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INTRODUCTION

The Co-Optimization of Fuels and Engines (Co-Optima) initiative is one of nine related technology areas that were reviewed during the 2017 Bioenergy Technologies Office (BETO or the Office) Project Peer Review. Co-Optima is new to the BETO portfolio as work under the initiative began after the last BETO Peer Review. While it is part of the Demonstration and Market Transformation (DMT) portfolio, Co-Optima was reviewed in a separate session due to its complexity and scale of work. In the Co-Optima session, six external experts from various related industries reviewed four presentations.

This review addressed a total U.S. Department of Energy (DOE) investment value of approximately $50 million, with BETO contributing $26 million and the Vehicle Technologies Office (VTO) contributing $24,500 (fiscal year [FY] 2015–FY 2017 spending). The funding for the initiative’s six technical teams is split between BETO and VTO, with BETO primarily funding the Market Transformation (MT); Analysis of Sustainability, Scale Economics, Risk, and Trade (ASSERT); and High-Performance Fuels (HPF) teams. BETO’s portion represents approximately 3.7% of BETO’s portfolio reviewed during the 2017 Peer Review. During the review, a principal investigator (PI) for each BETO-funded technical team and the overall PI of the nine-laboratory consortium project were given between 15 to 60 minutes to deliver a presentation and respond to questions from the Review Panel. Co-Optima was also reviewed at the 2017 VTO Annual Merit Review. That review evaluated the progress of the technical teams primarily funded by VTO: Advanced Engine Development, Fuel Properties, and Simulation Toolkit.

The Review Panel evaluated and scored projects based on their project approach, technical progress and accomplishments from FY 2015 to FY 2017, 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’s 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. In this capacity, Ms. Lindauer was responsible for all aspects of review planning and implementation.

CO-OPTIMA OVERVIEW

The Co-Optima initiative aims to simultaneously transform transportation fuels and vehicles in order to maximize performance and energy efficiency, minimize environmental impact, and accelerate widespread adoption of innovative combustion strategies. This research and development (R&D) collaboration between VTO, BETO, nine national laboratories, and industry is a first-of-its-kind effort to combine biofuels and combustion R&D, building on decades of advances in fuels and engines.

The Co-Optima initiative takes a three-pronged, integrated approach to identifying and developing the following:

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

35 Learn more on the VTO Annual Merit Review and Peer Evaluation web page: https://energy.gov/eere/vehicles/annual-merit-review-and-peer-evaluation
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. We are pursuing a systematic study of fuel blendstocks (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 Support of Office Performance Goals

Co-Optima activities support Office goals by developing the knowledge, data, and tools to expand the blendstock options available to achieve desirable fuel properties.

CO-OPTIMA REVIEW PANEL

The following external experts served as reviewers for the Co-Optima Technology Area session during the 2017 Project Peer Review.

<table>
<thead>
<tr>
<th>Name</th>
<th>Affiliation</th>
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<tr>
<td>F. Michael McCurdy*</td>
<td>Leidos</td>
</tr>
<tr>
<td>Andrea Slayton</td>
<td>Slayton Consultants</td>
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<tr>
<td>Brandon Emme</td>
<td>ICM Inc.</td>
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<tr>
<td>Troy Hawkins</td>
<td>Eastern Research Group Inc.</td>
</tr>
<tr>
<td>Phil Marrone</td>
<td>Leidos</td>
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<tr>
<td>Candace Wheeler</td>
<td>General Motors (Retired)</td>
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</tbody>
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*Lead Reviewer
TECHNOLOGY AREA SCORE RESULTS

Average Weighted Scores by Project

- Co-Optima Overview: 9.05
- Co-Optima High-Performance Fuels Overview: 8.79
- Co-Optima Analysis of Sustainability, Scale Economics, Risk, and Trade (ASSERT): 8.60
- Co-Optima Market Transformation: 7.70

Legend:
- Sun-Setting
- Ongoing
- New
CO-OPTIMA REVIEW PANEL
SUMMARY REPORT

Prepared by the Co-Optima Review Panel

Overview
The Co-Optima team will enable substantial transportation efficiency improvements by optimizing future engine and fuel designs contemporaneously. Custom fuels will be derived from biological sources while the future engine designs will move past traditional spark-ignition engines into higher-efficiency designs, which will have light- and heavy-duty vehicle applications. Key barriers to the adoption of the co-optimized fuel and engine technologies include such items as (1) qualification of the fuels for use on the road, (2) legacy spark engines and proving value of the new fuels, and (3) catalyzing engine development spending without the fueling infrastructure in place.

On behalf of the Peer Reviewers, we would like to thank the DOE Co-Optima team for the invitation to review the presentations and the presenters who took the time out of their busy schedules to summarize their projects to the public at large.

Impact
The potential impact of the Co-Optima initiative is immense. The “chicken and egg” problem is real, whereby the design and deployment of advanced engines is contingent upon the availability of high-performance fuels while the commercialization of high-performance biofuels has been stalled waiting for a market for the fuels to develop. We see the government’s focus in this area as particularly important as a linkage between two different private-sector spaces (i.e., transportation and fuels). While the private sector is willing to invest R&D and development dollars within its core competencies, the sector has been unwilling or unable to invest on a cross-sector basis. By linking these two sectors through the investments by BETO and VTO, DOE has the potential to be the catalyst that enables private investment for the better public good.

All members of the Peer Review Panel could see the potential value in the work, particularly in the (1) potential for customization of future fuels for performance, price, sustainability, or even for specific types of cars or engines; (2) performance benefits to the legacy fleet of engines and future engine designs that are not practical with the current fuel pool; and (3) access to new biofuel markets that would reduce carbon emissions and bring jobs and investment to rural America. Building the fuel properties database and modeling/simulation tools has the potential to drive near-term benefits as the information is transferred to those entrepreneurial companies who can bring the new engine and fuel products to market.

Innovation
The Co-Optima initiative is very innovative, pushing the limits of engine performance and new advanced biofuel production technologies simultaneously. This will benefit the automotive and biofuel industries, the environment, and consumers while promoting rural area jobs and investment. The collaborative approach undertaken by the national laboratories is very innovative, incorporating a selection process that will deliver results in the near- to medium-term, particularly in “Thrust I,” the spark engine fleet. Evaluation and selection of blendstocks based on their economic and environmental benefits should allow BETO/VTO to direct resources into delivering both near- and long-term benefits for the American consumer.

While it would certainly be a stretch goal for the initiative, the Peer Review Panel members noted the potential for new and innovative processes for the qualification of fuels and engines that may be possible with the coordinated efforts of BETO/VTO, the U.S. Environmental Protection Agency, and the private sector.
Synergies

The synergies within BETO/VTO programs are numerous, most notably that higher-oxygen biofuel components represent an unexplored category of chemicals for the transportation sector with the potential to dramatically increase the efficiency of existing spark engines and could enable advanced engine designs with substantial performance and efficiency gains. The Panel saw the initiative as a very natural extension of the DOE’s core competencies and that public investment in this under-funded linkage has spillover benefits to the transportation and biofuel sectors, with synergies across the entire fuel-based transportation sector.

The Panel saw opportunities for better integration of the DMT and Conversion R&D Programs with Co-Optima as the generation of fuels for testing has been a rate limiting step for Co-Optima and appears to be outside of the core mission of the Co-Optima initiative. By utilizing fuels produced at various private- and government-supported pilot and demonstration-scale facilities rather than producing the fuels internally within the national laboratories, the initiative would focus more keenly on the most promising technologies in the near term while informally pairing the new fuels and engine designs improving the speed to market. It was the opinion of the Panel that the production of the fuels for testing may be better located within the Conversion R&D Technology Areas (i.e., Thermochemical, Biochemical, and Waste to Energy) so that the funds could be used to advance the maturity of the technologies. Reducing expenses associated with fuel generation may also free up resources for more engine or combustion testing.

Focus

The Co-Optima area appears poised to generate a wealth of new data from which new fuels and engines can be designed and optimized. The focus on options analysis to down-select from the large pool of more than 300 Tier 1 potential technologies to the much smaller and focused pool of 40 Tier 3 technologies was very impressive to the Panel. There is a dizzying array of potential technologies available and the rigorous, property-based screening approach will be needed to ensure that the work stays on track.

The Panel would have liked to see more emphasis and strategic planning in the MT area as the handoff from the Co-Optima initiative to the private sector for execution and deployment is where U.S. taxpayers will see a return on their investment. While the Co-Optima team has identified the need for a handoff, the stakeholders that are to receive the data are not well-defined as of yet. Better definition of who may be receiving the information and how they will use it to catalyze deployment of the engine or fuel technologies will reduce the risk that the data are not used in a beneficial way for the public. The Panel and some public attendees noted that the qualification of new fuels and engines is not a trivial task, and that some attention to how the new technologies get qualified would be beneficial to the initiative.

Commercialization

Co-Optima appears to be at the optimal stage in the development pipeline in that it pairs fuels and engine technologies in similar development stages so that they may mature in their development together. Engine designers can focus on the properties of fuels that are likely to be available, while fuel producers can tailor their output to the markets that are likely to be available. With each side focusing on the best available technologies, this could speed up the technology deployment timeline. This focus on fuels and properties also provides an opportunity to identify regulatory issues early in the commercialization process so that they can be addressed during the maturation of the technology rather than when an engine/fuel solution is technically ready to go to market.

The Panel remarked how an early adopter test case using public transportation or school could be beneficial to Co-Optima in that it could provide some definition for
the rollout strategy under development by the MT team. The rollout strategy will be key to managing expectations and keeping the various initiative stakeholders on board as the work progresses.

Recommendations

Based on the Peer Review and the Panel’s experience, our top three recommendations to the Co-Optima Team are as follows (in no particular order):

• **Develop a Risk Matrix for Thrust 1 Market Transformation**: Given the primary goal of deploying new engine and biofuel technologies for the benefit of consumers, the environment, and for rural jobs, it was our opinion that the Co-Optima initiative could benefit from producing a matrix of the adoption risks and then adjusting the near-term work to mitigate those risks. Whether the risks are in the technologies, regulatory issues, consumer value proposition, stakeholder fatigue, or other unidentified item, analyzing the project design against a deployment goal could be beneficial in prioritizing project workflow for the maximum benefit.

• **Source Candidate Materials from BETO’s Conversion R&D and DMT Programs**: The goal of the Co-Optima initiative is the co-optimization of fuels and engines, not the development of new fuel production pathways. By sourcing material from the Conversion and DMT teams, the initiative could free up substantial resources which could be redirected into strengthening the combustion dataset and MT efforts. As a side benefit, private fuel producers may be willing to share more data for ASSERT and other models if Co-Optima is not viewed as a potential competitor.

• **Add Regulatory Issues to the ASSERT Models**: The ASSERT models appear to address the environmental and economic issues quite well, and the addition of a regulatory block within the models could make them much more robust in reflecting real-world adoption of the various candidate molecules. Private-sector analysts look at regulatory items as part of a three-legged stool of environmental, economic, and regulatory issues.

CO-OPTIMA PROGRAMMATIC RESPONSE

BETO sincerely thanks the Peer Review Panel for its time, active engagement, and constructive review of the Co-Optima initiative portfolio. In putting together the Co-Optima Peer Review Panel, it was our hope to welcome a wide range of perspectives, and thus we invited reviewers from the DMT, Analysis and Sustainability, and Conversion Technology Area Review Panels. The value of these diverse Panel members’ feedback was clear in the thorough and insightful comments and recommendations that were received. The Peer Review Panel’s praise of the potential value and impact of the work undertaken by the initiative is much appreciated, as well as the recognition of the spillover benefits to the transportation and biofuels sectors. The Peer Review Panel’s recommendations will be used to further enhance the effectiveness of the Co-Optima activities and contribution to the Office’s goals.

Reviewers provided feedback on the three BETO-funded Co-Optima technical teams’ activities. The Co-Optima leadership team is working with PIs to address this feedback to strengthen their 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 already working to incorporate these suggestions into priorities for FY 2018 and beyond.
Recommendation 1: Develop a Risk Matrix for Thrust I Market Transformation

BETO agrees that the development of a risk matrix would be a beneficial addition to the market transformation activities within Co-Optima and will work with the team to ensure that this is addressed in FY 2018.

BETO also agrees with the reviewers’ comments that a clear vision and strategy is needed for MT activities under Co-Optima. We are working with the national laboratory team to develop a program-level vision for market transformation that establishes a clear strategy around industry handoffs and fits under the current Administration’s priorities. In developing this strategy, we will draw on the input that has been received at the stakeholder listening days and during one-on-one visits with targeted stakeholders and will continue to work closely with the consortium’s external advisory board.

Recommendation 2: Source Candidate Materials from BETO Conversion R&D and DMT Programs

BETO appreciates this recommendation and the Review Panel’s suggestion to look for opportunities for better integration with BETO’s DMT and Conversion R&D Programs. While we have made an effort to coordinate with BETO’s Conversion R&D Program during the planning and execution phases of Co-Optima in order to understand linkages and ensure that there is no duplication across the technology area portfolios, we recognize that there are opportunities to strengthen this coordination and will continue to do so. In 2018, we will work to strengthen this coordination at the BETO staff level and among the national laboratory PIs.

Under the Co-Optima initiative, BETO works to identify and evaluate performance-advantaged biobased fuel components with desirable properties to accelerate the introduction of affordable, scalable, and sustainable high-performance fuels for use in high-efficiency, low-emission engines. While Co-Optima does not have a specific goal around development of new fuel pathways, BETO feels that some work on fuel development is appropriate and necessary to support the initiative’s goals. That said, when sourcing candidate materials, fuel blendstocks will be obtained from commercial sources and surrogates will be used when possible to effectively reduce costs. When commercial sourcing is not possible, we will look for opportunities to source materials from Conversion and DMT projects.

Recommendation 3: Add Regulatory Issues to the ASSERT Models

BETO thanks the reviewers for recognizing the ASSERT team’s capabilities in addressing environmental and economic issues and appreciates the recommendation to strengthen the capabilities around addressing regulatory barriers. At present, policy and regulatory variables in two models used by the ASSERT team, the Biomass Scenario Model and Automotive Deployment Options Projection Tool, implicitly address regulatory issues. Although there are no current plans to develop new models, Co-Optima is considering restructuring the portfolio so that market transformation analyses, which address regulatory barriers, are integrated under the ASSERT team.
**CO-OPTIMA OVERVIEW**

**Project Description**

The Co-Optima initiative is a DOE effort funded by BETO and VTO to identify the fuel properties and engine-design characteristics needed to maximize vehicle performance and affordability, while deeply cutting harmful vehicle emissions. The overall goal of the effort is to achieve a 25%–30% reduction in per-vehicle petroleum use by 2030 by enabling higher efficiency engines powered by fuels containing bio-blendstocks that are sustainable, affordable, scalable, and compatible with infrastructure. Multiple research efforts on spark-ignition and compression-ignition strategies are underway with the goal of identifying solutions applicable across the light-, medium-, and heavy-duty vehicle sectors. The fuel property focus of the R&D includes efforts directed toward characterizing and exploiting the unique properties available from biomass-based fuel blendstocks.

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<th>Recipient:</th>
<th>National Renewable Energy Laboratory, Argonne National Laboratory, Idaho National Laboratory, Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory, Sandia National Laboratories</th>
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<tr>
<td>Presenter:</td>
<td>John Farrell</td>
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<tr>
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**Overall Impressions**

- This is a very exciting initiative with a good marriage between the chemistry of potential blendstocks
for biofuels (and potentially petroleum-based fuel) and engine efficiency. Funding has the potential to affect several industry players rather than promote one company as with other projects. The focus on developing fuel blends specific to increased engine efficiency development takes it one step further (i.e., Thrust II). With the practical modeling of economic, environmental, and market metrics for each candidate, this initiative helps industry as a whole evaluate the potential blendstocks. The initiative appears to be very well-organized and managed. The missing links and apparently by design, are how to implement change and provide industry incentives to use the valuable information and tools that will be available for the BETO goals.

• Ideally, this work provides a better fuel quality metric for consumers than the octane rating used today. The team may want to consider how to best drive toward true “pay for performance” in our liquid fuels.

The team understands that hybrid vehicles, et al., create some additional layers of complexity to co-optimization and that ultimately the link to the drive train is what matters (i.e., a Co-Optima co-optimization). I would like to see some clarity how these factors impact the potential outcome of the initiative’s work with regard to having the greatest impact on the overall vehicle population/usage.

The industry practice of thrifting could have a market impact on realizing the environmental goals of the initiative.

• Co-Optima is an exciting new initiative that seeks to accelerate the introduction of affordable, scalable, and sustainable fuels that simultaneously take advantage of engine technology to gain efficiency and maximize vehicle performance. While a huge undertaking, this is an extremely valuable effort which could lead to radical changes in the energy and transportation sectors. It is great to see the collaboration between BETO and VTO as well as the nine different national laboratories and other university partners that are working on the initiative.

For an effort of this size and complexity it is not surprising to have a full-time project manager to ensure the direction and milestones of the work are met. The initiative appears to be well-managed with regular updates, conference calls, and milestones. Communication across working groups will be essential. Using a consortium approach is key in utilizing the expertise and skill sets of the various groups within the national laboratories. Also, it is critical to the success of the program to maintain close ties with the external advisory board and outside stakeholders.

A great deal has been accomplished in the short time the initiative has been going. The specific accomplishments of the individual teams will be address in the following reviews. However, overall, balancing the shorter-term work on Thrust I designed to improve near-term efficiency of spark-ignition engines with the longer-term work to identify fuel properties that enable advanced compression-ignition engines will be critical. Both are important, and while the majority of the vehicles on the road are spark-ignition engines, the advanced compression-ignition work has the opportunity to spill over into the medium- and heavy-duty fleets. It will be interesting to see if this initiative can identify and exploit the unique properties found in biomass-derived molecules that are not available in petroleum-based fuels.

The work appears to be tightly linked with results from one group feeding into the work of another. This type of co-development and collaboration is critical when working on the fuel and engine sides. If successful, this initiative would enable the development of new fuels specifically designed to significantly improve fuel economy and vehicle efficiency. This would reduce fuel use and vehicle emissions, while increasing energy security and rural devel-
opment. The mission is clear and the stakes high. However, it is no easy task. Overall, it is a great initiative with potential wins for the bioeconomy, automotive manufacturers, and the environment. Two of the greatest challenges will be in building out the infrastructure and navigating the regulatory process to get these fuels certified for use. Therefore, initial focus should be on blendstocks that could have high impact. This also requires addressing the question of whether the fuel will be used in new cars only versus the legacy fleet. Having the U.S. Environmental Protection Agency and the California Air Resources Board on the advisory board may help get at the question of how we get the fuel certified for deployment in the marketplace.

In general, future work includes completing Thrust I and then shifting resources for a greater focus on Thrust II. Work will continue to focus on engine architectures and strategies that provide higher thermodynamic efficiencies and new fuels which are required to maximize efficiency and operability. This amounts to simultaneously identifying fuel properties that maximize engine performance while identifying blendstock options that provide key engine efficiency properties.

• Overall, it is certainly a very impressive initiative with a large number of contributors with vast expertise. The analysis of 400+ chemicals and down-selection to 40 represents a lot of good work that has been accomplished to date. The co-optimizer tool represents a vast opportunity where end users could customize their fuel products, potentially creating a market pull for these co-optimized fuels that would increase market uptake. My only concern with the initiative is that unless it includes qualification of at least a limited number of fuels, the regulatory hurdles could be a fatal flaw that severely limits the utility of the work performed.

• This initiative, which attempts to improve vehicle efficiency and reduce fuel consumption through a fundamental rethinking of fuel choice and engine design, is essential and a showcase for what the national laboratories do best. This team provides value to industry by performing a thorough review of all possible fuel compounds derived from biomass and systematically examining each one to determine which will perform best. While this approach is critical to finding new breakthroughs, private industry would (unfortunately) never allocate the time or funding to do this type of work. One concern with all of this work is how it can be transitioned to and accepted by the fuel distribution industry, which may see no value to them in changing fuel blends and reducing/replacing the fossil fuel contribution and/or infrastructure.

PI Response to Reviewer Comments

• We thank DOE and the reviewers for organizing and executing the Peer Review. We appreciate the actionable feedback which we are acting upon to further improve the impact of the Co-Optima initiative.

We will share the positive comments with our researchers. Such comments help all of us understand the importance of what we do each day:

◦ “This is a very exciting initiative with a good marriage between the chemistry of potential blendstocks for biofuels (and potentially petroleum-based fuel) and engine efficiency.”
◦ “[T]his work provides a better fuel-quality metric for consumers than the octane rating used today.”
◦ “While a huge undertaking, this is an extremely valuable effort which could lead to radical changes in the energy and transportation sectors.”
◦ “A great deal has been accomplished in the short time the initiative has been going.”

The reviewers also provide important guidance. For example, “The mission is clear and the stakes
high. However, it is no easy task.” It is indeed not an easy task, and some of the challenges, also noted by the Peer Review Panel, include how we transition the work to industry. “The missing links and apparently by design, are how to implement change and provide industry incentives to use the valuable information and tools that will be available for the BETO goals.” At the same time, the Review Panel provides the means for us to overcome the challenge by staying close to vital stakeholders and how Co-Optima’s impact can be strengthened by external advisory board guidance. “[I]t is critical to the success of the initiative to maintain close ties with the external advisory board and outside stakeholders.” The Co-Optima leadership team works with our government sponsors to clearly define the roles of the laboratories, DOE, and industry. We work closely on linkages with leading stakeholders, including original equipment manufacturers, energy/biofuel providers, and regulators. All of this interaction with various stakeholders helps ensure that our scientific output addresses industry needs within market drivers and thus can lead to better fuels and engines.

The Review Panel also notes that we need to balance our shorter- and longer-term work to address transportation needs across the transportation sector. “[B]alancing the shorter-term work on Thrust I designed to improve near-term efficiency of spark-ignition engines with the longer-term work to identify fuel properties that enable advanced compression-ignition engines will be critical.” We agree. In fact, we are updating goals around light- and medium-/heavy-duty ground transportation, and plan our work around meeting the needs of a wide range of vehicle types.

We also appreciate the Review Panel encouraging us to clean up our messaging even as we plan around macrotrends within the transportation sector. “The team understands that hybrid vehicles, et al, create some additional layers of complexity to the co-optimization and that ultimately the link to the drive train is what matters (i.e., a Co-Optima co-optimization). I would like to see some clarity on how these factors impact the potential outcome of the project work with regard to having the greatest impact on the overall vehicle population/usage.” As a leadership team, we will continue to focus our research on the emerging needs of the transportation industry and hone the clarity in our communication of the corresponding goals.

We thank the Review Panel again for great discussion and important, insightful, and actionable suggestions. We close with this quote from the Peer Review Panel: “This initiative, which attempts to improve vehicle efficiency and reduce fuel consumption through a fundamental rethinking of fuel choice and engine design, is essential and a showcase for what the national laboratories do best.”
CO-OPTIMA HIGH PERFORMANCE FUELS OVERVIEW

Project Description

The HPF team identifies new biomass-derived fuel options for more efficient engines with lower harmful emissions for Co-Optima. This is accomplished via a fuel property-based approach to developing biomass conversion-fuel chemistry-engine performance relationships. This approach leverages and complements the Conversion R&D program area while identifying materials with the right fuel properties and working backward to identify conversion pathways from biomass. The HPF team integrates the capabilities of seven national laboratories to identify new bio-blendstocks, assess their fuel properties, and establish conversion pathways for promising materials. Among other significant technical accomplishments, the team has identified 40 high-octane molecules and mixtures for spark-ignition engines, all of which meet a rigorous set of fuel property criteria and provide key conversion pathway and fuel property data to other Co-Optima teams. The new materials span a wide range of functional groups, including hydrocarbons and oxygenates, and can be generated using biochemical, thermochemical, and

Weighted Project Score: 8.8

Weighting: For ongoing projects, there is equal weighting across all four evaluation criteria: Approach, Relevance, Accomplishments and Progress, and Future Work.
hybrid methods. A similar effort is underway for compression-ignition engines. The HPF team output also helps answer key questions in technical analysis. Thus, the HPF team’s efforts are directly relevant to BETO goals to improve the value proposition for biofuels and develop new markets for biofuels.

**Overall Impressions**

- Overall the project approach is very exciting and a good combination of industry stakeholder interaction, and DOE/national laboratory skill sets. The work appears to be one that is common sense to do and hopefully industry will eventually run with some of the information provided. It appears that the work is well-managed on every front with good management and technical approach along with good communication and collaboration. The technical analysis thus far is very impressive, especially the winnowing of chemical characteristics from 400, to 20, to 4–5 chemicals in a relatively short period. Presenter Dan Gaspar did an excellent job presenting the HPF testing work. It was clear by the additional technical accomplishments in the supplementary slides that more time could have been spent on this topic.

- I suggest considering holding the PI annual kickoff before the budget year starts to maximize resource allocation efficiency.

A lot of great work and progress in identifying and sourcing a large group of candidates, with a lot more to find. It will be good to see more integration with VTO to see where the work is going to quantify the potential gains on a few examples. I like the practice of ensuring backwards compatibility and stability/corrosivity of lead candidates.

I suggest establishing or communicating how the blends the team has looked at so far demonstrate how suboptimal the current engines are in order to validate the assumptions about efficiency gains up to 30%.

As the presenters commented, the merit function used for much of the development is currently best available but not perfect and is undergoing some improvements. It would be interesting to know if this can be used to benchmark existing commercial blends to understand the limitations of the present fuels to allow for advanced engines and applicability to hybrid, etc, engine developments.

It would be good to apply the characterization methods also to the high distillates that present blenders use to “thrift” the fuel when ethanol is added. There may be impacts (good and/or bad) from these low-quality distillates on any of the compounds identified—the team should establish if they will limit the ability to fully leverage the co-optima fuel fully.

- The HPF group works to better understand the relationship between the fuel’s properties and engine performance in an effort to determine new bio-derived fuel options for more efficient engines. The team actively leverages the expertise and data generated by others and uses stakeholder engagement to help guide the analysis. Due to the large and diverse team, communication will be essential to keep the work on track. It is great to see that the HPF group leverages work from other BETO programs and consistently provides iterative feedback between each of the activities.

It will be exciting if the group can capitalize on the unique properties of biomass-derived molecules to produce suitable biobased blendstocks not found in petroleum-derived fuels. The HPF group has been busy. They started by identifying and evaluating over 370 candidate biobased blendstocks. These were down-selected using guidelines developed by the group to 40 high-potential blendstocks meeting the screening criteria. The blending behavior of these 40 materials were measured, and ASSERT was used to select 20 materials for technical analysis. This is an extraordinary amount of work especially since many of these potential blendstocks were not
commercially available and had to be synthesized. Much of the information generated to date has been placed in an online fuel property database which is continually updated to reflect new research and information.

Progress has also been made on Thrust II, including developing criteria for initial candidate identification and testing.

In all of this work, it will be important to evaluate not only the fuel characteristics, but how scalable are they, how much will these fuels cost, and how sustainable are they. Techno-economic analyses and life-cycle analyses should be done on all high-potential fuels. Also, a key challenge to any of these fuels is compatibility with existing infrastructure. We have seen from E15 and E85 that infrastructure can pose a great risk to the deployment of these fuels. Also, it will be critical to understand what impact these materials have on the polymers and elastomers found in the vehicle’s fuel system. This will be especially important for the legacy fleet already on the road.

The HPF group’s goal, to determine new fuel options afforded by bio-derived fuels, including conversion pathways, for more efficient engines with lower harmful emissions, is highly relevant to today. Today’s cars are not maximizing the efficiencies that could be gained due to a lack of octane in the fuel. Optimizing the fuels and the engines could go even further to reducing fuel use, reducing emissions, and strengthening the bioeconomy by creating jobs and spurring rural development. These are worthy goals creating win/win scenarios across the value chain. It will be important, however, to get this information into the hands of decision makers who need to act on it. A strategy to include this information in the Bioenergy Knowledge Discovery Framework (KDF) as well as disseminate it more broadly should be considered. As mentioned above, techno-economic analyses and life-cycle analyses should be done, as well as compatibility testing with existing infrastructure and vehicle fuel systems.

A new fuel may work in engines but may not be a backwards compatible material and would have to be restricted to new vehicles moving forward. I would also recommend considering how much fuel (maximum) can be blended as well as determining the properties at various blending levels of the fuel. I would also suggest looking at the long-term stability of the blendstock as well as multiple blends and not just single compounds.

- This work appears to have gotten off track as it has gone from analysis of co-optimized blends into basic conversion research. Future work appears to be headed back to the stated goals of fuels-related work. It is important to focus on the chemicals and be agnostic to the production processes upstream as the pathways used in the private sector are unlikely to match the laboratory work performed to date.

- This HPF task is arguably the most important part of BETO’s portion of the Co-optima initiative. It is generating a highly valuable database of fuel properties of many different compounds that can be derived from biomass. This work represents tremendous effort by all involved and should be commended. It would have been even more interesting when attempting a project of this magnitude (i.e., identifying new fuel components with optimal properties) to have truly started from scratch in assembling the best fuel rather than keeping the predominant petroleum basis with ethanol and only looking for additives to this base as was done here.

- This is well-run work, with a strong, well-organized team, a good management plan, relevant research questions, and management who are effective and promoting collaboration.

The team’s goals, go/no-go decision point, and milestones are all well-defined for the next phase of the work. The next phase builds on the first phase
and the presentation demonstrated how the work undertaken in the second phase is responsive to the findings of the first phase.

Moving forward, important aspects of this work are to disseminate results, communicate key findings and lessons learned, and package the models and data such that they can be vetted, used, and contributed to by others inside and outside the DOE laboratories in future projects.

**PI Response to Reviewer Comments**

- We thank the reviewers for their insights and suggestions in the conduct of the HPF team review. We appreciate their observations including “[t]his is well-run work, with a strong, well-organized team, a good management plan, relevant research questions, and management who are effective and promoting collaboration.” Finally, we are gratified to hear the reviewers agree the “HPF group’s goal to determine new fuel options afforded by bio-derived fuels, including conversion pathways, for more efficient engines with lower harmful emissions, is highly relevant to today.” Their recognition of the “great work and progress in identifying and sourcing a large group of candidates” is also appreciated.

Several reviewer suggestions and questions address project management. First, we will consider moving the annual HPF PI meeting before the beginning of the FY as suggested. Second, two reviewers noted the importance of communication, between Co-Optima teams and within the HPF team, as well as in engaging stakeholders and disseminating the information to the broader research community. We agree, and are developing a more explicit strategy to disseminate our findings broadly, as well as to communicate key findings and lessons learned, and to package the models and data such that they can be vetted, used, and contributed to others inside and outside the DOE laboratories in future projects.

This may include incorporation of this information in the Bioenergy KDF. Finally, we will continue to leverage other BETO programs and provide feedback to them, as suggested.

Reviewers noted the importance of key fuel properties such as stability and compatibility with existing infrastructure. We agree and have more work planned to extend the current work to model and measure the compatibility of high-potential blendstocks with the entire fuel system (including vehicles). This will be especially important for the legacy fleet already on the road. The reviewer suggestion to evaluate stability of blended fuels, in addition to blendstocks, is an excellent one we will incorporate into our work plan.

There were several comments pertaining to blending and thrifting. We agree that determining the impacts of various base fuel components, including low-quality distillates, on Co-Optima blendstocks are essential and plan to evaluate these in FY 2018. The recommendation to consider maximum blend levels, and to measure performance at a range of blend levels is likewise useful. We note that we have blended at several levels already and will continue to do so based on use cases like those seen in the marketplace, and potentially new use cases arising from co-optimization.

The reviewers rightly note the role of techno-economic analysis and life-cycle analysis in determining “how scalable are they, how much will these fuels cost, and how sustainable are they. Techno-economic analyses and life-cycle analyses should be done on all high potential fuels.” We plan to continue to closely collaborate with the ASSERT and MT teams to ensure we understand the cost and sustainability of new blendstocks, and will continue to extend the number evaluated.
The reviewers asked several questions regarding the merit function, integration with VTO-funded teams, and better quantifying potential gains. We will continue to increase integration with the VTO-funded efforts, and evaluate impacts from merit function improvements to better understand how much fuel economy gain could be achieved. We note that we are comparing to commercial fuels in some cases; further application to hybrid and other drivetrains will require new merit functions.

We thank the reviewers again for their astute suggestions and observations, and plan to incorporate these to ensure the work of the HPF team has the maximum impact and benefit to the full range of stakeholders “creating win/win scenarios across the value chain.”
CO-OPTIMA ANALYSIS OF SUSTAINABILITY, SCALE ECONOMICS, RISK, AND TRADE (ASSERT)

Project Description

The ASSERT team of Co-Optima evaluates the blendstock and vehicle technologies under consideration within the program from an economic perspective while conducting R&D guiding analyses. The outcome of this team’s work is a common understanding among Co-Optima teams and stakeholders regarding environmental and economic barriers to deployment of co-optimized fuels and engines and routes to overcome them. The team carries out techno-economic analysis and life-cycle analysis of compounds and mixtures considered as potential biomass-derived blendstocks that could increase engine fuel economy when blended with gasoline (e.g., in the case of Co-Optima’s Thrust I for spark-ignition engines). Furthermore, the team investigates potential energy and environmental benefits and drawbacks of large-scale deployment of co-optimized fuels and engines through analyses of the vehicle fleet, biorefinery expansion, shifts in the type and amount

Weighted Project Score: 8.6

Weighting: For ongoing projects, there is equal weighting across all four evaluation criteria: Approach, Relevance, Accomplishments and Progress, and Future Work.
of fuel consumption, and job creation. As part of this impact analysis, ASSERT also investigates how bio-
mass feedstock companion markets may propel biomass from a currently available but largely untapped resource to available in large quantities that meet biorefinery specifications. ASSERT analyses contribute directly to the decision point and inform Co-Optima research teams regarding routes to cutting costs and environmental impacts of potential blendstock candidates.

Overall Impressions

- Overall, the project approach is very exciting and a good combination of industry stakeholder inter-
action and DOE/national laboratory skill sets. The work appears to be one that is common sense to do and hopefully industry will eventually run with some of the information provided. It appears that the work is well managed on every front with good management and technical approach along with good communication and collaboration. Development of new and existing tools and ASSERT information should provide industry with valuable resources for determining blending feedstock eco-

- The efforts of the ASSERT team form the founda-
tion of all of the other teams. The ASSERT team strives to understand the environmental and eco-
nomic barriers to the deployment of co-optimized fuels and engines and identify routes to overcome them. If the Co-Optima initiative identifies a novel fuel molecule that can be optimized for a new energy-efficient engine but that fuel is not sustainable, cannot be made at scale, is not economic, or poses a health risk, that fuel will never succeed in the marketplace. That is why this work is so important.

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- The team is familiar with the industry practice of thrifting the low-value distillates back into the gas-
oline when the ethanol is added. This artifact needs to have some consideration in regard to commer-
cialization to ensure the same limitations are not put on co-optima fuel. The team should establish if a market model can be defined for the distillate waste so that they could be feedstock for co-optima or made into another product to keep them out of the vehicle fuel.

- The team has already completed analysis on the top 20 potential blendstocks identified by the HPF group. Its analysis showed that all 20 candidates received a favorable rating for fossil energy consumption and feedstock cost and that no single candidate fared unfavorably overall. The data also showed that the early-development stage of many candidates resulted in an unfavorable rating for conversion state of technology readiness, but that candidates at or near commercialization received generally favorable ratings. This is a great start.
As stated earlier, this work is cross cutting and serves as a key foundation to the rest of the work. It also has close ties to BETO’s Analysis and Sustainability Program Area, making use of several models developed by BETO. The information generated in this activity will also inform ongoing projects in the Conversion R&D Program’s portfolio. The ASSERT team’s close ties with the external advisory board and other external stakeholders also help to keep the work focused and relevant. Insights gained through this research into barriers to large-scale deployment of co-optimized fuels and engines can help inform future BETO R&D priorities.

A critical component moving forward will be work regarding potential routes to market adoption and the potential benefits of this adoption. Infrastructure and navigating the regulatory environment will be huge potential roadblocks for the introduction and mass marketing of these fuels. Unique to Thrust II will be the evaluation of costs and sustainability of after-treatment devices. It will be critical to develop a rollout strategy for these fuels including considering the impact of these fuels on the materials of the fuel systems in existing vehicles. If these fuels are for new cars only, how do we overcome the “chicken and egg” problem? If we anticipate a gradual phase in, what would this look like and what would be the major barriers?

- Overall the ASSERT work was very impressive, and it appears that it will contribute a lot of value by focusing efforts into those co-optimized fuels and engines that have the lowest barriers to entry/most potential. Some research into the regulatory hurdles would make this work much more valuable.

- The efforts of the ASSERT team are significant and complement that of the HPF team by analyzing potential fuel candidates by generally non-technical criteria (e.g., environmental, economic, and emissions effects) that are nevertheless important in the overall choice of a viable compound. The techno-economic analysis and life-cycle analysis work is also important. Though the consideration of these factors addressed by the ASSERT team is clear, it would be helpful to more clearly identify exactly how the ASSERT team’s analysis and results impact the overall choice of viable fuel candidates by the HPF team.

**PI Response to Reviewer Comments**

- We thank the reviewers for their comments highlighting the foundational nature of ASSERT’s work, and recognizing the importance of economics, scalability, and environmental impacts beyond fuel properties in determining the viability of bio-blendstock candidates. In particular, the comment, “Overall the project approach is very exciting and a good combination of industry stakeholder interaction and DOE/national laboratory skill sets’ emphasizes the importance of the multi-laboratory collaboration, DOE support and involvement, and stakeholder interactions. We see engagement with stakeholders as critical to our efforts and we continue to engage with industry through outreach events coordinated with the MT team so that we can inform industry regarding the availability of Co-Optima analyses and tools.

Furthermore, as part of our future work plans, the ASSERT team is working toward a more in-depth analysis with the MT team to understand the value proposition and potential barriers for a range of Co-Optima fuels through the value chain. For the petroleum refiner’s perspective, we plan to apply a range of linear programming tools developed under the Analysis and Sustainability Program to evaluate the impact of fuel blending and potential economic viability for the petroleum refiner.
Moreover, we will carry out further analysis of infrastructure and for new cars for a range of Co-Optima blendstocks in collaboration with the MT team. While some compounds may face significant infrastructure hurdles, bio-blendstocks that have similar properties to existing hydrocarbon fuels may be a somewhat straightforward fit with today’s infrastructure. We will consider the advantages and challenges associated with a range of blendstocks across the full value chain and taking into account factors such as the regulatory process, which has been a focus of the MT team.
CO-OPTIMA MARKET TRANSFORMATION

Project Description

Co-Optima will identify improved fuels that in combination with new engine designs will reduce petroleum reduction through greater overall efficiency and substitution of lower-greenhouse gas life-cycle fuels for current market fuels. The MT Team will provide stakeholders with the comprehensive, objective, science-based, and actionable data on engine systems and transportation fuels required to identify the most promising options for large-scale commercial introduction. The stakeholders engage through monthly conference calls, one-on-one visits, listening day activities, and use of an external advisory board. The MT team’s mission is to identify and quantify barriers to the introduction of new fuels and vehicles in the U.S. market. We achieve this through examining the previous successes and failures of fuel and vehicle introduction into the U.S. market and mapping out the steps required to introduce new fuels into commerce. Facilitation of the fuel introduction process with stakeholders is an important focus for the team. Evaluation of biofuel candidate molecules under consideration are being evaluated in six metrics for their suitability/readiness for market introduction.

Weighted Project Score: 7.7

Weighting: For ongoing projects, there is equal weighting across all four evaluation criteria: Approach, Relevance, Accomplishments and Progress, and Future Work.
Additionally, market introduction scenario analysis with the Co-Optima ASSERT team demonstrates market acceptability for Thrust I fuel candidates and quantifies Thrust II improvements necessary for driving a second fuel specification.

**Overall Impressions**

- This is a very exciting project with a good marriage between the chemistry of potential blendstocks for biofuels (and potentially petroleum-based fuel) and engine efficiency. Funding has the potential to affect several industry players rather than promote one company as with other projects. The focus on developing fuel blends specific to increased engine efficiency development takes it one step further (Thrust II). With the practical modeling of economic, environmental, and market metrics for each candidate, this team helps industry as a whole evaluate the potential blendstocks. The work appears to be very well-organized and managed. The missing links, apparently by design, are how to implement change and provide industry incentives to use the valuable information and tools that will be available for the BETO goals. This could make reaching the goals difficult.

- The team is familiar with the industry practice of “thrifting” the low-value distillates back into the gasoline when the ethanol is added. This artifact needs to have some consideration in regard to commercialization to ensure the same limitations are not put on co-optima fuel. The team should establish if a market model can be defined for the distillates so that they could be feedstock for modification/Co-optima or made into another product to keep them out of the vehicle fuel.

There was discussion about how to get the fuel available/launched into the public. I suggest considering a model similar to the natural gas buses as a potential case: hubbed fuel where “users” (employees) just add the fuel. Municipal public transporta-

tion may be a possible microsystem to use to launch Co-optima.

- The MT team’s role in the broader Co-Optima initiative is to enable the introduction of new, co-optimized fuels and engines by facilitating the new fuel standards needed for introduction into the marketplace, identifying vehicle, distribution, and infrastructure compatibility of new candidate bio-blendstocks, and interacting with all market sector stakeholders for technology transfer. This role is make or break for the program.

In general, the Co-Optima initiative is great. It is targeted at the science and the engineering that only DOE can do. But it will not succeed without a strong infrastructure piece and the ability to certify and effectively navigate the regulatory process. This is where this team needs to focus. Identifying and mitigating the challenges of moving new fuels and vehicles into markets will not be easy. It will require engaging with all critical stakeholders (e.g., original equipment manufacturers, fuel producers, distribution networks, gas station owners, UL, regulators, and consumers) as well as understanding and addressing the many hurdles that need to be overcome. The MT team is looking at lessons learned. A key finding from those efforts is that a consistent policy and regulatory environment is critical to the successful introduction of a new fuel. It will be critical moving forward to make sure that supportive policy and regulation is in place to make the transition successful. That was not the case with the introduction of E85 or E15. It is critical that this group focuses on infrastructure compatibility, backwards vehicle compatibility, and developing the necessary codes and standards.

The MT function will determine the ultimate success of this work. Engaging with the appropriate regulatory agencies and standards organizations as well as outside stakeholders will be key. That means having ongoing meetings with the U.S. Environmental Protection Agency and the California Air...
Resources Board. It is good to see they are already at the table. If successful, this activity will bring co-optimized fuel and engine technologies to market creating new market opportunities and U.S. jobs in the biofuels industry.

Future work includes analyzing scenarios to maximize stakeholder value for all market segments with the ultimate adoption and acceptance of two fuel/vehicle combinations into the light-duty market beginning in 2025. This is an ambitious and worthy goal. I would also recommend that the group spend some time developing a roll-out strategy even if the pathway to full adoption and acceptance is in stages as overcoming the “chicken and egg” scenario for dedicated fuel/vehicle combinations will be difficult. Tackling the regulatory requirements will also be extremely beneficial to the overall success of the program.

- The MT portion of the work is a critical piece, and its effectiveness will be the biggest determinant for the success of the program. I would like to see a bit more definition as to what would be a successful outcome as it is a bit unclear at the moment.

- The inclusion of an MT team in the Co-optima initiative was a good decision since they will help in the transfer of new fuel and engine specifications to industry and the marketplace. This is no small task and likely an uphill battle no matter how good the results in other parts of the Co-optima initiative because of the general inertia of industry to change, particularly when there may be no clear financial advantage to certain key players such as fuel distributors and the petroleum industry. How to achieve buy in from these infrastructure entities is in fact a key challenge and risk for the Co-optima initiative. Active engagement of all stakeholders and documentation of what was and was not successful in past related efforts, which constitutes a major effort for the MT team, are essential for success of the overall initiative.

**PI Response to Reviewer Comments**

- We thank the reviewers for their thoughtful comments and suggestions regarding the Co-Optima MT team review. Your acknowledgement and recognition of the importance of MT activities is appreciated, and your suggestions will help us improve the Co-Optima initiative.

It is our responsibility to develop value propositions for all of the market sectors. They will enable us to identify the possible incentives that provide drivers for market place change and a successful Co-Optima fuel/vehicle introduction.

The reviewers adeptly pointed out the dilemma of how to introduce a new fuel and a new vehicle simultaneously into the market, and their insight is appreciated. Overcoming the “chicken and egg” scenario will indeed be difficult, as the lessons learned studies highlighted. Exploration of fleet introduction where the ability to provide controlled access to fuel/fueling options can be better managed is a good suggestion. We agree that the model’s cases of natural gas fleets and municipality fleets are indeed good ones to analyze and learn from. Other market introduction strategies will also be explored through our market introduction scenario analysis task currently underway this FY and will help us develop a pathway(s) to full market adoption and acceptance as a longer-term goal.

The reviewers’ emphasis on the importance of engaging with regulatory agencies as well as those who influence policy and regulations is appreciated. The current levels of engagement with the U.S. Environmental Protection Agency and the California Air Resources Board have likely been sufficient to date, but we would agree that we might need to increase interactions with others such as other California and Canadian agencies in order to develop appropriate, consistent standards across multiple regions. We see that the Co-Optima team can facili-
tate the development of a new fuel specification and the process required to meet the regulatory requirements. The intent to first develop a finished fuel specification based on the co-optimized fuel properties will need to be sufficiently rigorous to address the reviewer comment regarding the effects of the distillate portion composition.

We acknowledge the importance of infrastructure and vehicle backwards compatibility and agree with the reviewer comments. We have focused effort to date on understanding the level of compatibility for potential bio-blendstocks. The team using the Co-Optimizer metrics will determine any necessary cost/value trade-offs, and whether the affected stakeholders would be supportive of changes that would be needed on a case-by-case basis.