CO-OPTIMIZATION OF FUELS & ENGINES

TECHNOLOGY AREA

CONTENTS

INTRODUCTION

The Co-Optimization of Fuels & Engines (Co-Optima) initiative (or "consortium") is one of 14 sessions reviewed during the 2019 Bioenergy Technologies Office (BETO) Project Peer Review. Co-Optima was initiated in 2016 and was previously reviewed at 2017 BETO Project Peer Review. While it is part of the Advanced Development and Optimization (ADO) portfolio, Co-Optima was reviewed in a separate session due to the scope and crosscutting nature of the initiative. In the Co-Optima session, six external experts reviewed nine presentations.

This review addressed a total U.S. Department of Energy (DOE) investment of approximately $59,000,000 (Fiscal Year [FY] 2016–2019 obligations), which represents approximately 6.8% of BETO's portfolio reviewed during the 2019 Peer Review. The principle investigators (PIs) for the FY 2018 Co-Optima DE-FOA-0001919 were invited to present posters at the 2019 Peer Review and reviews are not included in this report. Co-Optima was also reviewed at the 2019 Vehicle Technologies Office (VTO) Annual Merit Review.[1] That review focused on the VTO-funded tasks and projects.

The review panel evaluated and scored projects based on their approach, technical progress, and accomplishments from FY2017 to FY 2019, 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 Co-Optima initiative, full scoring results and analysis, the Review Panel Summary Report, and BETO's Programmatic Response are also included in this section.

BETO designated Alicia Lindauer as the Co-Optima Technology Area Review Lead with contractor support from Mr. Robert Natelson (Allegheny Science & Technology). In this capacity, Ms. Lindauer was responsible for all aspects of review planning and implementation.

CO-OPTIMA OVERVIEW

The Co-Optima initiative aims to advance the underlying science needed to develop fuel and engine technologies that will work in tandem to achieve significant efficiency and emissions benefits. This research and development (R&D) collaboration between VTO, BETO, nine national laboratories, and over 20 university and industry partners is a first-of-its kind effort to combine biofuels and combustion R&D, building on decades of advances in fuels and engines.

Co-Optima research is focused on identifying blendstocks that offer efficiency and performance benefits for the entire on-road vehicle fleet, from light-duty passenger cars to heavy-duty freight trucks. The initiative takes a three-pronged, integrated approach to identifying and developing:

- Engines designed to run more efficiently on affordable, scalable, and sustainable fuels
- Fuels designed to work in high-efficiency, low-emissions engines
- Strategies that can shape the success of new fuels and vehicle technologies with industry and consumers.

CO-OPTIMA SUPPORT OF OFFICE STRATEGIC GOALS

Co-Optima's main goal is to identify the combinations of fuel properties and engine characteristics that maximize efficiency, independent of fuel composition or production pathway, to allow the market to define the best way to blend and provide these fuels. The initiative is pursuing a systematic study of fuel blendstocks

[1] U.S. Department of Energy. 2019. "Vehicle Technologies Office Annual Merit Review." https://www.energy.gov/eere/vehicles/vehicle-technologies-annual-merit-review.

(represented as classes of molecular families) to identify a broad range of feasible options. The objectives are to identify blendstocks that can provide target ranges of key fuel properties, identify trade-offs on a consistent and comprehensive basis, and share information with stakeholders.

Co-Optima activities develop the knowledge, data, and tools to expand the blendstock options available to achieve desirable fuel properties. Co-Optima seeks to identify technology options for commercial liquid fuels and high-performance engines powering the entire on-road vehicle fleet (i.e., passenger to light truck to heavy-duty commercial vehicles, including hybrid-electric-vehicle architectures). The aggressive research timeline is structured around researching fuel and engine technologies to the point that industry can consider product development with confidence, setting the stage for commercial introduction of better fuels and engines sooner than otherwise possible without federal support. This will provide an opportunity to create market demand for up to 25 billion gallons of advanced bio-derived blendstocks estimated in a billion-ton biomass economy,[2] diversifying our resource base and providing valuable flexibility to refiners to respond to significant evolving global trends in transportation fuel demand.

While the Co-Optima initiative is jointly funded by the Office of Energy Efficiency and Renewable Energy's (EERE's) BETO and VTO, this review focused on the BETO-funded work. The national lab consortium work was reviewed in a series of five presentations. Four projects selected from the FY 2016 Co-Optima Funding Opportunity Announcement (FOA) DE-FOA-0001461 were reviewed in the session.

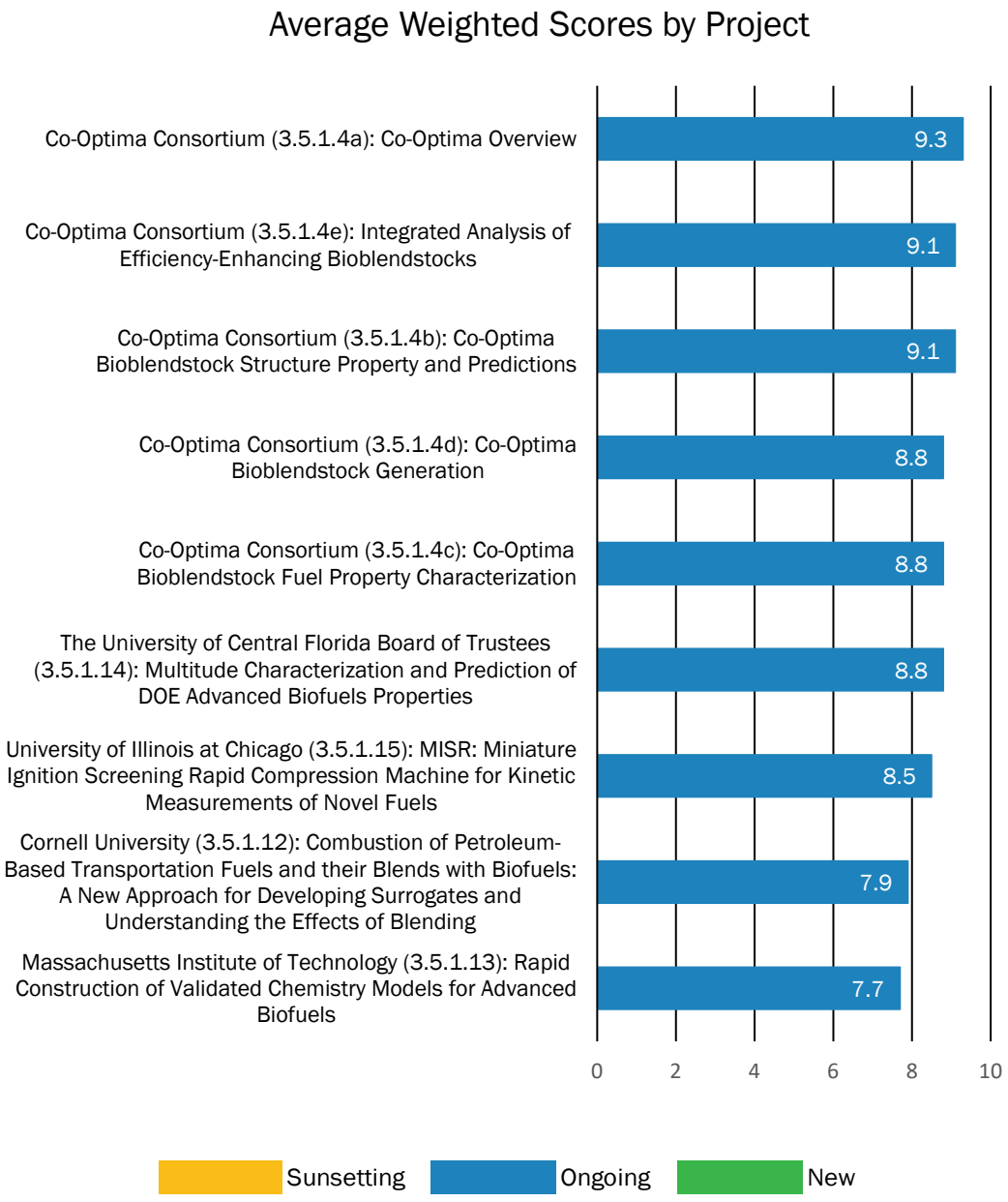
CO-OPTIMA REVIEW PANEL

Name	Affiliation
Harry Baumes*	Retired, U.S. Department of Agriculture
Charles Abbas	iBiocat
Cory Phillips	Phillips 66
Kristin Lewis	U.S. Department of Transportation – Volpe Center
Bhupendra Khandelwal	University of Sheffield
Steven Przesmitzki	Aramco

* Lead Reviewer

[2] Rogers, J. N., B. Stokes, J. Dunn, H. Cai, M. Wu, Z. Haq, H. Baumes. 2016. "An Assessment of the Potential Products and Economic and Environmental Impacts Resulting from a Billion Ton Bioeconomy." *Biofuels, Bioproducts & Biorefining* 11:110-128 (2017). http://doi.org/10.1002/bbb.1728.

TECHNOLOGY AREA SCORE RESULTS



CO-OPTIMA REVIEW PANEL SUMMARY REPORT

Prepared by the Co-Optima Review Panel

The Co-Optima portfolio is an important area of work within DOE. The program of work is co-led by BETO and VTO. The program objective is to advance the underlying science needed to develop and match new fuel and engine combinations for greater efficiency and lower emissions. BETO funds a large body of work focusing on biomass-derived fuels and the specific properties required for optimal performance including environmental and economic goals. Specific goals are (1) to identify low carbon fuel/engine combinations that increase fuel economy by 35% (light-duty) or 4% (heavy-duty) over a 2015 baseline, and (2) to achieve environmental performance benefits, particularly by lowering carbon intensity.

The peer review for the BETO-funded portfolio was held on March 7, 2019. The peer review panel was diverse and consisted of six members. The panel heard a total of nine presentations discussing the work; five of the presentations focused on BETO/VTO national lab co-led work: an overview; bioblendstock structure property relationships and property predictions; bioblendstock generation; bioblendstock fuel property characterization; and integrated analysis of efficiency enhancing bioblendstocks. In addition, there were four university research efforts led by PIs from Cornell University (combustion); University of Central Florida (UCF) (characterization and prediction of advanced biofuels properties); Massachusetts Institute of Technology (MIT) (rapid construction of valid chemistry); and University of Illinois–Chicago (UIC) (miniature ignition screening – rapid compression machine). The panel would like to thank the PIs for their innovative approaches, valuable contributions, and presentations. Based on the overall relatively high scoring of the projects, the panel members valued this work.

The national lab co-led projects by BETO/VTO had a strong team with crosscutting technical expertise and frequent team interaction, clear identified goals, and a desire to make work available/accessible to the public sector. Information sharing across labs and with BETO leadership was emphasized. While coordination is a key strength of these five projects, the university led projects do not seem to be as well integrated and linked into the experience and expertise of the national labs.

IMPACT

The Co-Optima initiative is working to develop new high-performance fuels, including biomass-derived fuels (identify and characterize fuel properties) that can boost engine efficiency and overall performance and cut emissions when combined with advanced combustion approaches. The 2019 Peer Review is the second peer review for Co-Optima, but the first that work has been conducted over a two-year period, and much has been accomplished. The entire portfolio has the potential to be significantly impactful to the biofuels industry and the bioeconomy in the process of providing/identifying efficiency enhancing bioblendstocks/fuels to technologically advanced engines design and control strategies. As evidenced by the Co-Optima overview and the individual presentations, the eight projects that were reviewed are unique and complementary. Therefore, it is difficult to identify any one project as being more impactful than another. Crosscutting goals are identified, including those that stimulate the domestic economy, create new bioeconomy jobs, and generate clean fuel options.

The Co-Optima portfolio comprehensively addresses identification of candidate bioblendstock molecules, the prediction and confirmation of candidate chemical performance, generation of candidate molecules from biological pathways, and potential for integration as viable and sustainable fuel options that should be further investigated. The approach adopted by BETO/VTO has been designed to execute on unique program areas, and to simultaneously share research results and accomplishments so they can be integrated with the other projects.

For example, the structure-property relationships and property prediction project focuses on chemical structure/property relationships (what is the molecular structure of advanced single-component biofuel

candidates and how are the property characteristics of these single compounds related to this molecular structure). These properties are used to extrapolate or predict the suitability of these multicomponent blendstocks using a broader mixture of individual biomass-derived molecules or molecular families.

This work feeds into the blendstock fuel generation and pathways work by selecting the most appropriate bioprocess to generate the larger volumes required to feed into the fuel property characterization work. Data and databases, models, and other tools have been and will continue to be developed and refined/expanded during the life of the program and made available to other Co-Optima team members, the national labs, and other stakeholders to facilitate and advance future research. Collectively, the work leads to integrated analyses/evaluation of co-optimized bioblendstock and engine technologies from environmental and economic perspectives while conducting R&D guiding analyses (techno-economic analysis [TEA], life cycle assessment [LCA], bioeconomy jobs, economic growth, etc.). Select impactful results are identified below.

The Co-Optima team has developed an approach to the bioblendstock candidate selection process that reduces costs and time to evaluate and assess suitability of blendstocks, enhances likelihood of developing a successful biofuel, and accelerates the time required to bring a bio-blend fuel to market. The Co-Optima team, through a defined filtering approach (tier fuel/desired performance/merit), started with 400 blendstock samples for boosted spark ignition and down-selected to 10 blendstocks for evaluation. This was further reduced to six blendstocks based on merit function scores (and fewest barriers to market).

The blendstock structure/property relationships and predictions and project approach is clearly defined and focused on chemical molecular structure/fuel property relationships to enhance the team's capability to identify potential blendstocks. The team utilizes machine learning and computational chemistry at the quantum level to correlate against a significant number of performance and operability parameters clustered within molecular classes. The approach of property/structure relationship for the fuel blend selection is an important step forward.

The merit objective function for light-duty engine efficiency was developed and is considered to be the most critically advanced engine tuning parameters from a multivariate standpoint allowing objective evaluation and optimization of fuel candidates for boosted spark ignition (BSI), multimode spark ignition (MMSI), and mixing-controlled compression ignition (MCCI) combustion modes. For light-duty engines, BSI and multimode (MM) engine modes, factor such as research and motor octane numbers, sensitivity, charge cooling, burn rate, and emissions are included in the measure. For medium-duty (MD) and heavy-duty (HD) MCCI engine modes, a different set of factors based primarily on fuel properties (e.g. cetane number, flash point, heating value) are weighed.

In the case of BSI, six blendstocks with the highest merit function scores (out of 24 screened candidates) were selected as having the fewest barriers to market specifically with technical readiness, economics, supply logistics, and environmental impact. The merit function has potential to become an industry standard metric in the future, not for fuel specifications but rather for biofuels R&D.

The Fuel Properties Database work has made very important progress. It has been expanded and now includes over 800 compounds and mixtures. The concept of the Fuel Properties Database will be essential for the success of Co-Optima and BETO’s Chemical Catalysis for Bioenergy Consortium (ChemCatBio). A fully searchable database with fuel property candidates supplied from multiple labs and researchers has been developed and was used extensively for BSI and MCCI candidate screening. A significant number of analyses have been performed, including on toxicity, levels of partitioning, and biodegradability. The latter two lead to a greater differentiation of the blendstocks than toxicity. The team was able to identify that synergistic effects of blending on spark-ignition (SI) performance are not just due to pure component octane numbers but also due to the ability to shut down the formation of low research octane number (RON) products in combustion. These data are forming the basis of multiple Co-Optima projects doing further investigation of blendstock candidates. The work helps to develop ASTM standards based on interactions identified between fuel effects and

combustion modes. This is critical for deployment and acceptance of fuels by the wider stakeholder community of biofuel manufacturers, distributers, auto original equipment manufacturers (OEMs), and regulators. The team has created the fully searchable Fuel Properties Database that is updated regularly and available online, with over 8,000 users in the last three years. The Co-Optima team will utilize the database for future screening.

The integrated analysis team has completed blendstock review and identified alcohols, olefins, and furans as the molecular families with the most likely high-efficiency candidates. Next, the team reviewed 23 bio-blendstocks based on initial screening through the use of the Analysis of Sustainability, Scale, Economics, Risk and Trade (ASSERT) model. The critical challenge of matching diesel energy density is harder than achieving efficiency. One of the most valuable elements of this project is the development and dissemination of many models and tools for the public that are being disseminated on GitHub.

All projects received relatively high scores from the panel members. The projects reviewed by the panel indicate the Co-Optima team is working toward its overall objective by conducting basic research on fuel properties and engines and by developing models, tools, accessible databases, and instruments. The Co-Optima program should have significant impact from dissemination and reporting of research results from the approximate 125 journal articles published and/or accepted for publication, approximate 50 technical reports, and the more than 90 presentations given to multiple venues by team members.

The overview and four national laboratory-led DOE projects tended to be scored higher than the four university-led projects. The range of the average panel ranking between the highest and lowest was 0.55 for the lab-led projects and 1.0 for the university-led projects. Further, no university-led project was ranked higher than any lab-led program. This should not be misconstrued to suggest that the university-led projects are any less valuable or important to the Co-Optima initiative. The lab-led projects are well coordinated and integrated, and this is an area in which the university-led projects could be improved, as identified in the recommendations.

Both the UCF and UIC presented impactful work on the effect of biofuels on engine-parameter-tuning uncertainty as well as, the miniature ignition screening rapid compression machine (MISR) instrument respectively. Both of these projects generate significant, sizeable quantities of relevant data quickly and efficiently while providing statistical analysis on traditional combustion kinetic parameters (e.g., laminar flame speed, soot volume fraction-shock tubes, rate constants, coking volume fraction). This work will be important for hardware design implications with MM, MCCI, and kinetically controlled combustion modes.

INNOVATION

This Co-Optima portfolio itself is innovative in a sense that the initiative is looking at many fuels, including biofuels (design, synthesis pathways, properties) and engines simultaneously and is focusing on what developing fuels (bio-based) are desired to optimize the advanced engines. This offers a unique opportunity to identify and generate novel bio-based blendstocks that meet chemical, economic, and sustainability criteria. As such, multidisciplinary efforts and resources are required, which calls for a great deal of management oversight and a high degree of integration and coordination among and between the individual projects. The Co-Optima portfolio overall uses an innovative approach to generate new opportunities for biofuel/engine advancement. The component elements are comprehensive and the national lab led projects are well integrated and coordinated. The four university-led projects appear to function independently of the others, but the work is valuable and contributing to the ultimate objectives of the Co-Optima program. The data, tools, and models being developed through the initiative will be valued across the portfolio, by other public and private sector researchers, and by bioeconomy stakeholders.

Many of the projects are utilizing state of the art analytical, informational science, and big data techniques, algorithms, and software to advance the project work and ultimately the Co-Optima portfolio. Computer learning techniques, predictive modeling, and data-mining techniques are examples of tools/software being

utilized and developed. They are using machine learning and computational chemistry at the quantum level to correlate against a significant number of performance and operability parameters clustered in molecular classes. The approach of the property/structure relationship for blend selection is an important step forward. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This will eventually help select the right blends.

The blendstock generation project has presented an impressive and clearly laid out approach of combining predictive modeling with retrosynthetic analysis to identify the method of production, then validate the production method. The team is also generating blendstocks for characterization (if unavailable from industry). This is one of the most innovative approaches in the consortium, because it ties the synthesis pathway into the evaluation activities, which is a more holistic approach.

The structure/property and prediction component of the Co-Optima project is crucial to the successful development of novel biofuel options in that it:

- Provides the predictive modeling and validation of blendstock characteristics
- Isolates the effects of specific functional chemical families or groups on fuel properties
- Provides a method for high-throughput screening level analyses of blendstock candidates
- Identifies unexpected structure/property relationships.

The data and models from this project will be extremely useful across the Co-Optima team but also for industry and other researchers. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This would eventually help in speeding up the process of biofuels and engines for better efficiency. This is also assisting in taking steps forward for achieving BETO objectives and technology area goals.

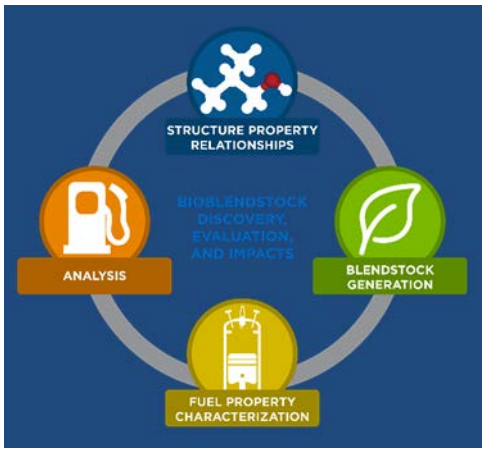
The MIT project is developing combustion chemical kinetics models for advanced biofuels to assess and predict potential performance. The approach combines computer modeling generalization to enable new compound analysis combined with real experimental data on fuels/chemistry. For combustion modeling, the key is to identify the most important reactions to include and capture in the modeling framework. The MIT project is world leading because it focuses on creating a machine-learning program to generate reduced chemical kinetics models in batches, rather than the traditional method of developing them one at a time by hand. This would be a breakthrough in the field once successful and widely deployed.

The UIC project is similar in motivation to the MIT project in that it seeks to automate an extremely expensive and time-consuming process, namely running a rapid compression machine. The project has the potential to generate more data in months than the previous body of research in this field did in years, if successful. Combining the results of the UIC and MIT projects could completely change the nature of fuel chemical kinetics modeling and make the current methods look antiquated by generating an order of magnitude more data in the same amount of time.

There are many innovative aspects to the Co-Optima initiative in addition to those technical items identified above. A strong management team is in place. The inclusion of an external advisory board (EAB) provides guidance and insights from various stakeholder perspectives. There is a strong effort to make methodologies, tools, models, and databases available and accessible to the public. The Co-Optima team actively engages with its stakeholders.

SYNERGIES

The Co-Optima Overview presentation identified the initiative's objective as, "Advancing the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental, and economic goals." As such the individual projects, particularly the five projects led by the national labs, have a great deal of synergies between them. The management structure of each project is similar: team expertise in cross-cutting areas (fuels, vehicle, infrastructure, etc.) for the specific projects, participation by multiple national labs, monthly and quarterly meetings focusing on progress, issues, and reporting to senior leadership (BETO/VTO). In many instances, individual project management members may participate in more than one project. The coordinated design of the Co-Optima projects (see figure to the right, titled "Approach of the Four Co-Optima National Laboratory Research Projects" is highly integrated, with results and accomplishments and feedback flowing from one project to another. There is a high degree of synergy; projects rely on similar inputs and tools. What is not clear is if these groups interact sufficiently to ensure good communication and streamlining of efforts to avoid redundancy.



Approach of the Four Co-Optima National Laboratory Research Projects

The four university-led projects are more distinct and do not exhibit the same degree of integration with the national labs or each other. There needs to be a better flow of information, results, and accomplishments from the four university-led projects to the other Co-Optima projects, especially information that could be added to databases and modeling.

The review panel supports the national lab-led projects to make data, databases, models, and tools available to and accessible by stakeholders and the public.

FOCUS

The Co-Optima program remains compositionally neutral on recommending future fuels. This approach needs to reconcile with BETO's need to satisfy the market with commercially viable fuels. There should be an effort to identify a deliberate driver to seek a natural overlap from both sides, or the overall approach will be inefficient and work will continue to move forward in silos rather than in a community approach.

The structure property relationships and property predictions and the fuel property characterization projects provide a tiered approach to the initial blendstock assessment, the results of which feed into most, if not all, of the other Co-Optima projects. The team has successfully narrowed a large field of candidates to a key set of highly likely candidates, incorporating not only chemical characteristics but also certain environmental performance criteria. Given the importance of biodegradability and low toxicity for these blendstocks for which sustainability and improved environmental performance will be critical, it makes sense to evaluate these blendstock elements as an early screening; these should be part of the Tier 1 screening rather than waiting until Tier 3.

Validation work should continue along with benchmarking against traditional hydrocarbons currently being produced in the refinery to establish precision and accuracy metrics. The structure property relationships and property prediction team has demonstrated the ability to predict synergistic non-linear combustion behavior which is an extremely important capability. The team should continue to provide fundamental insights on such counter-intuitive fuel blending properties or behavior.

The Bioblendstock Generation project team should keep expanding their fuel generation scope within the targeted viable biomass-derived fuel candidate classes by considering blends made up of alcohols, alkanes, and ethers together along with commercial hydrocarbons to form a true fuel matrix. Pure component data are only good to an extent for extrapolation to the blending values, which is what really matters.

Many of the surrogate fuel blends identified will require decades to enter the market, if ever. At least one panelist suggests the program consider having at least one track focused on engines specifically for hybrid-electric vehicles (HEVs), since hybrids will be likely the most common internal combustion engine by 2050. For example, a high-compression, lean Atkinson cycle engine running in a very small operation window can exceed the fuel efficiency of an MCCI engine operating over a wide range of speed-load points (per a reviewer's internal analysis from their company). Developing a new fuel for a narrow engine operating range of an HEV may significantly lessen the operating robustness requirements, making the fuel commercialization easier.

The potential barriers to introduce the new fuels (requiring new infrastructure) appear to have been somewhat trivialized. While not really an R&D issue, it should be considered somehow, perhaps as part of the integrative analysis component. This would require more interactions between the ChemCatBio and Co-Optima consortia. Analytical results presented infer a short time is required to bring a fuel to market, whereas it takes several years for approval and development of infrastructure (in some cases). Perhaps some ranking of the difficulty of introducing the fuel nationwide and worldwide could be added to the merit function, i.e., methanol would rank lower than ethanol on market introduction.

COMMERCIALIZATION POTENTIAL

The objective (per the Co-Optima overview presentation) of the Co-Optima initiative is to "Advance the underlying science needed to develop biomass-derived fuel and engine technologies that will work in tandem to achieve efficiency, environmental, and economic goals" by identifying low carbon fuel/engine combinations that increase fuel economy by 35% (light-duty) or 4% (heavy-duty) over a 2015 baseline, with reduced emissions. This is a long-term project and although there has been a great deal accomplished over the initial three years of the work, the target date to meet the object is 2030.

The project's value provides foundational knowledge of underlying science to understand and predict fuel properties to stakeholders to improve the value proposition for biofuels. The work that has been accomplished to date, such as the Fuel Properties Database, the merit function, and the retrosynthetic analysis tool, is laying a foundation for the future development of commercially available bioblendstock fuels for advanced light, medium-, and heavy-duty engines that provide efficiency, environmental, and economic benefits.

RECOMMENDATIONS

The review panel makes the following recommendations to BETO leadership.

1. Better leverage the industry, environmental, and technical expertise of the EAB.

    A. Review the composition of the EAB to ensure relevant stakeholder industries and sciences are represented.

    B. Add at least one environmental scientist, biochemist, and explicit fuel and vehicle OEM representative. Appropriate science expertise on the EAB would recognize and improve sustainability criteria (toxicity, biodegradability, miscibility) which need to be moved from Tier 3 to Tier 1 in the review of viable fuels. If a fuel is detrimental to the environment, then it should not be considered as viable.

    C. EAB should provide guidance on the review and analysis of complex blends.

i. Explore if the results can feed back to the catalytic conversion work and reduce conversion selectivity concerns.

2. Increase engagement with the fuel additive manufacturers (Afton Chemical, Innospec Inc., NALCO Champion, etc.) and other relevant stakeholders (such as potential biofuel producers beyond the existing supply chain of fossil fuels and blenders) for the purposes of resources, perspective, and risk mitigation:

   A. To study fuel impact on lubricants, ignition improvers, etc.

   B. Use the additives' engine dynamometer facilities

   C. Engage commodity processors and leverage new and evolving federal programs.[3]

3. Make a Co-Optima landing page with all models and data ready for the public.

CO-OPTIMA PROGRAMMATIC RESPONSE

INTRODUCTION/OVERVIEW

BETO sincerely thanks the review panel for its time, active engagement, and constructive review of the Co-Optima portfolio. In putting together the panel, it was our hope to welcome a wide range of perspectives, and thus we invited reviewers from the Analysis and Sustainability, Catalysis, and Biochemical Conversion review panels. The value of the diverse panel members' feedback was clear in the thorough comments and recommendations. The praise of the potential value and impact of the Co-Optima work is appreciated. The panel's recommendations will be used to enhance the effectiveness of Co-Optima activities and contribute to BETO's goals.

This was the first peer review where Co-Optima's university (competitive/2016 FOA) projects were presented. It was refreshing to see generally positive scores and comments for the university projects. The issue raised by the panel about an apparent limited engagement between the university projects and the national labs will be considered. Recurring stakeholder calls continue, and the arrangement of the recurring calls has been reorganized to facilitate more direct communication between specific stakeholders. Additionally, the new competitive university projects under the FY 2018 FOA (which, as mentioned, did not present at peer review) each have a specific liaison at the national labs to streamline Co-Optima stakeholder communication.

Reviewers provided feedback on the national lab and university activities. The Co-Optima Leadership Team is working with PIs to address this feedback to strengthen future work plans. The reviewers also provided feedback to the overall Co-Optima initiative, which was organized into three general recommendations. We greatly appreciate these recommendations and are working to incorporate these suggestions into FY 2020 priorities and beyond.

[3] One panelist felt BETO's Co-Optima efforts could be enhanced by reaching out to commodity processors of wood products and wood residues, citing that there is an opportunity to tie in with a new presidential initiative for a healthy forest that the Technical Advisory Committee (TAC) is now trying to tackle. With the great abundance of trees in the west and southeast regions (healthy and otherwise) there is a potential there to having significant volumes of feedstocks. With the right incentives, these feedstocks can be tapped into by the Co-Optima team.

Recommendation 1: Better leverage the industry, environmental, and technical expertise of the EAB.

BETO agrees that the EAB is a critical part of the Co-Optima organization. BETO will work with the VTO and the Co-Optima leadership team to review the EAB composition. Recent additions to the EAB include two new members representing the biofuels industry.

Recommendation 2: Increase engagement with fuel additive manufacturers and other relevant stakeholders.

BETO will continue working with VTO and the Co-Optima leadership team to prioritize stakeholder engagement, including with fuel additive manufacturers and OEMs.

Recommendation 3: Create a Co-Optima landing page with all models and data accessible for the public.

BETO agrees with the recommendation and is actively working to make models and data accessible to the public. A revised website was launched in August 2019 that features a searchable and sortable publications database that includes over 150 technical reports, journal articles, conference papers, and presentations produced under the Co-Optima initiative. Additional web content is being developed to highlight models, tools, and data as well as consortium capabilities.

COMBUSTION OF PETROLEUM-BASED TRANSPORTATION FUELS AND THEIR BLENDS WITH BIOFUELS: A NEW APPROACH FOR DEVELOPING SURROGATES AND UNDERSTANDING THE EFFECTS OF BLENDING

Cornell University

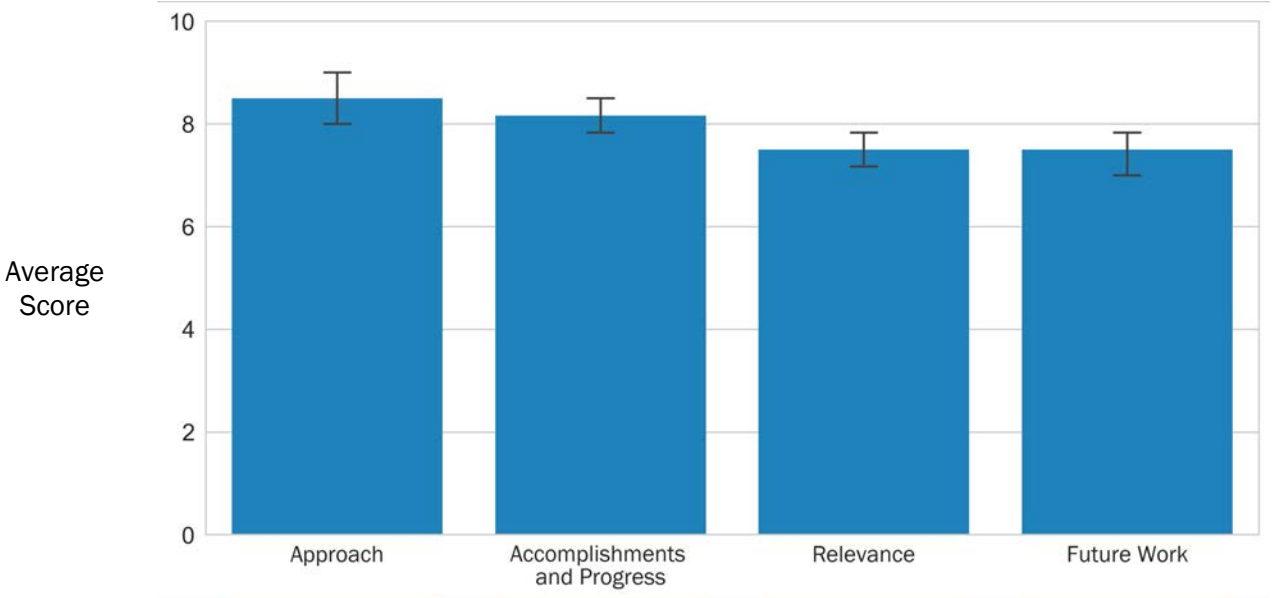
PROJECT DESCRIPTION

WBS:	3.5.1.12
CID:	EE0007978
Principal Investigator:	Dr. C. Thomas Avedisian
Period of Performance:	1/15/2017–9/30/2020
Total DOE Funding:	$1,131,791
Project Status:	Ongoing

The objective of this project is to develop surrogates for petroleum-based transportation fuels and their mixtures with bioblendstocks that are relevant to the Co-Optima initiative, and to determine the combustion kinetic mechanisms of the surrogates to enable numerical tools to predict performance of combustion engines. The project is aligned with MYP barrier ADO-E (Co-Development of Fuels and Engines) by its focus on a generalized simulation capability that can accommodate co-development of fuels and engines. The project is developed in two parts. The first examines a model biofuel binary blend comprised of heptane and isobutanol. The second part will examine more complex gasoline biofuel blends with the biofuels selected for their relevance to Co-Optima. A binary is the lowest order multicomponent system for a surrogate and is useful to assess the ability to predict mixture effects without complications of developing a surrogate or a kinetic mechanism for the mixture. These latter aspects will be addressed in the second period. The focus is on experiments and simulations with ostensibly known inputs in the first period. The burning configuration is that of an isolated droplet burning with spherical symmetry. This canonical liquid fuel burning configuration is among the very

Weighted Project Score: 7.9

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



I One standard deviation of reviewers' scores

few multiphase configurations that are amenable to detailed numerical modeling, yet also with a strong link to spray flames, which set the initial conditions in combustion engines. It is an attractive burning configuration that is devoid of many complexities of a spray flame, yet which nonetheless captures the inherent unsteadiness of liquid, gas and radiative transport, complex combustion chemistry, and moving boundary effects inherent to a spray flame. Heptane is a component of a primary reference fuel for gasoline and its kinetic mechanism is also sometimes used as a surrogate for diesel fuel; iso-butanol is a biofuel with a comparatively high merit function score from Co-Optima. The combustion kinetic mechanism of the binary is known and the ability to simulate burning is evaluated. In the first period of the project, the OpenSMOKE++ computational code was used with a kinetic mechanism consisting of 225 species and 7,645 reactions that also included unsteady gas and liquid transport, variable properties, and radiative transport. The heptane isobutanol mixture provides a simplified platform to assess the ability to predict mixture burning properties and to simulate combustion without the need to develop a surrogate. In the second period, surrogates for gasoline biofuel will be studied. The tasks will require formulating surrogates and new kinetic mechanisms. Selected burning properties of the petroleum fuel biofuel blends will be incorporated into the process of formulating a surrogate and validating its combustion kinetic mechanism. The presentation at the BETO 2019 Project Peer Review meeting summarizes results obtained to date for the first period. It includes experimental measurements of combustion properties and simulations for the model system.

OVERALL IMPRESSIONS

- This project will assist BETO and other government agencies and policy makers in addressing the challenges faced by lack of sufficient understanding of the burning characteristics of new biofuels in blends.

- The analysis of spray geometry is critical to modeling flame combustion characteristics, yet a dearth of information exists in literature. This project deals with this gap by providing single-drop flame characteristics that can be used in common engine modeling tools like CONVERGE CFD. The project team should continue to build out the experiments and show a clear connection to advanced engine design assumptions.

- The team is developing combustion kinetic mechanisms for biofuels. In order to do this, they have already developed a few mechanisms. The team is using a 1-D droplet burning configuration to get an understanding of how biofuels burn and prepare mechanisms accordingly. The appropriate combination of experiments and simulations has been presented in future work. Some risk factors have been considered. All the conventional combustion models are based on a pre-vaporized approach, whereas in this case the actual liquid droplet model is being developed. Development of biofuels combustion mechanisms is important to increase biofuels uptake, which aligns with BETO objectives.

- This project has effectively developed a method to test characteristics of fuel blendstocks and multi-component blends using a single droplet analysis, which will provide useful data for predictive modeling of fuels and blendstocks being tested at the bench scale. It would be helpful to outline how the outcomes of current work and the results of future work would be disseminated throughout the Co-optima team and integrated into the overall project execution.

- The objective of this project is to develop surrogates for petroleum-based transportation fuels and their mixtures with bioblendstocks that are relevant to Co-Optima, and to determine the combustion kinetic mechanisms of the surrogates to enable numerical tools to predict performance of combustion engines.

- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- A range of combustion configurations are used by a national laboratory and some co-Optima team members to provide data for validating kinetic mechanisms of biofuels and their blends with

transportation fuels. These include shock tubes, rapid compression machines, and jet-stirred reactors to name a few. They share a common element that the liquid phase is eliminated by pre-vaporization and the gas transport process is zero or one-dimensional. Ab-initio models then become viable for simulating the experimental data in a process for validating combustion kinetic mechanisms and associated property databases. However, sprays set the initial conditions for combustion in engines but cannot yet be modeled with this level of detail. Droplets represent the sub-grid element of sprays and are amenable to such detailed modeling. In particular, the 1-D droplet flame is an alternative configuration which the work of this project is designed to show and has value for validating kinetic mechanisms required for engine simulations. The kinetic mechanisms and property databases that result from using 1-D droplet flame data can supplement the configurations noted above by folding into the validation process properties with a direct link to liquid fuels and spray flames. A more stringent test of mechanism validation is then possible by eliminating the liquid phase from consideration.

RAPID CONSTRUCTION OF VALIDATED CHEMISTRY MODELS FOR ADVANCED BIOFUELS

Massachusetts Institute of Technology

PROJECT DESCRIPTION

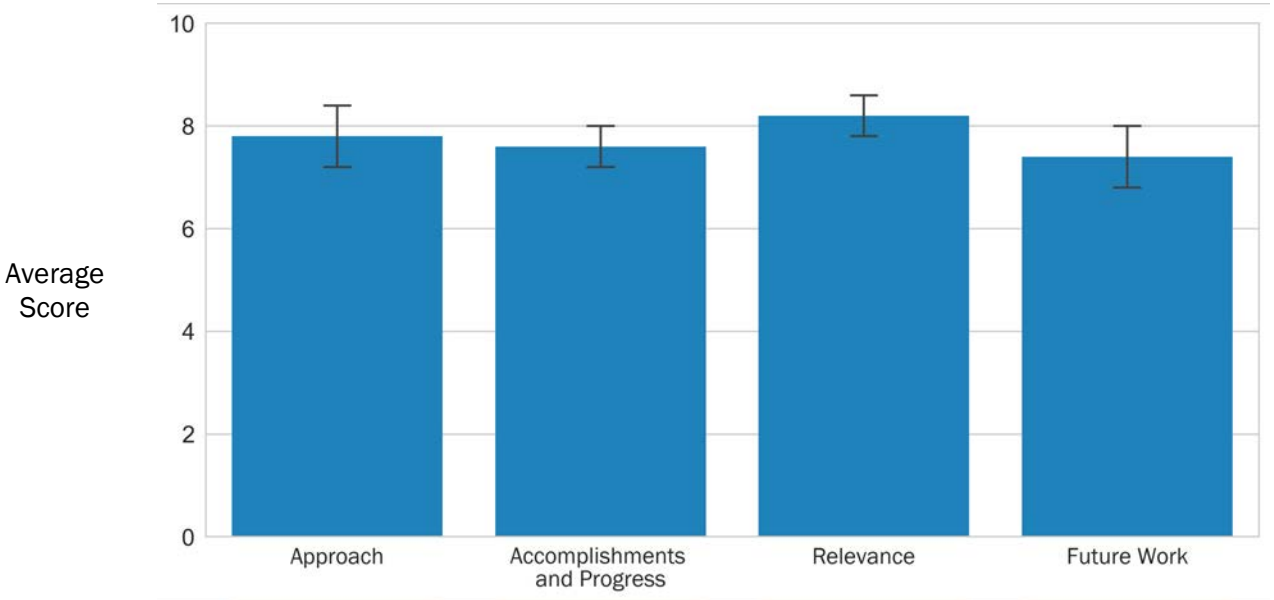
WBS:	3.5.1.13
CID:	EE0007982
Principal Investigator:	Dr. William Green
Period of Performance:	1/15/2017–3/30/2020
Total DOE Funding:	$893,427
Project Status:	Ongoing

One of the main concepts underlying the Co-Optima initiative is that co-optimization of new fuels with new engines can be greatly accelerated using computer power. In order to do this, one needs accurate computer models for the engine chemistry of each fuel of interest, so one can predict how they will perform under various engine conditions. The main objective of this project is to demonstrate the capability to rapidly generate accurate combustion chemistry models for advanced biofuels, using automated mechanism generation approaches and rate parameters derived from quantum mechanical calculations. We validate the new fuel chemistry models by measuring time-histories of combustion intermediates and ignition-delay times in a shock tube, using laser and spectroscopic probes, as well as by comparisons with experimental data measured by others in the Co-Optima team and any other data available. As part of this project, new experimental probes for reaction intermediates and improved biofuel modeling methods are being developed, documented, and disseminated. Some key technical lines of research of this project include:

- Improving the ability to rapidly identify important reaction pathways and intermediates and include them in the computer model, without including unimportant species and reactions that slow engine simulations without improving the accuracy of performance predictions.

Weighted Project Score: 7.7

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



I One standard deviation of reviewers' scores

- Development of suitable laser spectroscopic probe protocols for accurately measuring the time-profiles of low levels of combustion intermediates formed in shock tube experiments. Different approaches are needed at high pressure due to pressure-broadening leading to overlaps and interferences in the spectroscopy.

- Development of methods for accurately accounting for intramolecular hydrogen bond effects on the reaction kinetics of biofuels and biofuel oxidation products. Existing methods for computing rates were developed for simpler molecules which did not have any internal hydrogen bonds.

- Development of combined theoretical and experimental methods for modeling the ignition behavior of fuels which are complex mixtures.

The newly improved and validated capability to rapidly construct accurate computer models for many fuels is being used to develop accurate models for several of the Co-Optima initiative target biofuels. The fuel chemistry models constructed by this project are shared with other members of the Co-Optima program, in particular with those team-members doing engine simulations, making it possible for them to accurately predict fuel effects on engine performance.

Detailed chemical kinetic models will be constructed for several biofuels using an advanced computational approach. The models will be based on mechanism generation algorithms, computation of reaction rates through quantum chemistry, and experimental measurements. The models' predictive ability will be determined by comparisons to additional data.

At the time of this review, about 1.5 years into this ongoing project, we have constructed an apparatus and developed laser techniques to accurately measure the time profiles of the disappearing fuel and the rising reaction intermediates like formaldehyde (HCHO), ethylene (C2H4), and carbon monoxide (CO) even before the fuel ignites. We have also calculated the rates and thermochemistry of many key radicals using high level quantum chemistry. We have also developed new and improved methods for estimating rate coefficients and thermochemistry during automated mechanism construction. We have applied these calculations and methods to construct detailed models for the Co-Optima biofuels cyclopentanone and methyl propyl ether and compared the model predictions with our own experimental measurements and additional data measured by our collaborators.

OVERALL IMPRESSIONS

- The ability to rapidly construct models predicting characteristics and performance of novel biofuel blend stocks will provide a framework for predictive performance modeling for multiple characteristics that have not been measured experimentally. This project undertakes the model adjustment for characteristics found in biofuel blendstock candidates, such as hydrogen-bonding and complex reactions. If successful, this methodology will save time and resources during the exploration of new chemicals of any kind and should enable more rapid testing of novel fuel blendstocks. A suggested future milestone would be to engage standard-setting bodies (e.g., ASTM) to identify concerns and/or enable use of models to enable new fuel qualification for use. This would be valuable to ensure that novel fuels can be easily adopted.

- The premise of the work seems reasonable to help accelerate the development of accurate kinetic mechanistic combustion schemes with simple, clear objectives like, "pre-ignition species time-profiles are most useful." The work uses a machine learning methodology to help generate kinetic pathways followed by quantum verification in an iterative convergence technique. This really helps simplify and focus the work. The project team provided clear and compelling data describing the way the formaldehyde sensors work. The future engine implications for the experimental early carbon monoxide extinction curves should be stated. The machine learning approach should demonstrate that there are only a number of allowable paths for nature to choose and a systematic way to discriminate between them should be established. The project team should consider Consortium for Computational Chemistry

and Physics resources and other VTO collaborations when exploring the hydrogen bonding issues and effects on the kinetic calculations, as well as, other molecular interactions captured in aggregate constants like activity coefficients to increase the level of rigor. The project team should try to provide a better understanding of flow reactor data as related to internal combustion, real engine dyno-tuning activities and benchmarking with real test blends and primary reference fuels from an OEM perspective. Project lead has a very collaborative approach and ambitious technical approach of modeling first and comparing to experimental data. Several training dataset algorithms should be explored to help tune the models and measure the statistical approach to overfitting, as well as, adjust the hierarchical molecular clusters established for the kinetic pathways.

- The team is doing a good job of coming up with faster mechanisms for biofuel combustion calculations. The project would help make combustion calculations faster for biofuel combustion. Development of biofuels combustion mechanisms is important to increase biofuels uptake, which aligns with BETO objectives.

- The overall objective of the project is commendable; to demonstrate the capability to rapidly generate accurate combustion chemistry models for advanced biofuels and using automated mechanism generation approaches and rate parameters derived from quantum mechanical calculations.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The recipient chose not to respond to the reviewers' overall impressions of their project.

MULTITUDE CHARACTERIZATION AND PREDICTION OF DOE ADVANCED BIOFUELS PROPERTIES

The University of Central Florida Board of Trustees

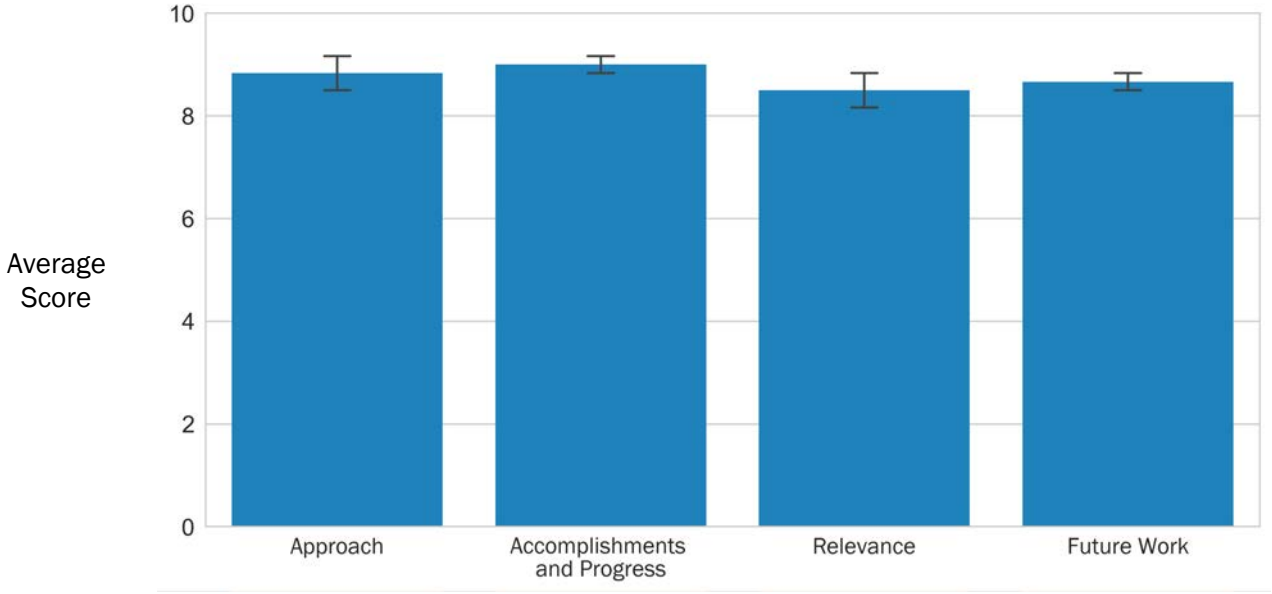
PROJECT DESCRIPTION

The goal of this project is to provide a detailed data set of multiple combustion experiments relevant to the engine combustion of Co-Optima fuels. The data and information for the fuel behavior will mitigate the potential for combustion operability issues due to the particular fuel being used. The research project accelerates the introduction of affordable, scalable, and sustainable high performance bio-based fuels for use in high-efficiency, low emission engines thereby achieving the Co-Optima and BETO outcomes.

WBS:	3.5.1.14
CID:	EE0007984
Principal Investigator:	Dr. Kareem Ahmed
Period of Performance:	1/15/2017–8/31/2020
Total DOE Funding:	$894,336
Project Status:	Ongoing

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

OVERALL IMPRESSIONS

- This project is an important part of the Co-Optima suite of projects by providing the experimental combustion data and correlation of structural correlation to properties for the Co-Optima blendstock candidates. This project is complementary to the other projects looking at fuel characteristics modeling and prediction. Some of the qualitative characteristics of the fuels (e.g., causticity) are important and should be documented as well.

- This project like several of the others in Co-Optima seeks further understanding through quantitative measurements and development of tools that can used to determine properties of new bio-blends.
- The project lead gave an excellent background on why the experiments are necessary and the approach ties back to OEM engine tuning. Further, this project has important implications on advanced engine design decision thresholds. Essentially this work is trying to solve the classic chicken and egg problem in engine-fuel design optimization by triggering the hardware modification as a result of the degree of approach toward parametric uncertainty thresholds caused by new fuel candidate testing. This is essentially the objective, uncertainty quantification which should involve statistical control charting techniques which is the classic method for measuring uncertainty (laminar flame speed, soot volume fraction-shock tubes, detail kinetics from synchrotron, coking volume fraction). This work will be important for hardware design implications with MM, MCCI and kinetically controlled combustion modes.
- The team is involved in providing a large amount of combustion and fuel systems related experimental data to the Co-Optima members. All the tests which are being done by the team are important for ensuring the compatibility and performance of different fuel blends. Clear plans of future work have been presented with appropriate milestones and these look feasible. Good integration with the national labs. The team has presented that they will test compounds of heavy fuels in the next 18 months.
- The goal of this project is to provide a detailed data set of multiple combustion experiments relevant to engine combustion of Co-Optima fuels. The product that will result from this project is data and information for the fuel behavior that mitigate the sensitivity of the alternative fuels.
- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The recipient chose not to respond to the reviewers' overall impressions of their project.

MISR: MINIATURE IGNITION SCREENING RAPID COMPRESSION MACHINE FOR KINETIC MEASUREMENTS OF NOVEL FUELS

University of Illinois at Chicago

PROJECT DESCRIPTION

This project is a combined experimental and modeling effort with goals of (1) the development of a small-volume high-throughput ignition delay apparatus, (2) the use of that apparatus to measure characteristics of candidate fuels and blends in the Co-Optima program, (3) and the development of mechanistic-based modeling tools to describe and predict ignition characteristics, especially in advanced compression ignition (ACI) engines.

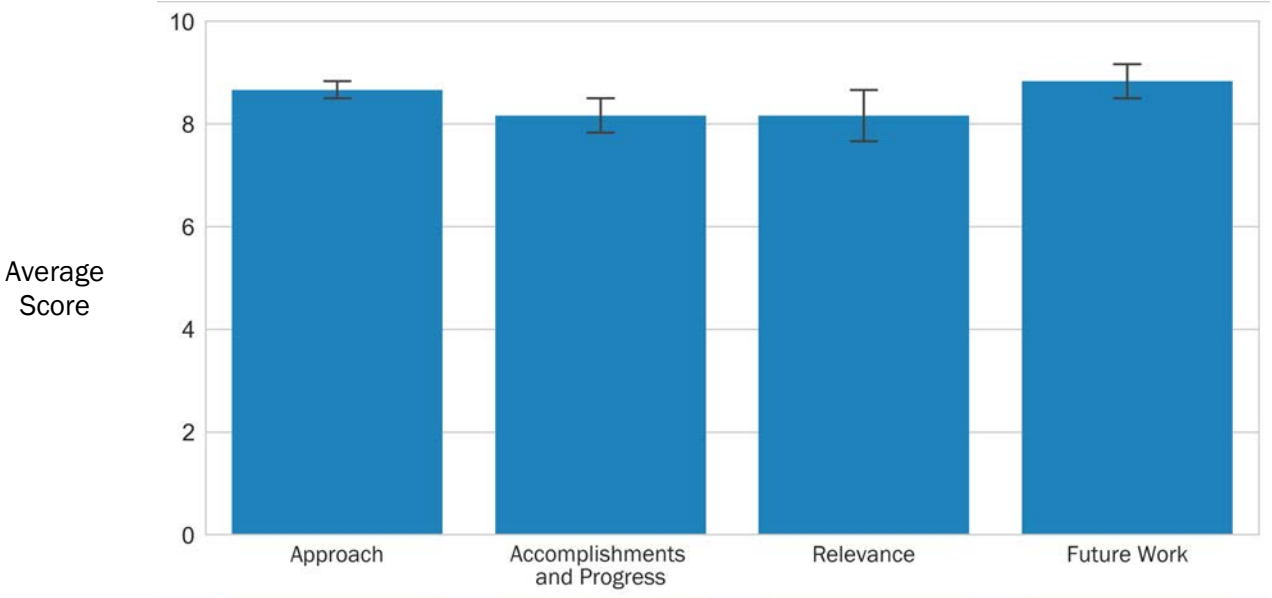
WBS:	3.5.1.15
CID:	EE0007985
Principal Investigator:	Dr. Patrick Lynch
Period of Performance:	1/15/2017–5/14/2020
Total DOE Funding:	$518,828
Project Status:	Ongoing

In this project, we are building and will use a novel miniature rapid compression machine suitable for high-throughput screening of ignition delay times: the MISR. This device will be used for characterizing properties from very small volumes of low-volatility fuels, less than 20μL per experiment. The MISR will operate with high repetition rate (~1 Hz), high repeatability, and can quickly map out a wide range of temperature and pressure conditions.

The modeling effort and analysis tools under development provide kinetic insights from extracting the temperature, pressure, and concentration specific constant-condition ignition delay times (i.e., a chemically based multiparameter map) from the MISR data using an inverse-staged Livengood-Wu integral technique. That complex ignition delay map can be convolved with the state history in other devices, like boosted SI

Weighted Project Score: 8.5

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



I One standard deviation of reviewers' scores

engines and particularly ACI engines to predict ignition characteristics and ultimately search for attractive configurations.

OVERALL IMPRESSIONS

- The MISR device for rapid throughput, lower cost blendstock analysis is intended to reduce the volume of material needed for analyses and increase throughput by orders of magnitude. If successful, this device will likely become a highly-desirable approach to analyzing small volumes of material for experimental testing and validation of modeling. It would be helpful to share a clear plan for making this device and/or testing capability available for the rest of the Co-Optima team.

- Once built, operated, and validated, MISR can provide a research tool to test labs on ignition properties of new bioblendstocks and components that is cost-effective and rapid.

- The premise of this work and the goals are exciting and lofty, but extremely important to revolutionizing the combustion characterization and flame diagnostics community, if successful. Here, a high-throughput screening (HTS) approach to running combustion experiments on the order 10^3/day as compared to shock-tube data, which is of the lower order, is at stake. The issue then becomes data management and visualization to guide R&D and kinetic elucidation. If the parameters emerging from these experiments have a 1:1 design impact on MM, MCCI and kinetically control combustion modes, then this could be the path to accelerate the industry. The project has an enormous potential and promise. The project team has to do early benchmark and calibration work to show that this method can predict current and well known measurement methods for performance and prove that it is suitable for ACI. The team has a special expertise and unique hardware design for correlating with advanced engine evaluation rigs. This has long-term potential to enhance or even replace Cooperative Fuel Research (CFR) rigs which continues to be the dream for many stakeholders in the petroleum and automotive industry. The responsibility assignment matrix was clear in the project, and there has been good initial progress in building the operating regime maps. The team has been quite active in the literature, and there appears to be an automation opportunity to process the Livengood-Wu differentials into the activated ignition delay maps. The first step is to successfully build the MISR rig, and this will take time.

- The team is going to develop a new test rig for testing the ignition characteristics of Co-Optima fuels. The approach which is being adopted is new and will use a very small quantity of fuels to complete the testing. The number of tests done within a small duration of time would also increase. This project will indirectly aid in achieving BETO objectives and technology area goals.

- This project is a combined experimental and modeling effort with goals of (1) the development of a small-volume high-throughput ignition delay apparatus, (2) the use of that apparatus to measure characteristics of candidate fuels and blends in the Co-Optima program, and (3) the development of mechanistic-based modeling tools to describe and predict ignition characteristics, especially in ACI engines.

- Current methods for testing the ignition performance of fuel blends are slow, costly, and require large quantities of fuel. The goal of this project is to design, develop, and produce a high throughput ignition screening device capable of quickly assessing the properties of small quantities of fuels and blends.

- Barriers addressed: Co-Development of Fuels and Engines (ADO-E).

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The project is integrated with the fuel properties team and the kinetics small group. We intend to receive direction for various fuels and blends through this group. This structure has worked well for coordinating testing of fuels and blends in the past.

- We agree. MISR targets are at longer ignition delays under low-to-intermediate temperature conditions.
- We agree with all these points. We agree in particular that this will be one of the first truly large data apparatuses for kinetic studies and effort needs to be spent on data management. The team has already developed analysis approaches to interpret and correlate the acquired data with those from conventional large-size apparatus, as well as kinetic modeling methods to further demonstrate the data as useful and novel targets to compare and validate kinetics. With the large amount of ignition delay data, the team has demonstrated a general approach to qualitatively analyze the effect of operating condition and fuel property on auto-ignition in both SI knock and ACI conditions.

CO-OPTIMA OVERVIEW

Co-Optimization of Fuels & Engines Consortium

PROJECT DESCRIPTION

The Co-Optima initiative is developing new high-performance fuels that can boost engine efficiency and cut emissions when combined with advanced combustion approaches. Internal combustion engines using liquid fuels will comprise a significant portion of the nation's vehicle fleet for the next several decades. Advanced combustion approaches have been identified that are capable of significantly improved efficiency and emissions, but new fuels are required to maximize benefits. There is an opportunity to exploit fuel properties and composition to enhance engine efficiency, particularly from biomass-derived fuels that offer unique properties in addition to lower carbon-intensity.

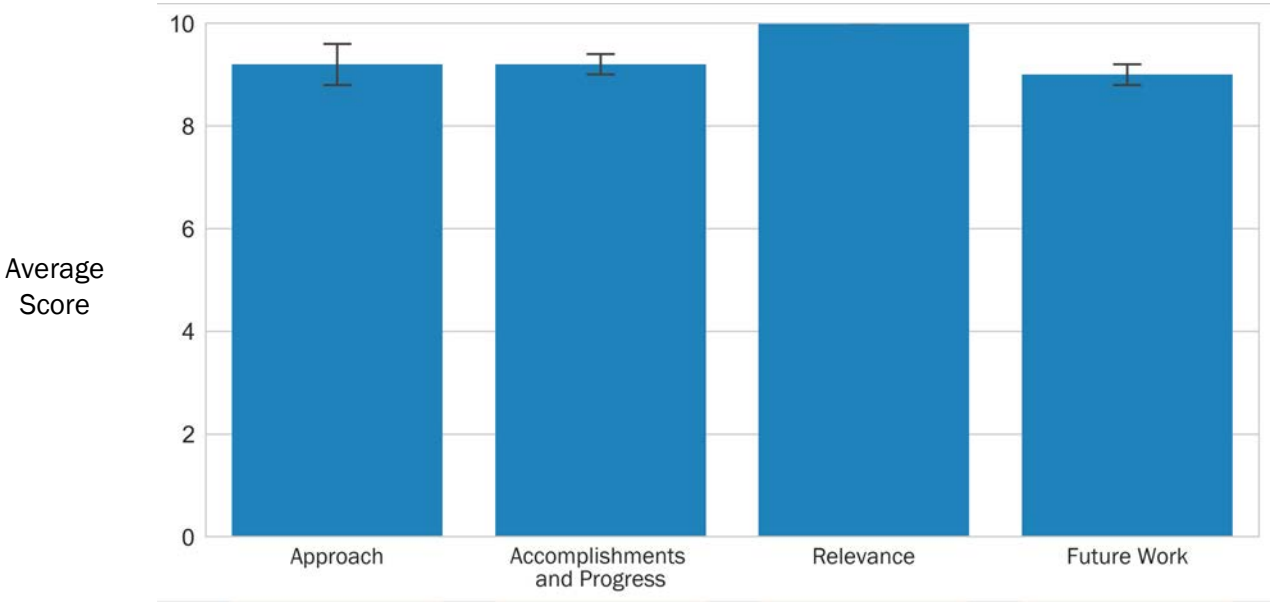
WBS:	3.5.1.4a
CID:	NL0029892a
Principal Investigator:	Dr. Daniel Gaspar
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	N/A
DOE Funding FY16:	N/A
DOE Funding FY17:	N/A
DOE Funding FY18:	N/A
DOE Funding FY19:	N/A
Project Status:	Ongoing

The Co-Optima team is composed of technical experts in analysis, biofuels, and engines from nine national laboratories and thirteen universities and funded by two DOE program offices. The team is supported by input and guidance from stakeholders and advisory boards.

Co-Optima is achieving its technical goals by (1) identifying fuel properties and engine operating parameters that enhance engine efficiency and reduce emissions for both light-duty and medium- and heavy-duty engines, (2) identifying high-performance blendstocks that are preferentially sourced from biomass, and (3) evaluating the potential economic and environmental impacts of the adoption of new engines and fuels.

Weighted Project Score: 9.3

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



Co-Optima is organized into technical teams possessing specific technical capabilities, with focused, integrated multi-team efforts centered on specific combustion approaches and enabling fuels for light-duty (BSI and multimode approaches combining compression ignition and SI) or medium- and heavy-duty (MCCI and kinetically controlled combustion) applications.

During the first three-year annual operating plan cycle, Co-Optima completed research on BSI fuel-engine technologies. Key outcomes include (1) quantification of fuel property impacts on efficiency, (2) identification of biomass-derived blendstocks imparting these fuel properties, and evaluation of impacts, including techno-economic, life cycle, refinery integration and benefits analyses. Research octane number, octane sensitivity, and heat of vaporization were determined to be the most important properties for engine efficiency. A series of low molecular weight alcohols, iso-olefins, furans, and cyclopentanone were found to have the highest engine-efficiency potential. An analysis of the benefits of adopting engines designed for fuels exhibiting these properties identified significant cost savings through higher efficiency and emissions reductions meeting or exceeding the advanced biofuel standard of 60%.

Co-Optima researchers will finish efforts in MCCI fuels and engines (diesel engines are the commercial example of this general class of engine) at the end of FY 2019. These MCCI efforts have identified key fuel properties including sooting tendency, cetane number, cold flow properties, and energy density. Research is ongoing to better understand how bioblendstock chemistry and properties can be leveraged for emissions reductions benefits in traditional and new MCCI approaches.

MM research builds upon the BSI approach and results and will conclude at the end of FY 2020. Several fuel properties, including octane sensitivity, flame speed, and phi sensitivity have been identified as important and blendstock measurements and evaluations are underway. Finally, nascent efforts in kinetically controlled combustion are underway to determine if reactivity control can be achieved by combining combustion approaches with bioblendstock fuel properties to meet operating and efficiency objectives.

Together, these efforts comprise the Co-Optima team's progress toward enhancing and understanding the value that can be provided by biomass-derived fuels.

Photo courtesy of Co-Optimization of Fuels & Engines Consortium

OVERALL IMPRESSIONS

- The Co-Optima project uses an innovative approach to generating new opportunities for biofuel/engine advancement. The component elements are comprehensive and well-coordinated, and the tools and models being developed through the program will be valuable throughout the team but also for other researchers and stakeholders. The various tools and resources being developed are not assembled in one location as of yet. The review panel suggested that it would be valuable to create a Co-Optima landing page on the Bioenergy KDF website (http://www.bioenergykdf.net) that brings people to the Co-Optima website and also provides links to all the various tools, resources, and datasets that are being developed.

- Given the promising bioblendstocks identified thus far, it seems likely the team will meet the target of identifying three bioblendstocks that exhibit specific target fuel characteristics, but it may be more challenging to achieve cost parity and greenhouse gas emission (GHG) reduction targets. The team has indicated identification of fuels meeting all these criteria as a go-no-go milestone. However, a "no-go" result, in which the team is not able to identify three molecules that meet these targets, should not lead to abandonment of promising blendstocks or the program necessarily if the fuels provide most of the desired characteristics. The team should have a strategy in place to identify how those remaining characteristics could be met e.g., if only the GHG criterion is not met, how would the team go about identifying better pathways to reduce GHG emissions, or if cost were the remaining barrier, how could/would the team (or other teams in the BETO portfolio) refocus on cost drivers and reduction?

- The project does not want to be a future fuel recommendation tool, but rather a database for physical, chemical, and performance properties. This posture should continue allowing for objective research and analysis to occur while staying mindful/thoughtful of any negative implications on BETO milestones and targets. The program has a strong budget which shows a serious commitment from all funding sources. The portfolio manager on staff to deal with the Work Breakdown Structure (WBS) elements and act as a budgetary oversight along with structured weekly meetings is good. It seems like there is an opportunity in this program to take advantage of predictive software algorithms. Oak Ridge National Laboratory should have some insight on opportunities in this area. The program should continue to engage cross-industry organizations such as, CRC Industries, Southwest Research Institute, SAE International, any other engine OEMs, ASTM International, the U.S. Environmental Protection Agency, and additive companies that operate dedicated fleets. VTO may want to consider purchasing an inexpensive fleet of hybrid-electric vehicles for this work. A renewable lubricant product maybe from LanzaTech should be used in such a project with the same fleet. Multivariate modeling algorithms could take engine performance and correlate it back to molecular structure to design fuel-appropriate fuel molecules. Make sure to include baseline data showing what the merit function is for conventional fuels. Blending fuel properties are equally as important as pure component properties. Establishing a blending matrix visualization will be a good way to communicate the available blendstocks in future engine applications.

- The project provides an overall view of the Co-Optima initiative. The team is strong and has the right skills to deliver on the project. It is good to see that the team has selected 10 fuel blendstocks to proceed, which is an important step. Strong management structures are in place to make sure the project progresses well and delivers what it is intended to deliver. Technical progress to date has been provided with a clear future plan.

- This project is highly relevant and focuses on needed fuels (bio-based) to optimize advanced engines. As such, there are multidisciplinary efforts and resources required, which call for a great deal of management oversight.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their insights and suggestions and are gratified that the reviewers found Co-Optima to be “fully aligned with BETO objectives and technology area goals,” and have “outstanding

technical accomplishments," with "a clear plan." The reviewers' assessment that Co-Optima has a strong team with the right skills and a sound management plan and structure, including our advisory boards, gives us confidence in the Co-Optima management approach.

- The reviewers' view that timelines are aggressive is consistent with our intent to provide foundational understanding that can lead to positive market and environmental impacts. Finally, we appreciate and will consider the suggestions to improve dissemination of results, models, and tools; evaluate more blendstocks composed of mixtures; consider biofuel/hybrid electric vehicle engines; and evaluate compatibility, toxicity, and environmental concerns sooner in our process.

CO-OPTIMA BIOBLENDSTOCK STRUCTURE PROPERTY AND PREDICTIONS

Co-Optimization of Fuels & Engines Consortium

PROJECT DESCRIPTION

The structure-property relationship and property prediction work in the Co-Optima program determines which bioblendstocks will be evaluated by the broader Co-Optima effort. We do so by establishing principles that relate the chemical structure of bioblendstocks to the physical properties and combustion behavior most important in internal combustion engines. We create these structure-property relationships by: 1) evaluating chemical families and a range of structural variants using published data and available predictive tools and 2) determining the underlying relationships that confer certain properties to given structures.

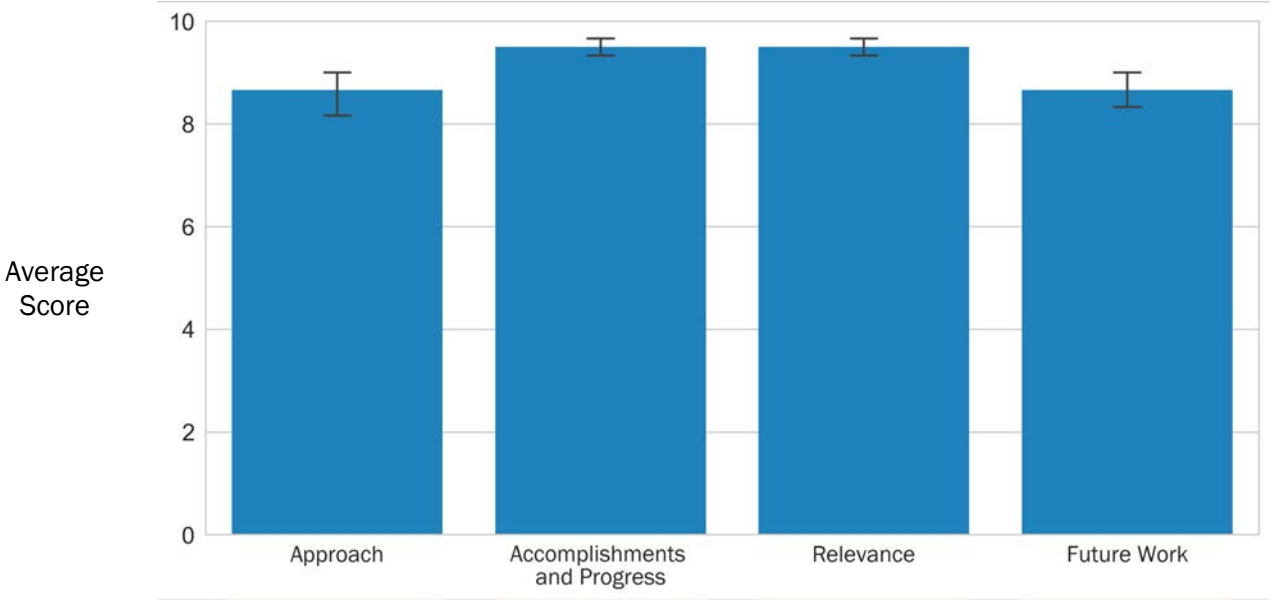
WBS:	3.5.1.4b
CID:	NL0029892b
Principal Investigator:	Dr. Anthe George
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$16,473,000
DOE Funding FY16:	$4,993,000
DOE Funding FY17:	$4,290,000
DOE Funding FY18:	$3,515,000
DOE Funding FY19:	$3,675,000
Project Status:	Ongoing

We can thereby broadly evaluate if a chemical family is suitable or unsuitable for a given combustion mode. Specific structural variants within suitable chemical families are evaluated in greater detail for important physical properties, and combustion behavior such as research octane number, cetane number, and sooting propensity. This is done by developing and building predictive tools, and by using theoretical chemistry techniques, mathematical models, and machine learning.

Key outcomes have included:

Weighted Project Score: 9.1

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



I One standard deviation of reviewers' scores

- Establishing important chemical families and identifying bioblendstocks for light-duty BSI and heavy-duty MCCI engines
- Transferring data and information to the Co-Optima Bioblendstock Generation, Characterization, and Analysis efforts
- Using the scientific understanding around biofuel properties developed in this activity to inform stakeholders beyond Co-Optima, including other core BETO programs
- Developing tools, methodologies, and understanding of how structure affects properties that can be applied beyond biofuels, to wherever understanding of a compound's performance is required.

We will continue to expand our focus on multimode combustion approaches and kinetically-controlled combustion by applying the workflow developed. Key properties for these approaches are octane sensitivity, phi-sensitivity, and flame speed. More research is being conducted to identify additional key properties for these advanced combustion approaches. This work, conducted to establish structure-property relationships and predict properties of bioblendstocks, underpins fuel-candidate identification and evaluation in Co-Optima.

OVERALL IMPRESSIONS

- As a whole, the Co-Optima projects seem to be well thought out and planned. The outcome of their combined effort will provide the necessary analytical tools to policy developers as new biofuels are adopted in the liquid fuel sector and engine designers.
- This component of the Co-Optima project is crucial to the successful development of novel biofuel options in that it provides the predictive modeling and validation of blendstock characteristics, isolates the effects of specific functional groups on fuel properties, provides a method for high-throughput screening level analyses of blendstock candidates, and identifies unexpected structure-property relationships. The data and models from this project will be extremely useful within the Co-Optima team but also for industry and other researchers. The team could consider engagement at ASTM to enable use of these predictive models to facilitate new fuel qualification under the ASTM Committee D.02.
- This underlying premise for this project is notable. It enables both bio and petroleum refiners the opportunity to explore molecular management at a new level. A nuclear magnetic resonance approach to deal with complex mixtures in a high-throughput, small-volume environment was established. This work deals with correlating the properties with the engine performance at the first principles level using a variety of multivariate modeling and machine learning algorithms for HTS. The approach is quite sound and considers the critical parameters responsible for engine efficiency. It appears that there may be an opportunity to develop a compositional-based specification that provides a window of acceptable physical and performance characteristics. Significant progress was accomplished, and validation work should continue along with benchmarking against traditional hydrocarbons currently being used in the refinery to establish precision and accuracy metrics. The opportunity for fuel design also emerges when properties can be correlated down to the quantum descriptors for optimized molecular structures (i.e., MM2 force field). Stochastic approaches can be coupled with it to devise a distribution of molecules that provide aggregate values for the performance parameters of interest. Basically, the fuel is being “built from scratch.” The project team has demonstrated the ability to predict synergistic non-linear behavior which is an extremely important capability. The team should continue to provide fundamental insights on such counter-intuitive fuel blending properties or behavior. Collaborations between the other projects that involve large databases is recommended as well (i.e., bio-information project, datahub project, RetSynth). AspenTech should be contacted to include the Statistically Associating Fluid Theory (SAFT) models after they are published highlighting the improvement in accuracy relative to classic activity coefficient theoretical approaches.

- Develop accurate chemical structure-fuel property relationships, and fuel property predictions from these, across a full set of chemical classes and structures. The structure-property relationship and property prediction work determines which bioblendstocks will be evaluated by the broader Co-Optima effort by establishing principles that relate the chemical structure of bioblendstocks to the physical properties and combustion behavior most important in internal combustion engines.
- Barriers addressed: Co-development of fuels & engines (ADO-E) and identifying new market opportunities for bioenergy and bioproduct (At-D).
- Property-structure relationships and selection of blends according to property required is an important approach of the whole Co-Optima initiative. Computational, experimental, chemical kinetics, and machine learning approaches are being used to deliver results. This would eventually help in speeding up the process of biofuels and engines for better efficiency. This is also assisting in taking steps forward for achieving BETO objectives and technology area goals.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- The recipient chose not to respond to the reviewers' overall impressions of their project.

CO-OPTIMA BIOBLENDSTOCK FUEL PROPERTY CHARACTERIZATION

Co-Optimization of Fuels & Engines Consortium

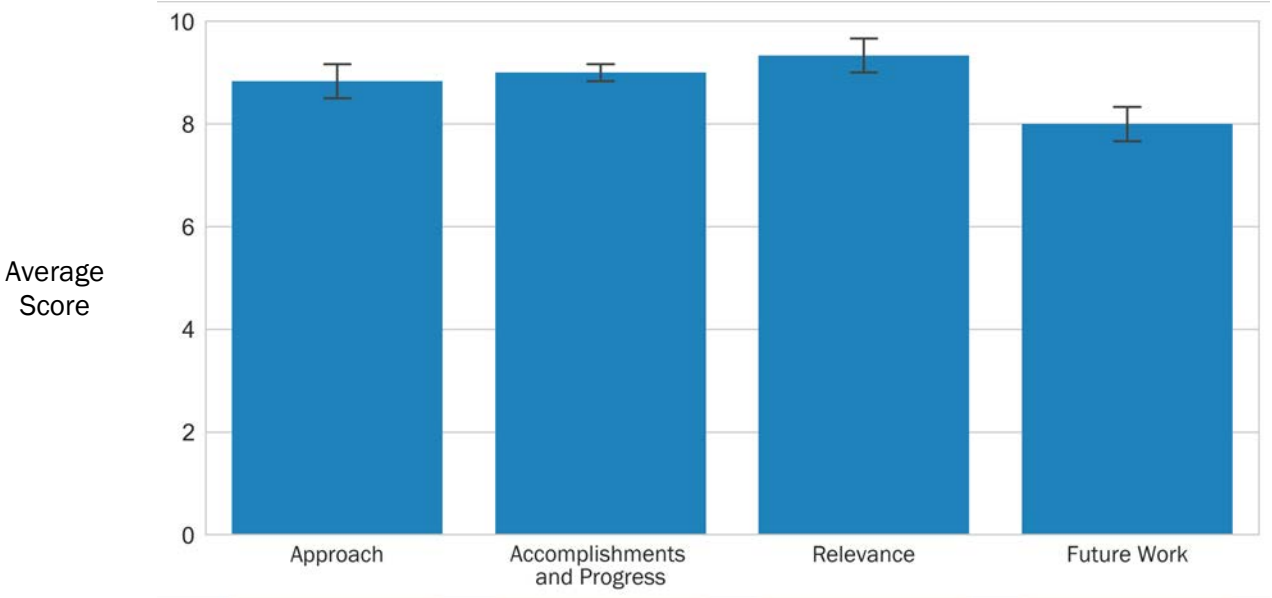
PROJECT DESCRIPTION

WBS:	3.5.1.4c
CID:	NL0029892c
Principal Investigator:	Dr. Robert McCormick
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$8,952,000
DOE Funding FY16:	$2,252,000
DOE Funding FY17:	$1,935,000
DOE Funding FY18:	$1,305,000
DOE Funding FY19:	$3,460,000
Project Status:	Ongoing

The Fuel Property Characterization (FPC) effort within the Co-Optima initiative focuses on the measurement of critical fuel properties. The goal of Co-Optima is to leverage unique fuel chemistries available from biomass to design more efficient engines, thereby reducing energy consumption and environmental impacts of transportation. FPC supports the on-going efforts of blendstock generation, structure-property relationships, and analysis, through multiple channels. FPC is responsible for the development, expansion, and, maintenance of the Fuel Properties Database (FPD), including acquisition of fuel property data. The FPD was heavily utilized during tiered-screening approaches to rapidly identify the most promising blendstocks for BSI and MCCI combustion. A key outcome of this endeavor is that it directly led to the identification and more in-depth evaluation of ten of the most promising blendstocks for BSI as well as the initial selection of 12 MCCI candidates for further consideration. Future efforts will also rely on the FPD as a screening tool as additional combustion approaches are investigated. FPC supports analysis efforts through the performance of compatibility and toxicology assessment of promising candidates. Through fundamental experimental measurements in a flow reactor, FPC provides critical feedback to the mechanistic understanding of soot precursor formation and the validation of kinetic mechanisms. These experiments combined with quantum mechanical calculations showed mechanistically why different functional group location could lead

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

to widely varying soot production—even for very similar molecules such as positional isomers. Additionally, experiments are beginning to reveal the chemical basis for non-linear blending effects for octane number which will allow the design of molecules with desired blending octane behavior in future endeavors. The outcomes of these efforts will help ensure that the Co-Optima program can identify fuel-engine combinations which achieve Co-Optima's efficiency, environmental, and economic goals.

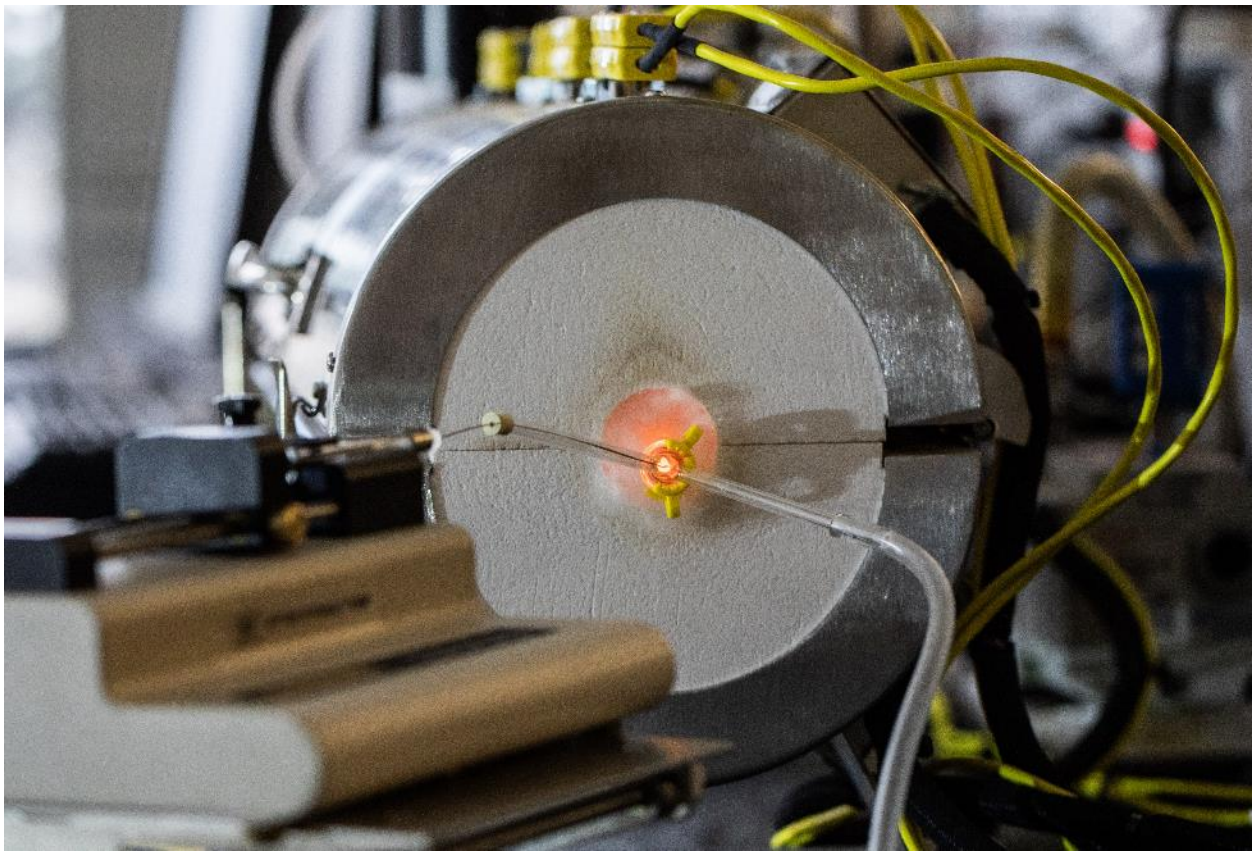


Photo courtesy of Co-Optimization of Fuels & Engines Consortium

OVERALL IMPRESSIONS

- This research will bring greater application of the existing and alternate biofuels that can be made and blended from the different fractions of biomass. This effort is greatly needed and can help inform the public, policy holders, governmental agencies, and departments as well as the auto and fuel industries.

- This project provides a tiered approach to the initial blendstock assessment, the results of which feed into most if not all of the other Co-Optima projects. The team has successfully narrowed a large field of candidates to a key set of highly likely candidates, incorporating not only chemical characteristics but also certain environmental performance criteria. Given the importance of biodegradability and low toxicity for these blendstocks, for which sustainability and improved environmental performance will be critical, it makes sense to evaluate these elements of the blendstocks as an early screening i.e., these should be part of the Tier 1 screening rather than waiting until Tier 3.

- The FPD has made really important progress. It includes over 800 compounds and mixtures. The team is working with next-level detection methods like vacuum ultraviolet spectroscopy. The concept of the

FPD will be essential for the success of Co-Optima and ChemCatBio. The project team should continue to coordinate efforts with the Bio-Information and Data Hub projects to leverage capabilities. Great progress has been made so far on publishing this database. There was a significant work effort here making blends and testing them. The team should continue to characterize real blends that include ethanol which is the foundational biofuel blendstock. The team should be applauded for looking at the toxicology and health, safety, and environment impacts early, as well as, fluoroelastomer responses. This is good progress. The ASTM outcome with D8076 is a very significant deliverable establishing the original working group and completing the statistics. The project team should make comments on future OEM partnerships and interactions as well as SAE collaboration with groups working on boosted direct injection spark ignition. The analytical scientific progress was evident with results from the flow reactor kinetic modeling showing the soot formation mechanisms in collaboration with the Consortium for Computational Chemistry and Physics team. The project team should consider both thermal oxidative and storage stability characterization opportunities.

- The FPC effort within the Co-Optima initiative focuses on the measurement of critical fuel properties. The goal of Co-Optima is to leverage unique fuel chemistries available from biomass to design more efficient engines, thereby reducing energy consumption and environmental impacts of transportation.

- The approach of providing one online location solution for all fuel properties is good. Interaction of different linear and non-linear properties while mixing is very important and has been covered. The database has been made easily accessible and easy to search. Providing fuel properties in an easy and accessible way is an important part of the Co-Optima initiative, as this helps in quick downselection of the final biofuels to be used. This would eventually help in speeding up the process of biofuels and engines for better efficiency.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We thank the reviewers for their insights, recommendations, and strong endorsement of our project approach that “is clearly defined” and “is crucial for team collaboration and future modeling.” We are grateful that the reviewers felt that “this work supports BETO’s mission to provide a fuel/engine pair,” and that “the relevance to the Co-Optima project is clearly defined.”

- Additionally, we appreciate and will consider the reviewers’ thoughtful suggestions for improvements to the project which include: potential upgrades to the flow reactor system to function under elevated pressures that are more relevant to real engine operating conditions, a more in-depth assessment of blendstock biodegradability and toxicology earlier in the evaluation process, and improvement of the distribution of information by a centralization of resources.

CO-OPTIMA BIOBLENDSTOCK GENERATION

Co-Optimization of Fuels & Engines Consortium

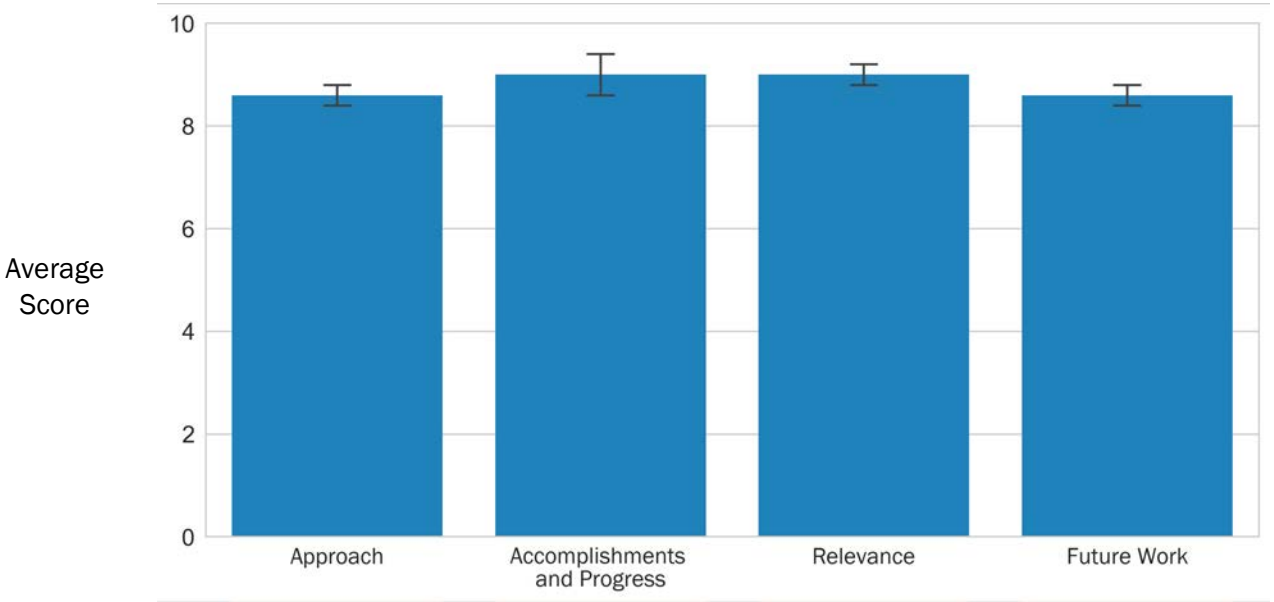
PROJECT DESCRIPTION

WBS:	3.5.1.4d
CID:	NL0029892d
Principal Investigator:	Dr. Derek Vardon
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$16,473,000
DOE Funding FY16:	$4,993,000
DOE Funding FY17:	$4,290,000
DOE Funding FY18:	$3,515,000
DOE Funding FY19:	$3,675,000
Project Status:	Ongoing

This project is part of the Co-Optima initiative that is working to identify blendstocks derived from biomass that can provide critical fuel properties and assess their benefits and barriers to adoption. The project provides a key function within Co-Optima by addressing gaps in fuel property and conversion knowledge for promising non-commercial bioblendstocks. This is done by (1) generating bioblendstock samples for fuel property characterization and (2) supplying preliminary conversion data for feasibility analysis. Project team members work with input provided by other Co-Optima researchers to determine which chemical families and molecular structures to target for advantaged fuel properties. We utilize in-house retrosynthetic analysis tools to help evaluate possible conversion pathways to investigate, and we produce bioblendstocks samples at increasing scales using a tiered approach that is informed by results from fuel property testing and pathway viability analysis. Efforts are coordinated with the BETO Conversion R&D program to ensure a focus on novel production pathways using the latest conversion tools and knowledge base. In concert with other Co-Optima teams, this project addresses the need to (1) provide a framework to derisk and evaluate novel bioblendstocks, (2) develop conversion pathway assessment tools, and (3) inform future conversion targets for the BETO core program. To date, this multi-year effort has generated novel and promising bioblendstocks that address both light-duty and heavy-duty vehicle applications. Key outcomes

Weighted Project Score: 8.8

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



include the (1) development of a scalable algorithm for the retrosynthetic analysis of potential conversion pathways, (2) evaluation of under-explored bioblendstocks with scaled production to validate their advantaged fuel properties, and (3) the development of new bioblendstock production routes for single and mixed compounds that can be tailored based on desirable fuel properties. Moving forward, our approach will be applied to emerging light-duty and heavy-duty combustion strategies that include multimode and kinetically controlled modes of combustion, respectively. Collectively, this project will help ensure the success of Co-Optima's mission for enhancing and understanding the value of blendstocks that can be obtained from biomass.

Photo courtesy of Co-Optimization of Fuels & Engines Consortium

OVERALL IMPRESSIONS

- This project is innovative and offers a unique opportunity to identify and generate novel bio-based blendstocks that meet chemical, economic, and sustainability criteria. There would also be value in executing predictive modeling on blendstock components from fuel producers who want to get them analyzed and perhaps ASTM qualified. I'm very glad to see that the data and retrosynthetic analysis (RSA) tool have been made publicly available on GitHub. It would be great to incorporate life cycle emissions, sustainability considerations, and economics into the selection process to prioritize the retrosynthetic pathways.

- Overall, the project is very comprehensive with a lot of moving activities, results, and deliverables which at a glance can appear disjointed. However, the mission to tie pathway discovery to advance engine fuel discovery under the same project is not an easy task, and team should be applauded for the breadth of space being pursued in this work. The project team has already shown proof that they can connect feedstock, process, and engine with physical samples. Now, additional resources and project organization efforts should be bolstered to balance out the discovery work with the process design engineering considerations. Significant progress has been accomplished in this project thus far and the amount of hard work given to this point is evident. This is a very large program especially when one has to generate their own blendstocks to study and send to collaborators.

- This research addresses gaps in fuel property and conversion knowledge for promising non-commercial bioblendstocks by (1) generating bioblendstock samples for fuel property characterization, and (2) supplying preliminary conversion data for feasibility analysis.

- The team has done good work towards bio blendstock generation. It is good to see that the team has done a detailed risk analysis of potential options. The team gets information on which bioblendstock is most desirable and can develop the method of producing it. This project directly aligns with BETO objectives and technology area goals.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- We appreciate that the reviewers found value in our approach to produce and evaluate novel bioblendstocks. Per the reviewers' suggestions, the project team will continue to assess novel bioblendstock candidates via retrosynthetic analysis and provide samples for fuel property testing and conversion data for production viability. In addition, future efforts will ensure the retrosynthetic analysis tools are publicly available and integrate sustainability and economic considerations. By working closely with the other Co-Optima teams, this effort will help address initial process design engineering considerations for promising bioblendstocks that are identified through the tiered screening process. The team thanks the reviewers for their support of this effort and constructive feedback for project next steps.

INTEGRATED ANALYSIS OF EFFICIENCY-ENHANCING BIOBLENDSTOCKS

Co-Optimization of Fuels & Engines Consortium

PROJECT DESCRIPTION

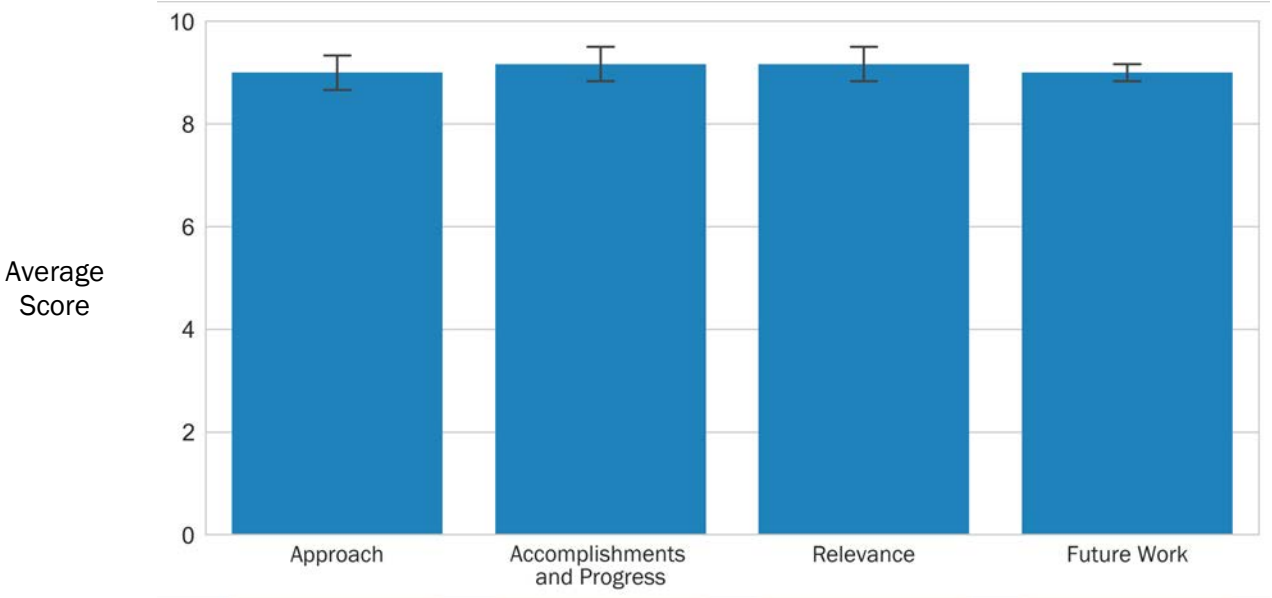
The Co-Optima ASSERT team carries out integrated analysis of efficiency-enhancing bioblendstocks that also reduce emissions. ASSERT supports Co-Optima by evaluating environmental and economic drivers and the scalability potential of perspective bioblendstocks, sharing these key outputs with the teams and stakeholders, and guiding Co-Optima's R&D. ASSERT leverages expertise at the national laboratories in TEA, LCA, refinery modeling, job creation modeling, and modeling of the biofuel industry. The team interacts extensively with other Co-Optima teams to gather data for use in analysis, to receive feedback on analysis parameters, scenarios, and assumptions, and to disseminate analysis results that inform research and development direction.

WBS:	3.5.1.4e
CID:	NL0029892e
Principal Investigator:	Dr. Jennifer Dunn
Period of Performance:	10/1/2018–9/30/2021
Total DOE Funding:	$13,270,000
DOE Funding FY16:	$3,631,000
DOE Funding FY17:	$3,120,000
DOE Funding FY18:	$3,394,000
DOE Funding FY19:	$3,125,000
Project Status:	Ongoing

Initially, ASSERT's focus was on analysis of bioblendstocks co-optimized with BSI engines. ASSERT screened 24 BSI bioblendstock candidates with desirable fuel properties, diverse functional groups, and diversity in production method. Each bioblendstock was categorized as exhibiting favorable, neutral, or unfavorable performance against 17 total technology readiness, economic viability, and environmental sustainability metrics. Isobutanol and aromatic rich hydrocarbons, based on significant technology readiness

Weighted Project Score: 9.1

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



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and economic and environmental feasibility, were the subject of detailed TEA and LCA. Furthermore, with a modeling suite customized for Co-Optima that estimates how the vehicle fleet and fuel consumption will evolve with the availability of co-optimized fuels and engines, the team estimated that as an upper bound, considering isopropanol as a bioblendstock at 30 vol%, 12% annual GHG emissions could be achieved in 2050 from the light-duty fleet.

Additional analyses characterized the potential economic value of bio-based blendstocks with favorable fuel properties for BSI engines to refiners. When octane was the only property considered, less bioblendstock than traditional high-octane fossil reformate was needed to boost fuel octane from the standard 88 RON to 95 RON. Furthermore, using actual product compositions from 15 different petroleum refineries in the United States, the analysis showed Co-Optima bioblendstocks would increase the refiners' profitability for every refinery studied.

ASSERT began to evaluate the potential value in pursuing bioblendstocks for the MCCI combustion approach that would limit engine-out emissions of oxides of nitrogen (NOx) and particulate matter (PM). We explored the range in potential aftertreatment device capital and operating cost savings through co-optimization of MCCI engines and fuels with a new modeling tool. We concluded that a smaller diesel oxidation catalyst, a diesel particulate filter, and selective catalytic reduction devices can reduce capital costs and lowering selective catalytic reduction urea use cuts operating costs. In an optimistic scenario, costs per mile for a heavy-duty truck could be reduced by over $0.50.

Going forward, ASSERT will continue to develop analyses for the MCCI combustion approach as well as for multimode (MM) and kinetically-controlled combustion approaches. This fiscal year, we will screen between eight and 12 bioblendstocks for MCCI or MM combustion approaches and explore the role of co-optimized engines and fuels in vehicles with hybridized power trains. Furthermore, the refinery analysis will expand to include bioblendstocks for MCCI and MM combustion approaches and integrate sustainability considerations.

Overall, ASSERT's research aims to enhance the bioenergy value proposition by identifying scalable, economically viable bioblendstocks that maximize engine performance and energy efficiency and minimize environmental impacts.

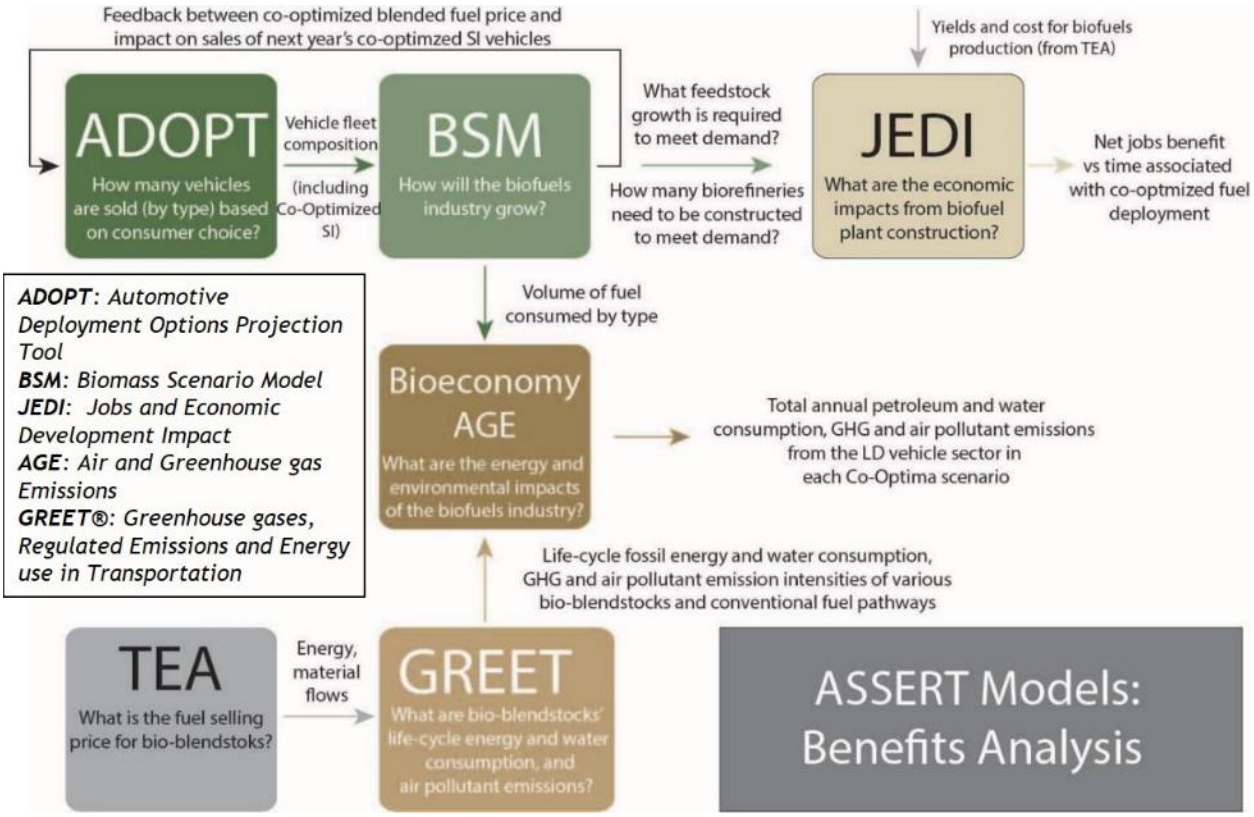

Photo courtesy of Co-Optimization of Fuels & Engines Consortium

OVERALL IMPRESSIONS

- The Co-Optima approach to bio-blends is relatively new but is necessary in light of the range of potential products that can be derived from biomass carbohydrate and lignin fraction. Looking at ways to develop a tool that integrates LCA and TEA makes a lot of sense as so far these two seem to be treated separately. I applaud the team of collaborators in working together in this effort. Looking at 8–12 potential bioblendstocks also is the right approach to develop sound research on properties and feasibility of these different feedstocks as biofuels. Process inputs can be optimized as more information and research is done and results are made available. The ASSERT approach is comprehensive and BETO should continue to develop such models that can be used to assess the wide range of impacts of increased uses of biofuels and other uses for biomass feedstocks and products derived from biomass.

- This project executes a critical aspect of the highly valued Co-Optima project, which is the screening of potential blendstocks to assess economic and sustainability implications. I strongly agree with the idea raised during the review of using both economic and environmental considerations into the retrosynthetic analysis tool in order to generate the most environmentally-sound production pathway for targeted blendstocks.

- Most existing advanced biofuel processes generate multiple products that are often directed to different markets. There may be value in assessing coproducts as part of this analysis.

- Given the potential to adapt/tweak some of the non-favored blendstocks that the Co-Optima team have identified if they offer other benefits (e.g., improved sustainability, etc.), it would be helpful to know if

there is a strong GHG LCA or other sustainability reason to focus on the slightly lower priority blendstocks.

- This is one of the most powerful projects in the Co-Optima portfolio. The use of Aspen PIMS™ along with ASSERT (TEA, GREET®, JEDI, ADOPT, BSM, BA) provides a realistic scenario on the possible outcomes and benefits to the nation when advanced engines are mapped strategically to high-performing biofuel candidates. This is an extremely comprehensive modeling approach. The team should continue their sound approach of engaging stakeholders. Pipeliners should come to the table (e.g., the Association of Oil Pipe Lines) in conjunction with the U.S. Department of Energy, American Petroleum Institute (API), SAE International, American Chemistry Council (ACC), and ASTM. This will be the "stakeholder village" necessary to increase the accuracy of the modeling scenarios. The project team is already highly collaborative and takes informs from across BETO and VTO.

- The team evaluates the blendstock and vehicle technologies under consideration within the Co-Optima program from environmental and economic perspectives while conducting R&D-guiding analyses.

- Barriers Addressed: Co-Development of Fuels and Engines (ADO-E) and Analysis to inform strategic direction (At-A).

- The team is helping the Co-Optima team complete TEA and LCA. The strategies and methodologies taken by the team to evaluate TEA and LCA are strong. The work of crosscutting teams is good. Their response to last year's reviewer views is good. There is a clear plan of future analysis. Screening of different bioblendstock candidates has been planned, in addition to co-deployment of co-optimized and hybridized vehicles.

RECIPIENT RESPONSE TO REVIEWER COMMENTS

- Reviewers of the ASSERT team of the Co-Optima initiative found value in the TEA and LCA of bioblendstocks under consideration within the program. Furthermore, the reviewers found the overall ASSERT analysis suite that includes the Biomass Scenario Model, the Automotive Deployment Options Projection Tool, the Jobs and Economic Development Impact model, the Greenhouse gases, Regulated Emissions, and Energy use in Transportation model, the Bioeconomy Air and Greenhouse gas Emissions model, and Aspen PIMS™ to be powerful and of value to BETO overall. The ASSERT team thanks the reviewers for the affirmation of the importance of the team's work. Per the reviewers' suggestions, ASSERT will continue to evaluate co-product influence on economics and sustainability of bioblendstocks, consider the interplay between biorefineries and petroleum refineries, and engage with additional stakeholders around the quantification of infrastructure costs and evaluation of bioblendstock viability based on infrastructure considerations.