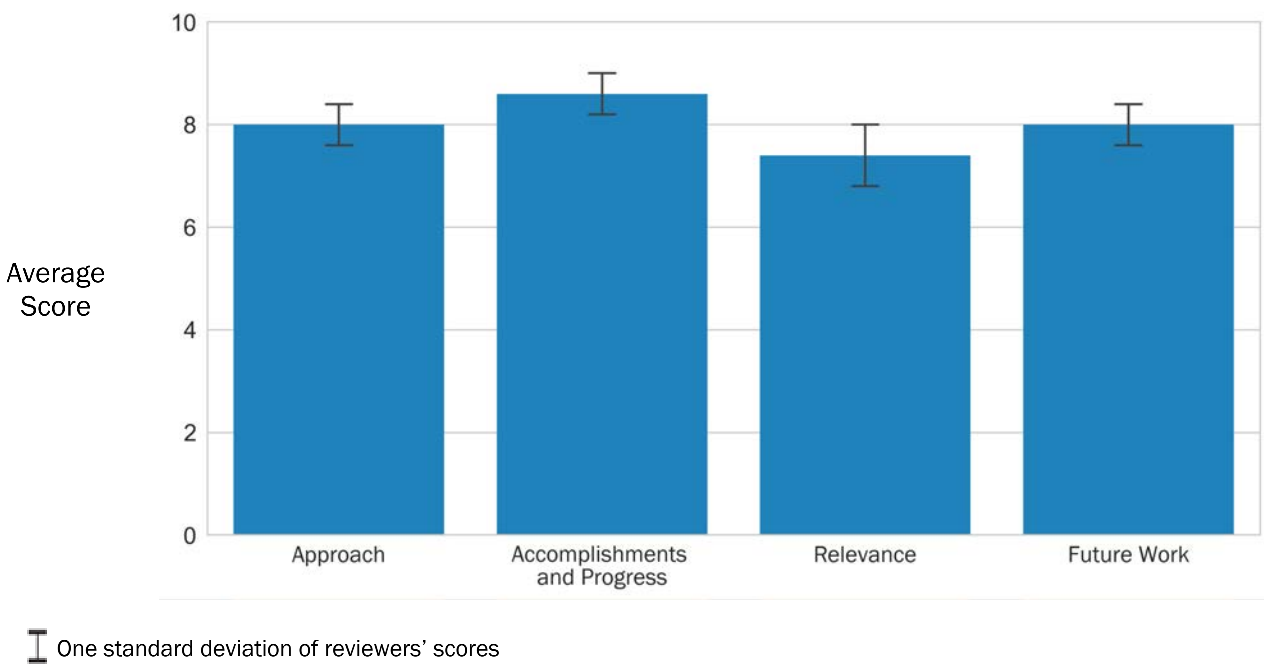
WBS:	4.1.1.70
CID:	NL0033867
Principal Investigator:	Dr. Anthe George
Period of Performance:	1/31/2018–9/30/2018
Total DOE Funding:	$100,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$100,000
DOE Funding FY19:	$0
Project Status:	Ongoing

Successful large-scale deployment of "drop-in" alternative jet fuels has been limited by their high cost of production compared to conventional fuel. Conventional jet fuels are limited by the crude oils from which they are made, the refinery technologies that can be applied, and the critical requirement to make consistent, on-spec fuels from hundreds of different feedstocks in hundreds of different refineries around the globe. These restrictions severely limit the opportunity to produce higher-performance jet fuels without massive investments in new refining equipment, and perhaps not even then.

Biomass resources and conversion technologies offer an opportunity to make types of components not accessible through petroleum refining and for the investment in making them to result in added production capacity, something that not even a costly retrofit of existing refineries could match. Simultaneously, if these new components can be designed to confer performance advantages, there is evidence that the benefits could offset at least some of the current cost differential. Through a recent workshop on jet engine fuel optimization, jet engine manufacturers defined the benefits they most desire: better operability, more efficient fuel combustion, and increased range payload. Therefore, we have the guidance needed to develop cost-competitive, sustainable, high-performance fuels (HPFs).

Weighted Project Score: 8.0

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



We began by benchmarking conventional jet fuels and relating key performance attributes to the properties of their various components on a molecular level. Based on this knowledge, we then proposed bio-based alternatives with the potential to optimize the combination of benefits sought by engine manufacturers and aircraft operators; this was based on published properties, structure-property correlations, and *ab initio* methods.

This presentation provides preliminary findings of the multiteam efforts on the identification of molecules, determination of their energy content, development of the Jet fUels blenD Optimizer tool (JudO) tool to determine "drop-in" blending, and how to achieve required energy content through Pareto front analysis of fuel composition. We also present preliminary results on the performance benefits of notional high-performance jet fuels.

Next steps in this work include:

- Improvements to the JudO tool by adding fuel attributes to meet drop-in ASTM requirements
- Molecule structure-property relationships on further key jet-fuel properties and associated structure-property trends
- Production of data on the laboratory-scale feasibility of HPFs, focusing on alkyl cycloalkanes and refined analysis of their value propositions.

This work will provide guidance on where R&D efforts in this space should be directed.

OVERALL IMPRESSIONS

- This project has the potential to assist industry with the identification of highest-value molecules for future work and could help shortcut failures and reduce the waste of resources. It does speculate with novel and previously unresearched molecules, but that should be the point of tools like this. I look forward to seeing the final product.
- The concept of designing a high-performance fuel *ab initio* based on desired characteristics to deliver specific benefits to a user is powerful, and the PIs make a compelling case in the project.
- The critical limitation at this time is that a clear dollars-per-gallon production cost target that makes the fuel economically viable has not been included. It is a relatively minor weakness at the early stage of this project, but it will become increasingly more relevant as the project advances.
- The approach is appropriate and applies to molecules regardless of their origin—fossil or bio—and it is intriguing that potentially superior performance might be obtained by bio-derived molecules. The different reduction state of the bio-derived molecule makes this consideration regarding the process pathway even more critical as the project evolves and will determine its increased or diminished relevance for the BETO mission.
- Nonetheless, these caveats on the economics should not prevent the team from seeing where the real value of these tools lie: the team provides a target, and it is up to other R&D efforts to see if such a target is realistic and reachable, both technically and economically. By providing a target that can fulfill required performance criteria, these tools, though they do not guarantee success, do ensure that R&D efforts are focused on molecules and the class of molecules that can indeed perform as required.
- This study was designed to understand the impact of various high-energy-density molecules on the performance of the jet fuel.

- The work followed a strategic and scientifically based approach to determine which bio-based compounds would have the best chance of positively contributing to jet fuel blends.
- The presenter did a good job of methodically explaining the process in an understandable manner.
- The current availability or whether the compound could be produced was not addressed, but it would add value.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We are sincerely grateful to the reviewers for their insight and their efforts in reviewing our program. We acknowledge the notes regarding the strengths of this aspect of the Co-Optima effort, and we limit our comments to the weaknesses sections of the review. In general, we note the comment that this is a small piece of work and that it would benefit from an expanded scope. Many of the comments pertain to work that was beyond the scope of this effort, which would nevertheless be valuable to accomplish.

GARDN COLLABORATION U.S.-CANADA AVIATION FUELS

Pacific Northwest National Laboratory

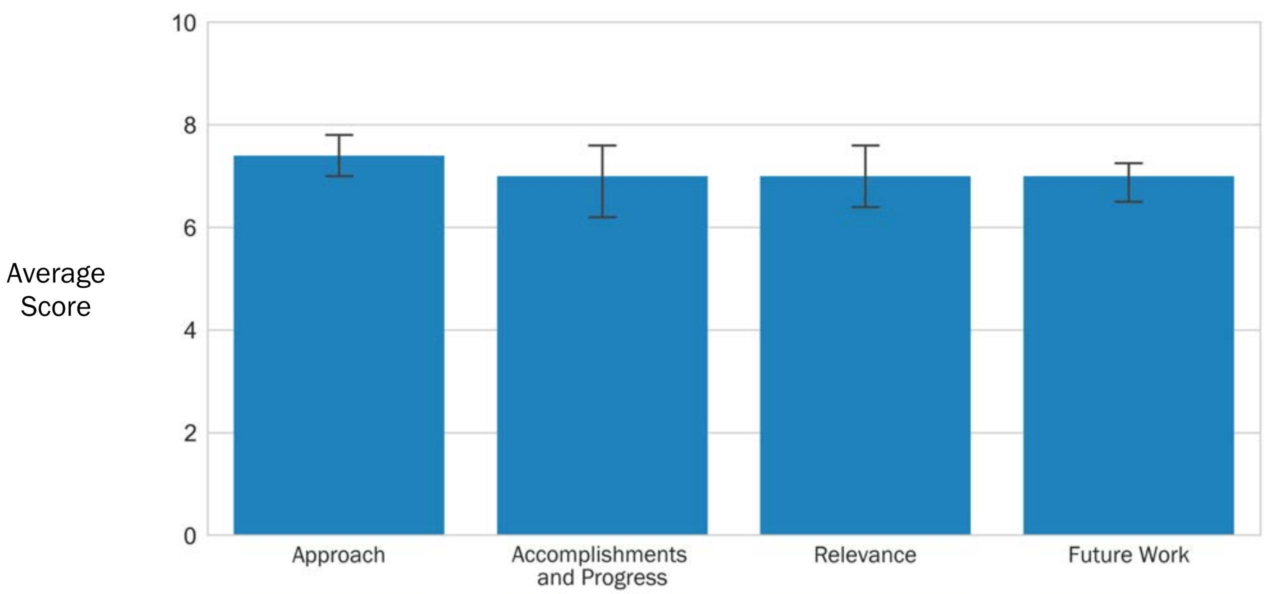
PROJECT DESCRIPTION

WBS:	6.4.0.9
CID:	NL0033748
Principal Investigator:	Ms. Corinne Drennan
Period of Performance:	1/1/2018–9/30/2019
Total DOE Funding:	$200,000
DOE Funding FY16:	$0
DOE Funding FY17:	$0
DOE Funding FY18:	$200,000
DOE Funding FY19:	$0
Project Status:	Ongoing

GARDN is a nonprofit organization funded by the Business-Led Networks of Centres of Excellence program of the Government of Canada and the Canadian aerospace industry. GARDN funds collaborative projects that can reduce the environmental footprint of the next generation of aircraft, engines, and avionics systems, and it helps members from academia and industry bring their innovative ideas to life. The Assessment of Likely Technology Maturation (ATM) pathways used to produce biojet from forest residues consortium, within GARDN, is tracking the performance and life-cycle impacts of forest residues to jet fuels via fast pyrolysis, catalytic fast pyrolysis (CFP), and hydrothermal liquefaction (HTL), involving partners from stakeholders of biojet fuels. PNNL was invited to participate in the ATM consortium for expertise in each conversion pathway as well as in hydrotreating, jet fuel preparation (e.g., fractionation, meeting specifications), and capturing life-cycle inventories associated with conversion processes. The consortium, led by NORAM and the University of British Columbia, includes the Canadian government CanmetENERGY laboratories, PNNL, $(S\&T)^2$ Consultants Inc., and SkyNRG, with support from the Boeing Company, Bombardier Inc., Air Canada, and WestJet Airlines Ltd.

Weighted Project Score: 7.1

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



One standard deviation of reviewers' scores

BETO, already coordinating on sustainable aviation fuels with Canada and Mexico, supported the majority of PNNL's participation in the ATM. In FY 2018, PNNL completed hydrotreating of the bio-oils biocrude from each liquefaction process (fast pyrolysis, CFP, and HTL), provided conversion performance data and biojet fuel products for fuel analysis, and provided general technical support in examining the three supply chains. A comprehensive report for the ATM's research is expected to be published in 2019. Through the collaboration, the ATM has demonstrated the feasibility of hydrotreating technology for upgrading bio-oils biocrudes from current thermochemical conversion technologies and established a model international collaboration network for building methodology and analysis of the complete supply value chain for biojet fuels from a single representative forest residue feedstock through conversion, upgrading, and fractionation. This international collaboration provides important experience and information to stakeholders of biojet fuels and will accelerate the acceptance of biojet fuel from biomass thermal chemical conversion processes.

OVERALL IMPRESSIONS

- This appears to have been a very short project that almost seems to have been designed to highlight the unsuitability of these feedstocks for aviation fuels; it might have been a result of the schedule or of the materials provided, but the overall gist seems to be that it is validating a negative result (i.e., do not consider this use). Hopefully the final report will be clearer and offer a broader explanation of the commercial applicability of the feedstocks.

- In general, this project has several points of merit. One is that it appears to demonstrate that the production of jet fuel from woody biomass is not a particularly attractive proposition. From a technical perspective, the comparison among different types of bio-oils is valuable because it highlights critical differences that are relevant when considering these materials regardless of the final application.

- A more detailed TEA would have been desirable, and the amount of hydrogen (H_2) upgrade necessary hints to a considerable hit on the GHG profile unless only renewable H_2 is used. A more detailed discussion on the GHG profile would have been needed.

- The conclusion on whether further investigation is warranted—and under which conditions—is not clear.

- This project, funded under GARDN, asked PNNL to participate in the ATM pathways to produce biojet fuel from forest residues.

- PNNL evaluated various hydrotreating options for pyrolysis oil to produce biojet fuel. PNNL found that the pyrolysis oil was not the best feedstock.

- This background research project focused on pathways from biomass to biojet fuel, accessing the overall sustainability.

- This project is of nominal overall value to industry.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Thank you for the considerations and comments. We agree that disseminating information about the differences between different bio-oils is important. A detailed TEA and LCA will be published this year. It is important to frame the results of this work in the context of woody biomass conversion via fast pyrolysis, CFP, and HTL. The results presented do not hold for the feedstock or conversion technology alone. For example, high-quality jet fuel is obtainable from woody biomass but by using a different conversion approach. Liquefaction technologies have the potential to produce quality jet fuel using different feedstocks or by blending different feedstocks with woody biomass.