# 5. Fuel and Lubricant Technologies

To strengthen national security, enable future economic growth, support energy dominance, and increase transportation energy affordability for Americans, the Vehicle Technologies Office (VTO) funds early-stage, highrisk research. The research will generate knowledge that industry can advance to deploy innovative energy technologies to support affordable, secure, reliable and efficient transportation systems across America. VTO leverages the unique capabilities and world-class expertise of the national laboratory system and works with partners across industry and academia to develop new innovations in electrification, including advanced battery technologies; advanced combustion engines and fuels, including co-optimized systems; advanced materials for lighter-weight vehicle structures and better powertrains; and energy efficient mobility technologies and systems, including connected and automated vehicles as well as innovations in connected infrastructure for significant systems-level energy efficiency improvement. VTO is uniquely positioned to address early-stage challenges due to its strategic research partnerships with industry (e.g., the U.S. DRIVE and 21st Century Truck Partnerships) that leverage relevant technical and market expertise. These partnerships prevent duplication of effort, focus U.S. Department of Energy (DOE) research on the most critical research and development (R&D) barriers, and accelerate progress. VTO focuses on research that industry either does not have the technical capability to undertake on its own-usually because there is a high degree of scientific or technical uncertainty-or it is too far from market realization to merit sufficient industry emphasis and resources.

The Fuel and Lubricant Technologies (FT) subprogram supports early-stage R&D to improve our understanding and ability to manipulate combustion processes, fuel properties, and catalyst formulations. This generates the knowledge and insight necessary for industry to develop the next generation of engines and fuels for light- and heavy-duty vehicles. As a result, co-optimization of higher-efficiency engines and high performance fuels has the potential to improve light-duty fuel economy by 35% (25% from advanced engine research and 10% from co-optimization with fuels) by 2030 compared to 2015 gasoline vehicles. The subprogram supports cutting-edge research at the national laboratories, in close collaboration with academia and industry, to strengthen the knowledge base of high-efficiency, advanced fuels and emission control catalysts. The FT subprogram utilizes unique facilities and capabilities at the national laboratories to create knowledge, new concepts, and research tools that industry can use to develop advanced combustion engines and co-optimize with fuels that will provide further efficiency improvements and emission reductions.

# Subprogram Feedback

DOE received feedback on the overall technical subprogram areas presented during the 2018 Annual Merit Review (AMR). Each subprogram technical session was introduced with a presentation that provided an overview of subprogram goals and recent progress, followed by a series of detailed topic area project presentations.

The reviewers for a given subprogram area responded to a series of specific questions regarding the breadth, depth, and appropriateness of that DOE VTO subprogram's activities. The subprogram overview questions are listed below, and it should be noted that no scoring metrics were applied.

#### Question 1: Was the program area, including overall strategy, adequately covered?

Question 2: Is there an appropriate balance between near- mid- and long-term research and development?

Question 3: Were important issues and challenges identified?

Question 4: Are plans identified for addressing issues and challenges?

Question 5: Was progress clearly benchmarked against the previous year?

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?

Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?

Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?

Question 10: Has the program area engaged appropriate partners?

Question 11: Is the program area collaborating with them effectively?

Question 12: Are there any gaps in the portfolio for this technology area?

Question 13: Are there topics that are not being adequately addressed?

Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

Question 16: Are there any other suggestions to improve the effectiveness of this program area?

Responses to the subprogram overview questions are summarized in the following pages. Individual reviewer comments for each question are identified under the heading Reviewer 1, Reviewer 2, etc. Note that reviewer comments may be ordered differently; for example, for each specific subprogram overview presentation, the reviewer identified as Reviewer 1 in the first question may not be Reviewer 1 in the second question, etc.

# Presentation Number: acs918 Presentation Title: Advanced Combustion Systems and Fuels R&D Overview Principal Investigator: Gurpreet Singh, U.S. Department of Energy

Question 1: Was the program area, including overall strategy, adequately covered?

# Reviewer 1:

The reviewer remarked that the program area was adequately covered and well described. This reviewer further recounted several items shown by the presenter: doubling of power density in ten years as related to engine trends; fuel economy (FE) increases as vehicles get larger; and regarding emissions trends, emissions have gone down while the number of vehicles and vehicle miles traveled have increased. The reviewer added that technologies to help the trend, which shows technology penetration, include gasoline direct injection (GDI); turbochargers (used with GDI); cylinder deactivation; engine stop/start; transmissions (six or more speeds); continuously variable transmissions. Overall, the reviewer commented that the program has been successful and continues to be successful due to industry, academic, and government collaboration.

# Reviewer 2:

This reviewer asserted that the strategy of Advanced Combustion Systems and Fuels R&D to reduce fuel consumption and emissions through higher efficiency and cleaner combustion-based power was clearly described. Further, the reviewer observed that a clear explanation of the impact of combustion-based vehicle power on the environment was also covered.

# Reviewer 3:

This reviewer indicated that yes, the program area and overall strategy are well covered.

Reviewer 4: This reviewer stated yes.

#### **Reviewer 5:**

The reviewer responded positively and observed brief but complete coverage of the program area, including overall strategy. The reviewer added that strategy was well described and seems very good.

Question 2: Is there an appropriate balance between near- mid- and long-term research and development?

#### Reviewer 1:

The reviewer affirmed that both near- and long-term R&D are balanced to achieve the overall R&D goals of the program.

#### Reviewer 2:

This reviewer responded positively; the work with industry affects near-term effectively. There is solid long-term science that greatly contributes to advancing engine knowledge and technology.

#### **Reviewer 3:**

The reviewer explained that the program looks at mid-term (advanced spark ignition [SI] research) and longterm (low-temperature combustion [LTC] research), fuel and fuel property effects, and aftertreatment for all combustion types. The reviewer continued that this balance is beneficial to the original equipment manufacturers (OEMs) and is well endorsed by them.

#### Reviewer 4:

This reviewer responded yes, and noted that a recent update to the Advanced Combustion and Emissions Control roadmap with priorities is integrated into plans. The reviewer also highlighted mixed mode for lightduty (LD) long-term and boosted SI for near-/mid- LD. Reviewer 5: The reviewer stated yes.

Question 3: Were important issues and challenges identified?

# Reviewer 1:

The reviewer commented that yes, the goals were well defined and developed with industry collaboration. Generally, this reviewer described the goals as a significant improvement in engine efficiency while maintaining low emissions and acceptable performance. The presenter showed how the research is successfully approaching these goals.

# Reviewer 2:

The reviewer stated yes; it was good to see slides showing the amount of oil saved by investing in internal combustion engines (ICEs). This reviewer further commented that ICE is clearly shown to be relevant long-term.

# **Reviewer 3:**

This reviewer commented that yes, the issues impacting current and future combustion-based vehicles were clearly identified and the challenges to meet future efficiency and emissions goals were adequately described.

# Reviewer 4:

The reviewer responded positively and further commented that the challenges were identified and related to the overall system issues.

Reviewer 5: This reviewer stated yes.

Question 4: Are plans identified for addressing issues and challenges?

#### Reviewer 1:

The reviewer reported that the presenter showed the areas of research that the program focusses on, the proposed research road map to reach the goals, and the technologies of focus that will allow that from fuels to engine parts to combustion systems to energy recovery systems to aftertreatment. This is a well thought out program that exemplifies how government and industry collaboration can benefit the United States as a whole.

#### Reviewer 2:

The reviewer replied yes; plans for developing enabling technologies for cleaner and more efficient combustion engines and fuels are clearly identified and outlined.

#### **Reviewer 3:**

The reviewer responded positively and added that plans seem solid and well thought out.

# Reviewer 4:

This reviewer stated yes.

#### **Reviewer 5:**

This reviewer indicated yes and noted that the emission control R&D slide could have also included challenges of cold start and catalyst light-off.

Question 5: Was progress clearly benchmarked against the previous year?

#### Reviewer 1:

This reviewer stated yes; the targets are carefully developed with industry input and are recently updated. The reviewer described goals as aggressive, but not unreasonable.

#### Reviewer 2:

The reviewer expressed that it is difficult to gauge progress on such a fine year-by-year timescale for such a large endeavor. However, this reviewer observed that year-to-year trends over the long haul are covered very adequately.

## Reviewer 3:

This reviewer referenced an original baseline that had been changed to a more recent engine. The reviewer further commented that the program was benchmarked against the previous year and prior years. The changing baseline made the gains look smaller, but the reviewer explained this is well thought out because it gives a better technological baseline to compare against future research. The reviewer opined that the Program Manager should be commended for making this change because it will give honest, but not inflated, improvements.

Reviewer 4: The reviewer stated yes.

# **Reviewer 5:**

This reviewer commented that some information was presented.

Question 6: Are the projects in this technology area addressing the broad problems and barriers that the Vehicle Technologies Office (VTO) is trying to solve?

# Reviewer 1:

The reviewer indicated yes; the projects seem well chosen to drive transportation technology in useful and effective directions.

#### Reviewer 2:

The reviewer explained that this program is focused on solving the technological barriers that the VTO office is trying to solve. The projects deal directly with improving the fuel consumption of engines and lowering the energy demands of vehicles.

#### **Reviewer 3:**

This reviewer responded positively and asserted that projects like SuperTruck II and Co-Optima are definitely addressing the "broad problems" that VTO is attempting to solve.

#### Reviewer 4:

The reviewer stated yes.

#### **Reviewer 5:**

This reviewer replied yes, to some degree. With respect to Co-Optima, the reviewer commented that near-/mid-term fuel for dilute downsized boosted SI should be the same fuel as that for longer-term mixed mode combustion.

Question 7: Does the program area appear to be focused, well-managed, and effective in addressing VTO's needs?

#### Reviewer 1:

The reviewer responded positively and was quite impressed with the leadership team, who are effective in leading a collaborative program. The leadership team's history and expected future are examples of how government should work to improve society.

# Reviewer 2:

This reviewer described the program as focused, well managed, and effective. Overall engine efficiency has increased significantly. The reviewer further explained that, thanks to this program, overall understanding of LTC concepts have gone from a science experiment to commercially viable (during parts of the engine map), and low-temperature (LT) aftertreatment that did not look possible now appears to be on the horizon.

# **Reviewer 3:**

The reviewer asserted that the program area is very focused, well managed, and generally effective.

Reviewer 4: The reviewer stated yes.

Reviewer 5: This reviewer stated yes.

Question 8: What are the key strengths and weaknesses of the projects in this program area? Do any of the projects stand out on either end of the spectrum?

#### Reviewer 1:

The reviewer asserted that all of the projects are well run and very strong.

#### Reviewer 2:

This reviewer commented that the program is extremely strong in all technical areas of need. The program manager is good at getting collaboration for industry and academia and it shows in the areas of research and research results. The only weakness observed by the reviewer was that the academic participation, while significant, was not as strong as the industry participation.

#### **Reviewer 3:**

The reviewer highlighted close involvement with industry, university, and lab teams as a strength. Further, this develops collaborative efforts toward major technical barriers. This reviewer also noted consideration of both LD and heavy-duty (HD) segments requirements. The reviewer described the tendency to emphasize collaboration to an extent that the overhead of coordination can become significant as a weakness.

#### **Reviewer 4:**

Key strengths observed by this reviewer include engagement of wide-range of resources from government laboratories, academia, and industry to tackle problems via a variety of projects and working groups. The reviewer commented that the program area actively seeks out and engages stakeholders to ensure that research remains focused on what all agree is important. However, coordination between labs and leveraging of their different strengths, while much better today than just a few years ago, could still be improved upon, as could encouragement of collaborative research projects between these labs and industry. The reviewer suggested that improved paths towards implementation of government-created tools and methodologies in the commercial sphere should be created and streamlined. Forums like Cross-cut Lean Exhaust Emissions Reduction Simulations and Advanced Engine Combustion memorandum of understanding are excellent examples of ways to share DOE learning with industry and how to provide a feedback mechanism to guide future research so that it remains relevant. The reviewer further indicated that projects like Co-Optima show a degree of coordination between the national laboratories that was sadly lacking just a few years ago.

#### **Reviewer 5:**

This reviewer described world-class researchers and research facilities as key strengths. A weakness identified by the reviewer is the ability to turn the fundamental research into something that will impact OEM product, and added that the 2025/2030 time frame is aggressive to impact OEM product plans.

Question 9: Do these projects represent novel and/or innovative ways to approach these barriers as appropriate?

#### Reviewer 1:

The reviewer remarked that the program's projects use technically feasible, but novel and innovative, approaches to solving the problems of increasing fuel efficiency in modern day vehicles while keeping the performance acceptable and the emissions low. Just this year, two auto manufacturers announced that they are producing vehicles using technologies developed in this program, which just 5 years ago were not thought possible due to the technical barriers. This is a testament to the diligence and hard work of DOE Program Manager.

#### Reviewer 2:

This reviewer indicated yes and thought this is an example of how government agencies should manage and drive technical solutions.

Reviewer 3: The reviewer stated yes.

Reviewer 4: This reviewer stated yes.

#### **Reviewer 5:**

Although these projects are well reasoned and logical ways to approach the issues being addressed, the reviewer was not exactly sure they represent novel approaches.

Question 10: Has the program area engaged appropriate partners?

#### Reviewer 1:

As noted previously by this reviewer, one of the strengths of this program is the degree to which partners in academia and industry have been combined with government resources to attack the problems at hand.

#### Reviewer 2:

This reviewer responded positively and observed very effective engagement of industry and university partners including OEMs, Tier 1 suppliers, and other suppliers.

#### **Reviewer 3:**

The reviewer commented that the program has engaged partners in industry and academia. The program managers regularly meet with their partners to discuss progress and program goals and are well covered in this area.

#### **Reviewer 4:**

This reviewer described collaboration with LD OEMs as strong.

#### **Reviewer 5:**

The reviewer stated yes, but suggested better engagement with more universities to provide proper human resources to the industry in the future. This reviewer further commented that support to universities is relatively low-cost compared to national laboratories.

#### Question 11: Is the program area collaborating with them effectively?

#### Reviewer 1:

The reviewer indicated yes; the combination of collaborative research programs and information sharing forums appeared to be very effective.

# Reviewer 2:

This reviewer stated yes and nicely done. Further, very effective collaboration was observed by the reviewer.

## Reviewer 3:

The reviewer explained that program managers have set up several avenues for industry and academia to collaborate with them. This collaboration is how they have been successful in achieving their goals.

## **Reviewer 4:**

The reviewer commented yes and noted many interactions and collaborations among national laboratories.

# Reviewer 5:

This reviewer remarked that the U.S. Council for Automotive Research and U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability (U.S. DRIVE) are good approaches to maintaining awareness for both teams (DOE and industry).

Question 12: Are there any gaps in the portfolio for this technology area?

# Reviewer 1:

No major gaps were found by this reviewer.

# Reviewer 2:

No significant gaps are noted, but the reviewer suggested that an emphasis on eliminating barriers towards early and fast commercialization of tools and learning should be maintained and fostered.

# Reviewer 3:

This reviewer reported that in recent years, due to budget cuts beyond the program managers' control, funding to LTC techniques and LT aftertreatment has decreased.

# **Reviewer 4:**

It was unclear to the reviewer how the "kinetically controlled" (KC) combustion mode would be achieved. Further, the reviewer commented that this mode is essentially homogeneous charge compression ignition (HCCI), which has not been working out well in practical application so far.

#### **Reviewer 5:**

The reviewer asserted that addressing cycle emissions, including cold start, should be increased.

Question 13: Are there topics that are not being adequately addressed?

#### Reviewer 1:

This reviewer commented that all the topics have been addressed well.

Reviewer 2: The reviewer stated no.

#### **Reviewer 3:**

There were no topics inadequately addressed observed by this reviewer.

#### **Reviewer 4:**

This reviewer suggested that greater consideration of promoting ways that combustion-based power can be merged in a more effective way in the trend towards greater electrification of power trains could be pursued, e.g., range extenders, etc.

#### **Reviewer 5:**

The reviewer stated yes and referenced prior comments.

Question 14: Are there other areas that this program area should consider funding to meet overall programmatic goals?

#### Reviewer 1:

The reviewer explained that the budget seems adequate to keep the needs in hand, though no one would complain about more funding.

#### Reviewer 2:

This reviewer noted the cost of lean aftertreatment.

#### **Reviewer 3:**

The reviewer highlighted controls as they might aid in application of LTC combustion concepts to enhance stability over the entire operating range of the engine. This reviewer also indicated that integration of multiple alternative fuels in future engines or even more complex hybrid power trains could be potential funding opportunities.

#### **Reviewer 4:**

This reviewer remarked that more effort in LTC and LT aftertreatment are needed, and opined that this is the next area of research that will be needed to achieve DOE goals.

#### **Reviewer 5:**

Many studies on chemical kinetics were observed by this reviewer, who added that there do not seem to be as many spray studies.

Question 15: Can you recommend new ways to approach the barriers addressed by this program area?

#### Reviewer 1:

This reviewer observed a great approach and stated to keep up the good work.

Reviewer 2:

The reviewer indicated not at this time.

**Reviewer 3:** This reviewer stated not applicable.

# Reviewer 4:

As LTC becomes more prevalent, this reviewer explained that fuel properties will be more important. Subsequently, the reviewer suggested that DOE needs to engage fuel manufacturers more.

#### **Reviewer 5:**

The reviewer recommended making it easier for multiple labs to enter into collaborative research arrangements (e.g., cooperative research and development agreements [CRADAs]) with industry might help reduce barriers and promote better leveraging of the different strengths of the various national laboratories.

Question 16: Are there any other suggestions to improve the effectiveness of this program area?

**Reviewer 1:** The reviewer commented to keep going.

Reviewer 2:

The reviewer stated this is not applicable.

# Reviewer 3:

This reviewer suggested to continue addressing barriers to production implementation of new ICE technologies.

# **Reviewer 4:**

The reviewer advised to continue the trend towards building collaborative research programs and forums for combining industry, government, and university research.

# **Reviewer 5:**

A larger budget for combustion and aftertreatment was recommended by this reviewer.

# **Project Feedback**

In this merit review activity, each reviewer was asked to respond to a series of questions, involving multiplechoice responses, expository responses where text comments were requested, and numeric score responses (*on a scale of 1.0 to 4.0*). In the pages that follow, the reviewer responses to each question for each project will be summarized: the multiple choice and numeric score questions will be presented in graph form for each project, and the expository text responses will be summarized in paragraph form for each question. A table presenting the average numeric score for each question for each project is presented below.

## Table 5-1—Project Feedback

| Presentation<br>ID | Presentation Title  | Principal<br>Investigator<br>(Organization) | Page<br>Number | Approach | Technical<br>Accomplishments | Collaborations | Future<br>Research | Weighted<br>Average |
|--------------------|---|---|----------------|----------|------------------------------|----------------|--------------------|---------------------|
| ft037              | Co-Optimization of Fuels<br>and Engines (Co-Optima)—<br>Overview  | John Farrell<br>(NREL)                      | 5-13           | 3.20     | 3.30                         | 3.70           | 3.20               | 3.31                |
| ft051              | Co-Optimization of Fuels<br>and Engines (Co-Optima)—<br>Fuel Property<br>Characterization and<br>Prediction | Gina Fioroni<br>(NREL)                      | 5-19           | 3.50     | 3.75                         | 3.63           | 3.63               | 3.66                |
| ft052              | Co-Optimization of Fuels<br>and Engines (Co-Optima)—<br>Fuel Kinetics and<br>Simulation Tool<br>Development | Matthew<br>McNenly<br>(LLNL)                | 5-23           | 3.33     | 3.50                         | 3.33           | 3.33               | 3.42                |
| ft053              | Co-Optima Boosted<br>Spark-Ignition and Multi-<br>Mode Combustion, Part 1                                   | Scott Sluder<br>(ORNL)                      | 5-26           | 3.50     | 3.50                         | 3.67           | 3.50               | 3.52                |
| ft054              | Co-Optima Boosted<br>Spark-Ignition and Multi-<br>Mode Combustion, Part 2                                   | Chris<br>Kolodziej<br>(ANL)                 | 5-29           | 3.63     | 3.50                         | 3.75           | 3.63               | 3.58                |
| ft055              | Co-Optima Boosted<br>Spark-Ignition and Multi-<br>Mode Combustion, Part 3                                   | Scott Curran<br>(ORNL)                      | 5-33           | 3.33     | 3.00                         | 3.83           | 3.00               | 3.19                |
| ft056              | Co-Optima—Mixing-<br>Controlled and Kinetically-<br>Controlled Compression<br>Ignition Combustion           | Charles<br>Mueller (SNL)                    | 5-37           | 3.40     | 3.40                         | 3.50           | 3.30               | 3.40                |
| ft057              | Co-Optima—Emissions,<br>Emission Control, and<br>Spray Research   | Josh Pihl<br>(ORNL)                         | 5-43           | 3.50     | 3.70                         | 3.40           | 3.60               | 3.60                |

| Presentation<br>ID | Presentation Title  | Principal<br>Investigator<br>(Organization)        | Page<br>Number | Approach | Technical<br>Accomplishments | Collaborations | Future<br>Research | Weighted<br>Average |
|--------------------|---|--|----------------|----------|------------------------------|----------------|--------------------|---------------------|
| ft062              | Characterization of<br>Biomass-Based Fuels and<br>Fuel Blends for Low-<br>Emission, Advanced<br>Compression Ignition<br>Engines (Co-Optima) | Ajay Agrawal<br>(U. of<br>Alabama)                 | 5-47           | 2.88     | 3.13                         | 2.88           | 2.88               | 3.00                |
| ft063              | Micro-Liter Fuel<br>Characterization and<br>Property Prediction (Co-<br>Optima)   | Ingmar<br>Schoegl<br>(Louisiana<br>State U.)       | 5-51           | 3.00     | 3.00                         | 3.25           | 2.88               | 3.02                |
| ft064              | The Development of Yield-<br>Based Sooting Tendency<br>Measurements and<br>Modeling to Enable<br>Advanced Combustion<br>Fuels (Co-Optima)   | Charles<br>McEnally<br>(Yale U.)                   | 5-55           | 3.25     | 3.42                         | 3.58           | 3.42               | 3.40                |
| ft065              | Dynamic Species<br>Reduction for Multi-Cycle<br>Computational Fluid<br>Dynamics (CFD)<br>Simulations (Co-Optima)                            | George<br>Lavoie (U. of<br>Michigan)               | 5-60           | 2.90     | 2.80                         | 2.80           | 3.10               | 2.86                |
| ft066              | Reduced Petroleum Use<br>through Easily Reformed<br>Fuels and Dedicated<br>Exhaust Gas Recirculation  | Tom Briggs<br>(Southwest<br>Research<br>Institute) | 5-64           | 2.88     | 2.88                         | 2.38           | 3.00               | 2.83                |
| Overall<br>Average |   |  |                | 3.25     | 3.30                         | 3.35           | 3.27               | 3.29                |

# Presentation Number: ft037 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)— Overview Principal Investigator: John Farrell (National Renewable Energy Laboratory)

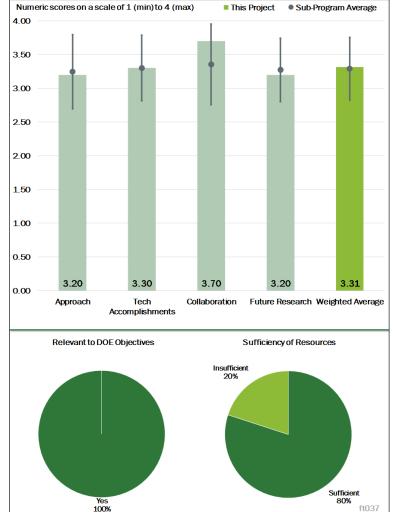
#### **Presenter** John Farrell, National Renewable Energy Laboratory

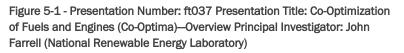
Reviewer Sample Size A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

# Reviewer 1:

The reviewer opined that this is a complex program, involving a broad range of stakeholders, and a very important undertaking. To move towards sustainable global mobility systems, optimizing the power plant and energy carrier systems will be necessary. In the long-term, the reviewer wanted to include the integration, or substitution, of synthetic energy carriers into the fuel system. Yet, the reviewer remarked that this must be done in a transitional way such that legacy fleets are not compromised. Co-





Optima has established a collaborative structure with nine national laboratories and representative of stakeholder communities. The reviewer offered that the work is challenging and results in Co-Optima's needing to respond to a wide range of short-term constraints and long-term objectives. The reviewer proposed that the structure the team has put in place should facilitate this complicated task.

# Reviewer 2:

According to the reviewer, the overall approach is reasonable for the high-level goals defined in this Overview report. While some of the key technical barriers have been identified, the metrics for gauging successful resolution of the technical barriers are not clearly defined. For instance, the reviewer remarked that emissions have been identified as a barrier/goal. However, no metric/target has been defined for emissions compliance. Considering that Co-Optima is targeting a 2030 engine, the reviewer suggested that at the very least, the engine-out emissions should be at a level consistent with meeting Tier 3 emissions requirements with available technology.

The LD fuel-economy target for Co-Optima, which is currently specified as 10% improvement beyond the 25% gain from business-as-usual (BAU) improvements in engine technology, appeared to be too optimistic the

reviewer. The 10% FE improvement is expected to be obtained from changes in fuel properties (e.g., research octane number [RON] and sensitivity) and reduced pumping losses at low loads (advanced compression ignition [ACI] modes). However, the reviewer said that the 25% BAU engine improvements will address some of the same efficiency enablers, specifically compression ratio (CR) and reduced pumping losses, which may pose a challenge to realizing the 10% FE improvement from Co-Optima research.

While electrification is out-of-scope for Co-Optima, the reviewer stated that greater electrification (belt starter generator/integrated starter generator) in conjunction with technologies like continuously variable cylinder deactivation (e.g., Tula) is likely to compete with ACI/KC combustion modes. The reviewer indicated that it may be worthwhile to consider the impact of such technologies, which are expected to be mainstream by 2025, on Co-Optima-based combustion modes and fuel blendstocks.

The reviewer asked that the 2015 baseline for LD engines be clearly defined. At present, the engine configuration or fuel consumption has not been stated explicitly.

#### **Reviewer 3:**

This reviewer commented that while the following hypotheses may be true, the program seems to ignore combustion modes or architectures that may yield high efficiency, low emissions such as an engine that operates using gasoline compression ignition (GCI) across a full engine map for LD applications: Central Engine Hypothesis—that there are engine architectures and strategies that provide higher thermodynamic efficiencies than are available from modern ICEs, and new fuels are required to maximize efficiency and operability across a wide speed load range; and Central Fuel Hypothesis—that if we identify target values for critical fuel properties that maximize efficiency and emissions performance for a given engine architecture, then fuels that have properties with those values (regardless of chemical composition) will provide comparable performance. Starting from a clean slate and using "mixed mode" operation, the reviewer asked why GCI is out of the question.

#### **Reviewer 4:**

The reviewer commented that the approach is hypothesis driven to find optimum fuel and engine combustion strategies. The approach is logical, but the main barrier is that the predictive models for both fuels and engine combustion studies have not reached the appropriate level that can address the barriers. The reviewer asserted that the results are often limited to the scope of the tested operation. Using the results for broad operating regions of engines will lead to erroneous conclusions. There are too many questions that need answering, while the funding is limited. The reviewer preferred that the project be further focused; thus, meaningful results can be obtained. Otherwise, the reviewer saw that it will be a combination of several fundamental studies.

Given there are different engine platforms and modeling accuracy varies among projects, the reviewer highly recommended that the program directors require "uncertainty analysis" along with "sensitivity analysis" for each of the results from different projects. Thus, the outcome from different projects can lead to informative conclusions. The reviewer noted that many of the projects did not have or presented uncertainty analysis for their findings.

#### **Reviewer 5:**

The reviewer stated that a 10% FE-improvement is claimed due to Co-Optima alone. The reviewer inquired as to why the 25% from a base engine is added to the 10% to show a total of 35%. The reviewer found that to be confusing and noted that it gives the impression that Co-Optima is claiming all 35% if one neglects to read the footnote. Also, if the engine improves by as much as 25%, then the reviewer said that the remaining opportunity to get another 10% improvement becomes very, very challenging, given the challenges of mixed-mode combustion.

Pertaining to the central fuel hypothesis, the reviewer stated that fuel structure (molecules) affect aftertreatment operation and performance to a large extent, and perhaps also engine performance (e.g., fuel

composition affects cold start performance to a significant effect). The reviewer questioned whether enough work has been done to make a statement about the validity of the hypotheses.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

## Reviewer 1:

In 2017-2018, the reviewer commented that there were several noticeable accomplishments: Refinement of the merit function for boosted SI engines, use of pressure-temperature domain to develop a fundamental understanding of auto-ignition and the impact of fuel composition on ignition delay, simulation toolkit development, improved chemical kinetic mechanisms, and spray characterization and particulate emission studies. The reviewer agreed that the aforementioned accomplishments, along with others, demonstrate progress towards DOE's higher level goals.

#### Reviewer 2:

While the reviewer disagreed with the research pathways that some of the LD research has taken, the reviewer saw great value in the research that has been done. Research into the beyond-RON and beyond-motor octane number (MON) space is helpful to engine designers and fuel manufacturers alike. It allows both the auto and fuel industries to understand the needs of future engines. This reviewer also saw great potential for the research into how chemical structure impacts fuel properties, and asserted that this research will be of great benefit to the fuel industry.

#### **Reviewer 3:**

The reviewer found that the getting this complex organization functioning has been impressive. The organization has been very active in soliciting, accepting, and acting on shareholder feedback. The result is evolving into more tightly focused projects and adjustments in objectives. The reviewer indicated that this complex organization is well into the learning curve of functioning effectively and is actively pursuing opportunities to make it better.

The reviewer agreed with the decision of pursuing mixed-mode combustion for LD engines—KC combustion at light to intermediate loads and transitioning into flame propagation combustion at high load—but expressed surprise that pursuing full map operation with KC combustion was retained for the medium-duty (MD)-/HD activities. It seemed to the reviewer that the constraints that make KC combustion unattractive for heavy load in LD applications also hold true for MD/HD.

The reviewer thought that it will be important for Co-Optima get buy-in from stakeholders that the proposal to introduce a higher RON, higher sensitivity fuel is a starting point, not an end point. The proposed fuel change will preserve the operation of the legacy fleet, enable the immediate introduction of more efficient engines, and will be the basis from which engines using advanced combustion technologies can be introduced into the future.

#### **Reviewer 4:**

The reviewer pointed to major progress in the project by characterizing merit functions for different combustion regimes, fundamental understanding for boosted SI operation, and identifying key fuel properties for optimal engine performance. The reviewer saw the integrated results utilizing related projects as missing. Integrated results looking into engine efficiency while meeting emission constraints are further needed. It was not clear to the reviewer how results from different platforms will lead to cohesive conclusions. Multimode operation seems a good option for maximum engine efficiency and minimal engine-out emissions, but much more work is needed.

#### **Reviewer 5:**

Multimode SI/ACI is slated to end October 2020. The reviewer wanted to know if this allows enough time to overcome the barriers listed on Slide 13 (transient control, cold operation, combustion noise, etc.). The

reviewer opined that the time is not sufficient. For example, there are still significant barriers existing just to commercialize lean, SI flame-propagation combustion because of a lack of an efficient, cost-effective lean exhaust aftertreatment system.

Question 3: Collaboration and Coordination Across Project Team.

# Reviewer 1:

Having worked for over a decade at a national laboratory, the reviewer had never before seen the level of cooperation and collaboration at all levels of the national laboratories as in this program.

# Reviewer 2:

The reviewer stated that collaboration is the basis for this entire program and the participants are doing it well.

# Reviewer 3:

The reviewer commented that increased collaboration among the participating national laboratories has been one of the strengths of the Co-Optima program. In addition, a concerted effort has been made to schedule and update stakeholders with periodic updates. The reviewer encouraged further interaction with regulatory agencies (California Air Resources Board/U.S. Environmental Protection Agency) to ensure that potential barriers to commercialization of new fuel-blending components are identified early.

# Reviewer 4:

The reviewer indicated that the program includes an excellent network of researchers (9 national laboratories and 13 universities). The network is there and different events (Octane Workshop series in July 2018) are well-planned. But, the reviewer pointed out that there are still cases where further collaborations between modeling and experimental groups can be improved. For instance, the project FT065 (computational fluid dynamics [CFD] modeling) will require proper engine experimental data (e.g., cycle-to-cycle residual gas measurements to understand engine dynamics), but the data are not available from the experimental group(s), and this will limit the outcome of the work.

#### **Reviewer 5:**

Collaboration is certainly very good across the laboratories and now recently academia. However, the reviewer noted that there are really a very small number of stakeholders who really count, including those who build and sell engines as a business and those who make and sell fuel as a business, and perhaps the fuel distribution and retail industry. Thus, the reviewer encouraged that the input of these two stakeholders should be given more weight.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer commented that it is critical that the Co-Optima members maintain active engagement with the stakeholders to make sure that important barriers are being addressed. The Co-Optima members are doing this now; the reviewer recommended to keep it up.

#### Reviewer 2:

The proposed research is outstanding and well defined to meet the programs goals, according to the reviewer, who did not see much in the way of things to criticize.

#### **Reviewer 3:**

The reviewer stated that the proposed future research is in line with the goal of the Co-Optima program to help develop ACI/mixed-mode compression ignition (MCCI)/KC combustion concepts that are targeted at

providing high-efficiency, low-emissions solutions for both light- and HD applications. Transient control and low engine-out emissions are critical for production viability and should be key considerations as go/no-go decisions are made regarding ACI/MCCI/KC combustion modes. While not explicitly stated, the reviewer recommended pursuing fuel spray studies and numerical toolkit development going forward.

#### **Reviewer 4:**

The reviewer said that the proposed future research has logical next steps and was pleased to see the emphasis on cold start, transient controls, mode switching, and engine-out oxides of nitrogen  $(NO_x)$  and particulate matter (PM) emissions in the future research list.

However, the reviewer noted that the funding is limited so the work needs to further narrowing to reach to productive outcomes unless the project budget is substantially increased. For instance, the project could focus more on engine operation in electrified powertrains because these powertrains will present the main powertrain portfolio for 2030 and beyond. This will limit the scope of the project; thus, the budget will be spent more effectively with more concrete outcomes.

#### **Reviewer 5:**

The reviewer advised that more thought should be given to down selecting to one or two practical, scalable fuels of known composition. Further, this reviewer recommended more emphasis on how fuel properties and compositions affect engine combustion performance and exhaust aftertreatment performance.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer remarked that this is a huge but important undertaking. The program is working to balance the introduction of engine and fuel combinations in the near-term and facilitate the introduction of more advanced engines with advanced combustion approaches in the future. The reviewer said that this is an appropriate activity for the government laboratories.

# Reviewer 2:

The reviewer noted that the improving existing engine combustion technologies, identifying desirable fuel properties, and developing new biofuels are all expected to contribute to DOE's goal of petroleum displacement.

#### **Reviewer 3:**

The reviewer observed that this program directly aims at DOE's objectives of lowering petroleum consumption through detailing pathways for engine and fuel manufacturers to use alternative (bioderived) blendstocks to design new efficient engines and fuels.

#### **Reviewer 4:**

The reviewer stated that the program aims to increase FE by 10% in LD vehicles (35% compared to model year 2015) and by 4% in HD vehicles. This program includes great efforts on providing clean-energy options, reducing vehicular fuel consumption, and reducing carbon dioxide greenhouse gas emissions.

#### **Reviewer 5:**

The reviewer stressed that engine performance and exhaust aftertreatment are certainly dependent on fuel properties (and composition), and so this work is very relevant.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

## Reviewer 1:

The reviewer indicated that resources are sufficient if available on a yearly basis for a timeline that ends way beyond October 2020. In fact, there should be no timeline imposed on projects like this as they benefit industry in bits and pieces on a continual basis.

# Reviewer 2:

The reviewer said that the established scope of work is consistent with the budget. The coverage of topic areas seems appropriate.

# **Reviewer 3:**

According to the reviewer, the resources are sufficient to achieve the stated milestones because the project is well-planned.

# Reviewer 4:

The funding is sufficient for the proposed work.

# Reviewer 5:

Given the scope of this project, the reviewer observed that substantially more funding is required to lead to conclusive and transformative results unless research platforms are reduced. There are too many fundamental problems that need to be understood, and the simulation tools have not reached the capability to be fully predictive.

# Presentation Number: ft051 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)—Fuel Property Characterization and Prediction Principal Investigator: Gina Fioroni (National Renewable Energy Laboratory)

**Presenter** Gina Fioroni, National Renewable Energy Laboratory

**Reviewer Sample Size** A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

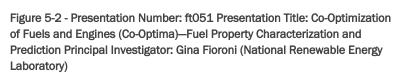
# Reviewer 1:

The reviewer complimented this project for having developed exceptional methods for better measuring/predicting fuel properties and generating valuable data for mechanism validation. The reviewer stated that the project could be significantly better if the flow reactor can be upgraded to be capable of operating at higher pressure, which is critical to validate reaction mechanisms at conditions closer in ICEs.

# Reviewer 2:

The reviewer commented that this is

Numeric scores on a scale of 1 (min) to 4 (max) This Project Sub-Program Average 4.00 3.50 3.00 2.50 2.00 1.50 1.00 0.50 3.50 3.75 3.63 3.63 3.66 0 00 Approach Tech Collaboration Future Research Weighted Average Accomplishments Relevant to DOF Objectives Sufficiency of Resources



very nice work. The detailed measurement of the connection between the fuel's chemical structure and its operational characteristics (vapor pressure, auto ignition characteristics and emissions formation potential) is critical, fundamental information. The reviewer stated that it would be wonderful if measurements made could have been made under elevated pressure.

Yes 100%

#### **Reviewer 3:**

The reviewer found the approach to filling needs for information on fuel properties to be good. Many detailed experiments and simulations must be included. A concern the reviewer had is that with 145 individuals in 86 organizations, it seems that the coordination/communication/status reports required could become a significant workload, taking resources away from actual work.

# **Reviewer 4:**

According to the reviewer, the approach presented is a very systematic methodology for understanding fuel structure and its impact on fuel properties, combustion, and emissions. The fundamental understandings this

Sufficient

100%

ft051

project strives to achieve will guide more accurate combustion and kinetic model development required for advanced combustion simulations.

The reviewer commented that measurement of heat of vaporization (HOV) coupled with a mass spectrometer is critical in understanding which compounds vaporize first. The challenge with the results presented is the atmospheric boundary conditions. Fuel injection in direct injection engines occurs at significantly elevated pressures and temperatures, both of which can affect vaporization and ignition characteristics. The other challenge with the presented HOV results is that it is not clear how a fuel spray, with a lean periphery and a rich core, might vaporize. The reviewer proposed that this line of research is probably not appropriate for this project, but would be an interesting experiment.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer pronounced the methods developed to reveal alcohol on Reid vapor pressure and using multiple instruments to quantify HOV on gasoline evaporation as phenomenal. The flow reactor generated valuable data for auto-ignition, kinetic-mechanism development, and validation.

#### Reviewer 2:

Progress in several areas seems to be very good, according to the reviewer, who also said that important findings are coming out.

#### **Reviewer 3:**

The reviewer commented on the very interesting and important results, e.g., ethanol-suppressing aromatic evaporation.

#### **Reviewer 4:**

The reviewer reported that the results from the fundamental experiments conducted have identified weaknesses in the kinetic models used for combustion research, especially soot mechanisms. This is an important discovery that will lead to more accurate kinetic models. The combination of the HOV and mass spectroscopy (MS) results show the evolution of different fuel compounds that can drastically impact combustion chemistry. It was not clear to the reviewer how this is impacting kinetic simulations or modeling efforts. The methodology to use less than 0.1 milliliter (ml) of a fuel to estimate RON and octane sensitivity (OS) is very impressive. The OS predication is not as good as RON using the Gaussian process, an explanation of which would have been helpful to the reviewer.

Performing the HOV and MS at elevated pressures might yield different results. The reviewer recommended considering an upgrade to the hardware to tolerate high pressure. The reaction kinetics will change according to pressure so instead of attempting to correlate experiments at atmospheric pressure, it might be more worthwhile to correlate experiments to representative combustion pressures.

**Question 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

According to the reviewer, there was outstanding collaboration with universities and OEMs.

#### Reviewer 2:

The entire Co-Optima program is dependent on strong collaboration, and the reviewer noted that this project appears actively engaged with collaborators.

#### **Reviewer 3:**

As expected from the Co-Optima program, the reviewer said that there is significant interaction and contribution from multiple facilities and researchers. This continues to be one of the strongest points of the program. The results of this project can be seen to influence multiple different projects and enable more accurate model development.

## **Reviewer 4:**

The reviewer said that there seems to be good collaboration, but it was hard to judge because there are so many stakeholders. It must be difficult to be aware of projects that should face off. A concern the reviewer had is that with 145 individuals in 86 organizations, it seems that the coordination/communication/status reports required could become a significant workload, taking resources away from actual work.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

# Reviewer 1:

The reviewer commented that the future research is effectively planned in a logical manner, considered the objectives to the overall Co-Optima program.

# Reviewer 2:

The reviewer suggested that data at higher pressure would be a great enhancement to the program.

# **Reviewer 3:**

The directions seem to be correct to the reviewer, who said that it is a good idea to upgrade the flow reactor to run at higher pressures; one might expect the chemistry to have pressure dependencies. For example, phi sensitivity of fuels is known to be pressure dependent.

#### **Reviewer 4:**

The reviewer stated that the proposed future work addresses the open questions identified in the project update. An improvement would be to upgrade the HOV and MS hardware to tolerate high pressures for more accurate combustion conditions.

Question 5: Relevance—Does this project support the overall DOE objectives?

# Reviewer 1:

The reviewer called this work foundational to the modeling efforts in developing new fuels, predicating their properties, and understanding their impact in combustion. This project is instrumental in the Co-Optima program and, as such, is instrumental in the goals of DOE in increasing engine efficiency, decreasing engine pollution, identifying novel and locally sourced fuels, and improving energy security.

#### Reviewer 2:

As part of the Co-Optima program, the reviewer stated that this project will develop invaluable methods/data for a better understanding of fuel properties, which are crucial for co-optimizing engine and fuel technologies, and definitely support the overall DOE objectives.

#### **Reviewer 3:**

This reviewer described Co-Optima, in total, as a very important set of technologies and projects for DOE's goals of efficiency subject to meeting emissions standards, and energy independence.

# Reviewer 4:

The reviewer referenced prior comments and remarked that this project is an important fundamental aspect of the Co-Optima effort.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

If additional resources would allow high-pressure measurements, the reviewer said it would be money well spent.

#### Reviewer 2:

The reviewer stated that funding is sufficient for most of the tasks involved; however, funding will need to be increased to achieve the higher pressure capability needed for more accurate HOV and MS measurements.

#### **Reviewer 3:**

The reviewer said that there are sufficient resources to achieve the stated milestones.

#### **Reviewer 4:**

There seem to be a lot of people and facilities involved, according to the reviewer, who commented that the effort seems sufficient.

# Presentation Number: ft052 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)—Fuel Kinetics and Simulation Tool Development Principal Investigator: Matthew McNenly (Lawrence Livermore National Laboratory)

**Presenter** Matthew McNenly, Lawrence Livermore National Laboratory

**Reviewer Sample Size** A total of three reviewers evaluated this project.

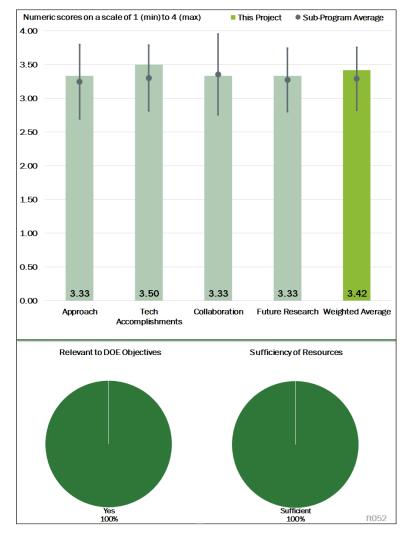
Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

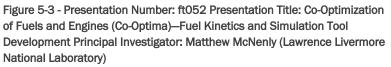
# Reviewer 1:

The reviewer observed an outstanding approach to performing the work, and had no further comments.

# Reviewer 2:

The reviewer asserted that the project approach is very sound in nature. A systematic evaluation of fuel kinetics and ignition delay times is being done with both experiments and numerical studies. One of the criticisms the reviewer had about the work is the lack of consideration of turbulence in the evaluation of ignition delay times. In





addition, some measurement of flame speeds at different pressures will be helpful for model validation.

#### **Reviewer 3:**

Overall, the reviewer pointed out that the approach is well-focused on improving the capabilities to predict fuel chemical properties, covering a comprehensive range of fundamental and applied areas. As the project team stated, the relevant engine combustion areas to be tackled include dilute gasoline combustion, clean diesel combustion, and low-temperate and multimode combustion. The reviewer stated that it is important to note that each technical area has its own barriers and requires a specifically tailored approach. The reviewer suggested that the project team should consider clearly laying out the goal, approach, and accomplishments having relevance to each of the above-mentioned areas. For instance, on Slide 6, it is hard to see clearly what approaches the project team is taking to improve the fundament kinetics knowledge/capabilities on clean diesel combustion and multimode ACI combustion.

The reviewer understood that an advanced fuel ignition delay analyzer (AFIDA) provides rapid ignition time delay measurement and can serve as an efficient screening tool. But, it was not clear to the reviewer to what

extent it can help kinetic mechanism development considering the physical processes involved. The spray physics in AFIDA may also be different from that in the ACI mode so the value of CFD simulations needs to be clarified. To search for the right fuel chemistry for the multimode ACI/SI operation, the reviewer commented that the project team needs to present a merit function to rank different combinations. In addition to phi-sensitivity and OS, RON may be another parameter that needs consideration. For a proper evaluation, the practical value and the fidelity of the kinetic tools, the reviewer recommended that CFD simulations should eventually be conducted in actual SI, ACI, and diesel engine conditions. To make the knowledge more transferrable to the industry, mechanism reduction is critical and should be addressed.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer noted that the team has made good progress since last year. The work on AFIDA is extremely impressive, and it seemed to the reviewer that it is very useful for this work with high through-put. In general, this reviewer was happy with the progress of the project.

#### Reviewer 2:

The project team has made good progress to address the key project tasks and the overall Co-Optima goals, according to the reviewer.

#### **Reviewer 3:**

The reviewer remarked that progress was outstanding and had no further comments.

**Question 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

The reviewer reported the collaboration to be outstanding and had no further comments.

#### Reviewer 2:

The reviewer found a high degree of collaboration among national laboratories in the project, but encouraged the project team to seek out some industry collaboration. The reviewer noted that there are some industry partners on the external advisory board but did not see an OEM or a fuels company included.

#### **Reviewer 3:**

The reviewer commented that the project is well coordinated and has excellent collaborations among national laboratories and universities. The involvement of the Coordinating Research Council and the Advanced Engine Combustion working group is also beneficial. In addition, the reviewer suggested that the project team should consider further strengthening the interactions with OEMs so that the outcomes of the research can be of more practical value and transferrable to industry. Also, the reviewer wanted to see the project team develop closer coordination with the Co-Optima experimental teams on ACI and diesel combustion activities.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer said the proposed future research was outstanding and had no further comments.

#### Reviewer 2:

The reviewer called the proposed future work satisfactory; however, the reviewer urged thinking about including the effects of turbulence in chemistry as that is the missing piece in the puzzle. In addition, the

reviewer asked if the rapid compression machine (RCM) could be converted into a rapid compression expansion machine (RCEM). There might be opportunity for probing species concentration evolution in a RCEM, which can be used for further validation of the species evolution from the chemistry mechanisms.

#### **Reviewer 3:**

The further work is overall well-planned to address the remaining technical challenges, according to the reviewer, who suggested adding other areas for consideration, such as developing a merit function for ACI/SI multimode combustion; and incorporating polycyclic aromatic hydrocarbon (PAH) chemistry in the diesel surrogate model, kinetic mechanism reduction, and CFD simulations in actual SI, ACI, and diesel engine conditions.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

By improving the fundamental kinetics knowledge and developing high-fidelity predictive tools, the reviewer highlighted that the project is an important element to support the Co-Optima goals and the overall DOE objectives.

#### Reviewer 2:

The reviewer affirmed that definitely this project is very relevant to the Co-Optima effort and in general for DOE.

#### **Reviewer 3:**

The reviewer reported that the proposed future research was outstanding and had no further comments.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer said that the proposed future research was outstanding and had no further comments.

#### Reviewer 2:

The reviewer stated that \$1.4 million for fiscal year (FY) 2018 shared across various laboratories for both computational and experimental work is reasonable and sufficient for the completion of the work.

#### **Reviewer 3:**

According to the reviewer, the resources are sufficient to achieve the milestones and address the technical barriers.

# Presentation Number: ft053 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 1 Principal Investigator: Scott Sluder (Oak Ridge National Laboratory)

#### Presenter

Scott Sluder, Oak Ridge National Laboratory

**Reviewer Sample Size** A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer noted that this work is aimed at increasing the understanding of the impact of high-RON, highsensitivity fuel on downsized, boosted SI engines, which is a pathway that the LD industry has committed to for the foreseeable future. Thus, the reviewer exclaimed that the potential impact of this work is huge.

# Reviewer 2:

The reviewer pointed out that the Co-Optima-boosted SI and multimode SI/ACI efforts focus on an experimental and computational approach to identify

Numeric scores on a scale of 1 (min) to 4 (max) This Project Sub-Program Average 4 00 3.50 3.00 2.50 2 00 1.50 1.00 0.50 3.50 3.50 3.67 3.50 3.52 0 00 Future Research Weighted Average Approach Tech Collaboration Accomplishments Relevant to DOF Objectives Sufficiency of Resources Yes 100% Sufficient ft053 100%

Figure 5-4 - Presentation Number: ft053 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 1 Principal Investigator: Scott Sluder (Oak Ridge National Laboratory)

fuel properties and allow researchers to use a SI/multimode merit function to choose fuel properties for engines. Once refined, this will be a very useful tool.

# Reviewer 3:

The reviewer commented that the project is reasonably designed and planned.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

## Reviewer 1:

The reviewer stated that the project has evaluated varying fuel properties in advanced SI engine allowing researchers and engine designers to better understand the relationship between combustion abnormalities, such as knock and fuel properties. While engine manufacturers study this phenomenon in current engines, this research focuses on future engines and technologies allowing the industry to better understand how the changes in technologies are affected by fuel properties.

#### Reviewer 2:

The reviewer indicated that excellent progress and results have been achieved.

#### **Reviewer 3:**

The reviewer remarked that knock is the main barrier to designing a high-performance engine. The knock model is very important for predicting knock onset and hence it is crucial for engine-design optimization. However, the use of knock-intensity extrema in the knock model may be too conservative to be used in the design optimization, and it could lead to a design of less than the true optima. Moreover, all modern engines have incorporated a knock sensor. The reviewer suspected that the knock model without the consideration of the knock-sensor operation may also be too conservative.

**Question 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

While Co-Optima is a national laboratory-only effort, the reviewer mentioned that researchers have collaborated with OEMs, fuel manufacturers, academia, and national laboratories to perform this research. This work is a great example of how to collaborate with industry and national laboratories.

#### Reviewer 2:

According to the reviewer, excellent collaboration exists among the laboratories conducting engine experiments, RCM experiments, and simulations over the range of fuels of interest.

#### **Reviewer 3:**

The reviewer stated that collaboration exists and the partners are fairly well coordinated.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer suggested that this work should continue for both engine experiments and simulations. The proposal to test the effect of MON at high engine speeds and loads and high-intake temperatures needs to be given high priority.

#### Reviewer 2:

The reviewer commented that the proposed future research will allow the Co-Optima program to determine the fuel properties needed to enable advanced SI engines.

#### **Reviewer 3:**

The plan seemed effective to the reviewer.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer asserted that this project focuses on the impact of fuel properties on down-sized, boosted SI, gasoline-engine performance and so is extremely relevant; it should not be prematurely terminated.

#### Reviewer 2:

The reviewer remarked that the research is going into information that will be used by engine designers to develop engines that use less fuel, therefore lowering our dependence on petroleum.

#### Reviewer 3:

The reviewer noted that the project can potentially achieve the DOE goal of Co-Optima.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

Reviewer 1:

Current level of resources should be maintained for the foreseeable future, according to the reviewer.

Reviewer 2:

The reviewer found the research to be on track to meet its goals with the resources it is allocated.

**Reviewer 3:** 

The reviewer said that the team members have sufficient resources.

# Presentation Number: ft054 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 2 Principal Investigator: Chris Kolodziej (Argonne National Laboratory)

# Presenter

Chris Kolodziej, Argonne National Laboratory

**Reviewer Sample Size** A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer found the project to be very well-designed as it combines experiments, simulation, and tool (Co-Optimizer) development. The work significantly improves the understanding of fuel impact on engine performance.

#### Reviewer 2:

According to the reviewer, the approach is on target with emphasis being placed on the correct areas (fuel property effects on auto-ignition, simulation support, using the Co-Optimizer, and using the Merit Function to grade candidate fuels).



The reviewer noted that the project is gathering octane-relevant data with well-designed experiments at conditions relevant to boosted SI engines.

#### **Reviewer 4:**

The reviewer commented that the experimental approach in this project is logical and looked into the effect of fuel properties on knock intensity and auto-ignition. The approach for the uncertainty and sensitivity analysis is very valuable and can be used in other projects as an example. However, the approach in the Co-Optimizer (simulation) area needs further thinking. Two major items to consider are that the Optimizer can produce the proper outcome only if there are enough data used to cover all major nonlinearities, and the process for knock/auto-ignition is not Gaussian for broad engine operation. The reviewer asked how residual gas composition/fraction and cyclic variability effect are seen in the defined merit on the presentation slides.

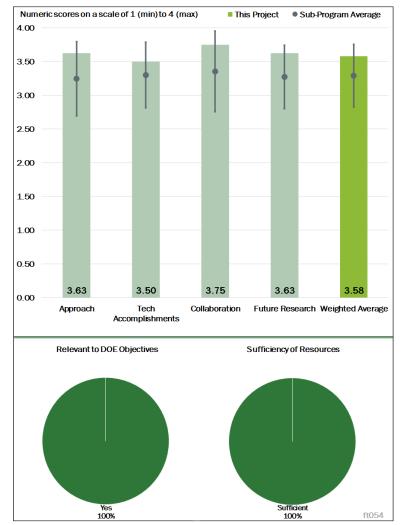


Figure 5-5 - Presentation Number: ft054 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 2 Principal Investigator: Chris Kolodziej (Argonne National Laboratory) In exhaust-gas recirculation (EGR)-diluted combustion (barrier 1), the cyclic variability and combustion stability are major concerns. It was not clear to the reviewer how this is addressed in this project because the focus is mostly on knock and auto-ignition.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer remarked that the work on RON and HOV is providing new knowledge and increased understanding of how these fuel properties affect engine performance. Knock-correlation work with various knock metrics has also provided new information that industry can use. The virtual constant-pressure flow rig (CFR) is a clever approach and will save time and resources in the long run.

#### Reviewer 2:

The reviewer found that significant progress has made in learning how HOV and RON affect auto-ignition. The experiments were very well-conceived. CFD helped to explain the transition between knocking and normal SI combustion. Co-Optimizer is a useful tool supporting decision making.

#### **Reviewer 3:**

The reviewer complimented the project as being some nice work, and especially liked the virtual CFR and the CFR with compensation for HOV and boost.

#### **Reviewer 4:**

The reviewer commented that CFD model validations and understanding knock in boosted SI operation are the major accomplishment of this project. The project also provides helpful knowledge for understanding the tradeoffs among engine performance, fuel cost, and uncertainty. However, the reviewer stated that the project shows limited accomplishments in the areas of robust lean-burn and EGR-diluted combustion control and determining factors limiting LTC and method to extend limits for the barriers identified as the program objectives.

**Question 3: Collaboration and Coordination Across Project Team.** 

#### Reviewer 1:

The reviewer stated that there was excellent collaboration among national laboratories and with OEMs, universities, and energy companies.

# Reviewer 2:

According to the reviewer, there are lots of collaborations; involving the right kinds of skills and facilities in an effective way. The reviewer said that it was nice to see experimentalists and modelers in close proximity programmatically.

#### **Reviewer 3:**

The reviewer said that collaboration with many relevant organizations exists.

#### Reviewer 4:

The reviewer pointed out that there exists a strong collaboration within the Co-Optima team. The reviewer noticed that the requests from this project team for more data/inputs from experimentalists, as these are essential for the Co-Optimizer to generate quality outcomes. Similarly, further data are required for proper training of the artificial neural-network model for covering broad conditions.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

#### Reviewer 1:

The reviewer especially liked the idea of a boosted CFR to measure RON/MON at more boost-relevant conditions.

#### Reviewer 2:

The reviewer indicated that the proposed future work is laid out in a logical manner, with little risks.

#### **Reviewer 3:**

The reviewer asked whether one or two of the high-RON, high-sensitivity candidate fuels being tested can be recommended as being the best overall fuel for downsized, boosted SI engines.

#### **Reviewer 4:**

The proposed plan includes important remaining topics to be studied. The reviewer noticed only 3 months left in the project. Finishing all the proposed future research within 3-month timeframe would be very difficult.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer asserted that the project aims to increase efficiency of ICEs by providing better understanding of combustion in SI engines and generating an innovative Co-Optimizer tool to minimize fuel consumption and cost. This directly addresses the DOE objective to reduce vehicular fuel consumption and improve energy security.

#### Reviewer 2:

The reviewer said that high engine efficiency is targeted for downsized, boosted SI engines, a pathway that the LD industry has committed to. So, much of this work can directly be implemented in the very near future.

#### **Reviewer 3:**

The reviewer found the work to be well-aligned with the overall goal of Co-Optima. This project advances our knowledge of fuel-engine co-optimization, which supports the DOE objective of improving efficiency.

#### Reviewer 4:

The reviewer mentioned that Co-Optima goes to the root of DOE's energy independence and efficiency missions while considering limits on emissions.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer noted that there are sufficient resources to achieve the stated milestones.

# Reviewer 2:

The reviewer found the resources to be sufficient.

#### Reviewer 3:

The reviewer commented that there are sufficient resources as long as a strong collaboration exists with experimental groups in the Co-Optima program to provide the required experimental data for this project.

# **Reviewer 4:**

Resources seemed appropriate, although more funding might accelerate the results. OEMs are already near the time for committing designs for production, and that is near the time that Co-Optima is scheduled to end so the data cannot come too soon.

# Presentation Number: ft055 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 3 Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

# Presenter

Scott Curran, Oak Ridge National Laboratory

#### Reviewer Sample Size

A total of three reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

#### Reviewer 1:

The reviewer indicated that the team is performing well in this project with a healthy blend of experimental work and numerical computations. This is a welldesigned project.

#### Reviewer 2:

The reviewer stated that employing measurements in metal and optical engines and using CFD modeling are good approaches to enhancing synergistic work performance and effectively addressing the technical barriers of the research scope.

#### **Reviewer 3:**

3.50 3.00 2.50 2.00 1.50 1.00 0.50 3.33 3.00 3.83 3.00 3.19 0.00 Approach Tech Collaboration Future Research Weighted Average Accomplishments Relevant to DOF Objectives Sufficiency of Resources

This Project

Sub-Program Average

Numeric scores on a scale of 1 (min) to 4 (max)

4 00



Figure 5-6 - Presentation Number: ft055 Presentation Title: Co-Optima Boosted Spark-Ignition and Multimode Combustion, Part 3 Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

In general, the reviewer noted that all subprojects have identified key barriers and have worked towards addressing those barriers. As the work on multimode/ACI combustion modes progresses, the reviewer offered a few suggestions. Firstly, for ACI modes that rely on high intake temperatures, there is a need to demonstrate that the high temperatures can be achieved using internal EGR/hot residuals. Alternatively, the team needs to account for the energy required to provide the hot air temperatures while estimating the efficiency of the ACI mode. Secondly, as transient operation for multimode/ACI combustion is investigated, the reviewer said that it is also important to demonstrate that the ACI-mode enabling conditions (e.g., air temperature, valve timing, valve lift, and variable compression ratio [VCR]), can also be achieved in realistic time durations (few cycles instead of few seconds). Thirdly, as the various ACI combustion modes are investigated, especially those involving lean combustion, engine-out emissions should be taken into account while calculating efficiency improvements (e.g., catalyst regeneration, nitrous oxide emissions). Past DOE/industry projects have demonstrated high thermodynamic efficiencies for ACI modes, but have been limited by the inability to meet criteria emissions. Lastly, the reviewer remarked that sensitivity studies for ACI combustion modes should also include variation in fuel composition for a given specification to capture best- and worst-case market fuels. In other words, information on how tightly a fuel specification would need to be controlled would be

extremely valuable in determining the feasibility of a combustion mode plus fuel combination. A blendstock by itself may be affordable, scalable, sustainable, and compatible, but if the finished fuel needs to be controlled to very tight specifications, then it may not be commercially viable.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

#### Reviewer 1:

The reviewer praised this project as having made good progress over the past year and summarized some of the notable accomplishments of the project, including engine-out soot measurements as a function of particulate matter index (PMI) for nine different fuels. The work that is focused on variations in spray characteristics that influence particulate emissions but are not accounted for by PMI is valuable and should be pursued further. As the blendstocks are varied, the reviewer suggested that the variations in combustion stability/duration should also be tracked, especially for ACI modes to understand the sensitivity to variations in fuel composition. Production applications need to operate without knowledge of fuel composition; thus, the ACI combustion mode needs to be robust to account for variations in fuel composition. The reviewer thought that the quantitative wall-wetting diagnostic technique is a powerful tool for studying soot production. Investigating the impact of fuel composition on wall wetting and soot production for similar operating conditions would be valuable information for assessing the suitability of different blendstocks for SI/ACI combustion modes. Additionally, the reviewer said that any investigations during transient operation that can help minimize soot production during transient maneuvers would also be very valuable. The reviewer had a comment about determining the temperature variation between the maximum temperature that allows knockfree, high-load SI operation and the minimum temperature that enables low-load HCCI operation. While this information is useful, the high load investigated is not high enough. For multimode operation, ACI modes are expected to be coupled with downsized boosted operation. While 9-bar indicated mean effective pressure (IMEP) may be a high load for naturally aspirated (NA) applications, it is only a medium load for downsized boosted applications. If the ACI modes need to be used in conjunction with NA SI combustion, the reviewer explained that this would drive a larger engine size and would come with associated friction losses. The aforementioned accomplishments are in line with the overall goals of the Co-Optima program.

#### Reviewer 2:

According to the reviewer, overall technical accomplishments are in line with project expectations. In terms of CFD modeling, it was unclear to the reviewer where the flame-speed data at higher pressures are made available for the G-equation flame propagation model for the exotic Co-Optima fuels. This is crucial for knock predictions. The two-step VCR engine for enabling multimode is good work for the future and will only be meaningful with transient cycles. In some sense, the reviewer opined that the project gives a feeling of mixing two OEM approaches: the Nissan VCR engine approach and the Mazda SKYACTIV-X approach.

#### **Reviewer 3:**

The reviewer mentioned that progress in addressing technical barriers seems to be rather slow compared to previous years. The figures in Slide 18 indicate that change in temperature (dT) alone is not enough to characterize multimode operation. The reviewer offered that the suggestion of another parameter seems to be necessary. Also, the dT metric seems to be a function of the CR, and the researchers even seem to intend to explore high CR engine operation. However, the reviewer opined that the current scope and approach of multimode combustion are clearly limited by the range of CR of interest (that of conventional gasoline engines). This will significantly limit the application of the multimode combustion concept.

#### Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer called having Ford, GM, and Toyota in the team as fantastic and noted that collaboration with other national laboratories is also a plus. This is truly a very cooperative effort.

#### Reviewer 2:

The reviewer found excellent collaboration among participating national laboratories as well as industry partners. The reviewer said that it is worth noting that coordinating the activities across multiple teams/researchers requires a lot organization and the effort is worth applauding.

# Reviewer 3:

The reviewer commented that the collaboration was well-organized based on assigned tasks, though the reviewer encouraged more involvement by industry partners.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

# Reviewer 1:

The project has made good progress thus far and the reviewer encouraged continuation of several of the ongoing efforts. For the Sandia National Laboratories (SNL) mixed-mode/SI work, the reviewer said that, in addition to lower RON fuels, the impact of low MON should also be investigated to determine the effect on load range. As CR is increased for enabling both ACI modes and efficient SI combustion, engine operating conditions under high-speed, high load conditions with hot intake air temperatures may be closer to MON operation. For the Argonne National Laboratory (ANL) multimode work, the reviewer suggested that as new fuel properties are determined/defined that enable ACI operation, care should be taken that in a multimode engine, the same fuel needs to be used for high-load SI combustion as well.

While the scope of work is limited to low technology readiness levels (TRLs), the reviewer asserted that the project should keep practical considerations such as aftertreatment requirements and transient controls in mind while analyzing results and assessing the feasibility of the combustion concepts being proposed.

#### Reviewer 2:

The reviewer found that adding lower RON fuels to the test matrix is encouraging as are expanding efforts on load transients, start studies on cold-start effects, and developing and validating a CFD approach for lean SI combustion. The reviewer had questions about what the major factors would be to validate in lean SI engine simulation, and what kinds of parameters to consider to identify influential fuel properties for multimode ACI operation. Some of the tasks seem to be tough to achieve, e.g., to identify/define new fuel properties that impact engine performance under ACI operation with the nine fuels considered. But the reviewer still encourages these efforts.

#### **Reviewer 3:**

The reviewer remarked that it is highly important to conduct transient work (at least snap throttles at various speeds) to study the transition between ACI and SI, which will be at different CRs. This work is critical for OEMs to adopt this technology. The reviewer noted that the controls work is non-trivial; it is very important that there is a gentle transition between the regimes without noise, vibration, and harshness and/or misfiring/knocking events. In addition, the emissions characteristics during the transients will be important for certification.

Question 5: Relevance-Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer commented that achieving the tasks suggested for future research would definitely support the DOE objectives for several reasons: knowing ways to improve ACI operation model will be possible; developing optimal fuels for specific engine operation mode will be possible; and understanding what the major limiting factors/road blocks are in improving gasoline engine efficiency in ACI/SI mode will be possible.

# Reviewer 2:

The reviewer stated that the investigations being undertaken as part of this project are in line with the overall DOE goal of petroleum displacement.

#### **Reviewer 3:**

The reviewer affirmed that this project is highly critical to the Co-Optima goals and the DOE objectives in general.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

According to the reviewer, the FY 2018 budget looks sufficient for the different tasks proposed in the project.

#### Reviewer 2:

The reviewer found the funding to be sufficient for the proposed work.

# Reviewer 3:

Experimental resources seemed to be enough to the reviewer to perform the suggested tasks. However, the reaction mechanisms and fuel properties prediction model are mature enough to be reliably used in multi-component fuel CFD modeling.

### Presentation Number: ft056 Presentation Title: Co-Optima— Mixing—Controlled and Kinetically-Controlled Compression Ignition Combustion Principal Investigator: Charles Mueller (Sandia National Laboratories)

### **Presenter** Charles Mueller, Sandia National Laboratories

# **Reviewer Sample Size** A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer stated that the project is very well designed using multiple diagnostic and simulation tools for an in-depth understanding of fuel spray and mixing controlled compression ignition.

### Reviewer 2:

The reviewer found the project to be well-designed and well-planned.

### Reviewer 3:

According to the reviewer, this presentation did a very good job of showing how the different experimental programs within Co-Optima fit together

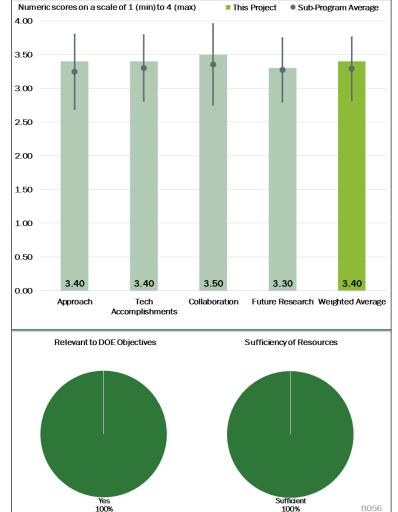


Figure 5-7 - Presentation Number: ft056 Presentation Title: Co-Optima-Mixing-Controlled and Kinetically-Controlled Compression Ignition Combustion Principal Investigator: Charles Mueller (Sandia National Laboratories)

to cover the overall objectives of the program. The reviewer stated that it was an excellent presentation, but it will be difficult to offer detailed comments about any of the projects covered because they were covered at such a high level.

### Reviewer 4:

It was obvious to the reviewer that trying to pack five projects into one review is too much. Generally, what could be conveyed in the review time showed that most of the projects have a good approach. The reviewer noted that the Advanced Compression Ignition: Fuel Effects (ACI-F) project seems tightly aligned with LD, while the MCCI project seems aligned with HD, and the spray projects are cross-cutting. The reviewer trusted that each project is coordinating with industry input to help guide the approach with respect to relevant industry constraints, but with a future-looking orientation.

### **Reviewer 5:**

The reviewer commented that the studies in the individual tasks are generally good and are addressing various technical barriers. However, the reviewer described the overall project as somewhat messy. It seemed to this

reviewer that the goal is to look at fundamental spray/fuel interactions and then how that process ends up impacting the combustion process. It is not clearly linked as presented, and it seemed to the reviewer as if there is just too much going on in too many directions. The reviewer expressed some concern that the projects will end up going in different directions without consistent datasets that we can use to derive lessons that will help with development of future engines or fuels.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

The reviewer praised the overall progress of the individual projects as excellent, and indeed it appeared to the reviewer to be contributing to the objectives of Co-Optima relative to the effects that fuel characteristics can have on the various phenomena associated with engine operation.

### Reviewer 2:

The reviewer commented that the principal investigators (PIs) have made excellent progresses on all subtasks. The mixing controlled combustion (ducted fuel injection [DFI]) is quite interesting, but the reviewer was not sure how to implement it on ICEs. Hopefully, the PI can come up with a solution.

### **Reviewer 3:**

The reviewer said that the liquid extinction images of two fuels show very distinct differences in spray structure and penetration. The explanation that this is based on distillation effects might not be complete because the two fuels could have very different surface tensions and viscosities, which will lead to atomization and resulting droplet sizes.

### Reviewer 4:

The reviewer summarized and commented on the technical Accomplishments for ACI-F as follows: According to the milestones, this project seemed to be on task and doing well. The work seems very detailed and thorough. The reviewer believed that the use of very high intake-manifold temperatures is for kinetic understanding and less about engine operation performance. Using relevant engine conditions for kinetic validation and development is extremely good. Many times, kinetic models are validated with conditions that are just not relevant to today's engine states. The reviewer requested that the project team is sure that the conditions used in this work are aligned well with high power density engines for best use across industries and markets.

Regarding the technical accomplishments for MCCI, the reviewer reported that these are some of the most interesting and potentially breakthrough work in the DOE portfolio. These accomplishments have the potential to disrupt the NO<sub>x</sub>-soot trade-off and shift energy and commercial sectors. Progress seems to be moving towards in-engine understanding with the optical engine experiments and in-cylinder soot quantification. If this is going to be disruptive, the reviewer said that an enormous amount of work needs to happen regarding design parameters, sensitivities, durability, fuel effects, deposits, materials, and thermal/mechanical fatigue. Validation of many things needs to happen before this goes to production.

According to the reviewer, mixing controlled combustion is dominant and will not be displaced by KC combustion concepts for a multitude of technical, scientific, and economic reasons. More DOE effort needs to be pushed towards mixing controlled combustion system scientific understanding, computational modeling, and technology generation. The reviewer urged the project team continue strong support of this DFI project and consider increasing the budget and scope. It was refreshing to the reviewer to see MCCI technology work because ACI has been a focus for a very, very long time.

Regarding the technical accomplishments for spray/combustion—optical imaging (SCO), the reviewer pointed out that the milestone chart says things are pending so it seems that this is a little behind. This fundamental spray work helps everyone in engine combustion because sprays are the starting point for today's fuel-air

mixtures. The building of a new, high-flow vessel is no simple task. The reviewer found this new capability to be excellent because it allows for high temperatures and pressures to be achieved, which are needed to be relevant to today's high-power density engines. It was good progress.

As far as technical accomplishments for the Sprays: X-ray Imaging (SX) project, the reviewer remarked that again, this spray-related project is making good progress. It is no small task to get functioning sprays at relevant boundary conditions for high-fidelity imaging. The reviewer suggested considering allocating more funding to help upgrade the X-ray spray capability and asked if putting a combustion vessel at the X-ray facility has been considered.

Regarding the technical accomplishments for the Sprays: Simulation (SS) project, the reviewer had difficulty assessing progress for this project, but getting better thermo-physical properties into three-dimension (3-D) CFD combustion simulations is outstanding. This is a real gap in present simulation codes used within industry, specifically concerning the fuel and spray processes. The reviewer encouraged the team to continue and to make sure that code or sub-models that are developed can be integrated by the industry into relevant CFD codes.

The reviewer was not sure about DOE's playbook on intellectual property and commercialization in this software/model/code area. The reviewer wanted to know if these code developments are open source and whether DOE or the laboratories wish to monetize the output of these simulation products. The reviewer asked if there is a guideline on how these things will happen because taxpayer dollars are used to develop these simulation tools. The reviewer was thinking about the path that the Lawrence Livermore National Laboratory (LLNL) Zero-RK is taking and was not sure if industry could obtain the better chemistry solver for their own use.

### **Reviewer 5:**

The reviewer stated that there appears to be decent progress on activities in all of the tasks, but it was completely unclear what work is connected to Co-Optima as compared to other work. For ACI-F, the same results were presented both as Co-Optima results as well as results from the combustion activity funding. The reviewer wanted to know what work is actually related to Co-Optima and whether it is distinct in some way from the combustion funding. Also, the reviewer inquired whether the fuels investigated here are consistent with those from the SI and mixed-mode Co-Optima tasks. Another question from the reviewer dealt with knowing if there is more definition of the fuel properties and chemistry available as the reviewer could not really tell from the material presented.

For the MCCI work, the DFI is technically interesting, but it did not seem to the reviewer at all related to Co-Optima at present. From a practical standpoint, it also seems very problematic for durable manufacturing; small features like this in the combustion chamber tend to erode and break under the thermal and mechanical stresses of combustion. It seemed to the reviewer as if this work should be funded elsewhere in the DOE and should step back to consider some basic mechanical and thermal issues before going forward with combustion development.

The SCO work was quite interesting to the reviewer, who wanted to see more focus in this area; there have been questions on how biofuels and other non-conventional fuels behave in sprays for decades, and this is something that ought to be understandable with today's diagnostics and simulation tools The reviewer would argue that the spray work should be the biggest part of this task right now, and the engine combustion work should be used primarily to generate data for comparison and framing of the spray studies. Once we understand the spray better, more effort can be put into the combustion systems.

As for the SX, the reviewer said that it coordinates well with the SCO work and the same comments apply. The reviewer remarked that it would be good to know how the SS work integrates with/coordinates

with/duplicates the other modeling tasks funded through the VTO. It was difficult for the reviewer to tell what is different here from what we saw in other presentations from the VTO modeling teams.

Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

The reviewer found very impressive collaboration among the different laboratories and the stakeholder industries.

### Reviewer 2:

The reviewer said there was outstanding collaboration with OEMs, universities, and among national laboratories.

### **Reviewer 3:**

Collaboration seemed excellent to the reviewer, who commented that there was enough collaboration to have one PI present five projects worth of material so that seems to be good justification. Also, much of this research is regularly seen at other review presentations with good discussion and engagement.

### **Reviewer 4:**

The reviewer remarked that there was good collaboration, and the partners participate and are well coordinated.

### **Reviewer 5:**

It was not clear to the reviewer that there is really any coordination across the project team; the studies do not seem particularly supportive of each other or building on each other. In general, the reviewer stated that the various Co-Optima thrusts appear to be doing a lot of overlapping work that could be better integrated and coordinated.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

According to the reviewer, the future work is planned in a logical manner to realize the proposed targets; there are no major risks.

### Reviewer 2:

The plan seemed effective to the reviewer.

### **Reviewer 3:**

It was difficult for the reviewer to answer questions like this because the presentation covered multiple projects at a very high level. It seemed to the reviewer that the projects are being effectively carried out and the planned future work addresses the important barriers.

### **Reviewer 4:**

The reviewer had no problems concerning proposed future research for four of the five projects as they are either fundamental, cross cutting, or potentially disruptive. The ACI-F project seemed well-aligned with the Co-Optima LD focus, but the reviewer was very unsure that ACI has a significant place in future engines regardless of the market or class of engine. It seemed to the reviewer that the LD OEMs have pushed for a fuel that is optimal for boosted SI and ACI, which may be too near-term in focus and potentially dictating physics. As the power system for transportation changes, the reviewer opined that there are continued, non-combustion technologies eroding the area of opportunity for ACI. The reviewer urged continuing research towards a

future-looking state, but with active industry engagement about the entire power system constraints. Engines will be turned off or only operated at the most efficient location. There are many things that interact with combustion, and ACI needs fully accounting for these likely future interactions. According to the reviewer, a good example is that once electrification, hybridization, and near-zero NO<sub>x</sub> emissions regulations come into place, ACI must provide a more efficient, lower cost, as capable, and synergistic solution than other combustion concepts in order to be viable.

### **Reviewer 5:**

The reviewer liked the overall plans for the SCO and SX tasks; using these diagnostics to dive into how these new fuels behave in sprays and what that does to mixture formation is fundamental and essential to the codevelopment of fuels and engines. The two engine tasks (ACI-F and MCCI) seem weakly planned. It was unclear to the reviewer how the ACI-F task is unique compared to the boosted SI and mixed mode work being performed, and it seemed overly split between some fuel testing and working on surrogate mechanisms that the reviewer would have expected to be an LLNL activity. The MCCI task seems to have too much focus on DFI in the future plans. If understanding how to co-develop a mixing controlled combustion system with new fuels is wanted, the reviewer suggested starting without something like DFI and fully understanding how the fuels interact with more conventional combustion system design variables, while the DFI is more fundamentally investigated outside of Co-Optima. Subsequently, it can be determined how and why it works and whether it actually could be made in production-robust way.

Question 5: Relevance-Does this project support the overall DOE objectives?

### Reviewer 1:

The reviewer commented that an in-depth understanding of fuel spray is crucial for co-optimizing fuels and engines. The project is well-aligned with the goals of Co-Optima program and definitely supports the overall DOE objectives.

### Reviewer 2:

The reviewer affirmed that all of these projects support the DOE initiative of reducing energy consumption through various fundamental understanding or new technologies.

### **Reviewer 3:**

The reviewer responded that the project can potentially achieve the DOE goals of Co-Optima.

### **Reviewer 4:**

While the project does support DOE objectives, it also seemed to the reviewer to overlap too much with other DOE VTO funding for the combustion programs, and it does not seem to be pushing in directions that could significantly impact industry ability to make use of the co-optimization idea. The more fundamental spray work is really good for addressing the objectives, but the reviewer stated that the engine-level work just does not look as if it will do much for meeting the objectives.

### **Reviewer 5:**

The reviewer referenced prior comments.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

The reviewer said that these projects seem sufficiently funded and any specific differences were commented on in the Technical Progress section.

### Reviewer 2:

According to the reviewer, there are sufficient resources to achieve the stated milestones.

### Reviewer 3:

The reviewer remarked that the team members have sufficient resources.

### **Reviewer 4:**

At a high level, the reviewer commented that the budget for the project is good. The reviewer would prefer having seen the funding moved more towards the fundamental side for now and later bias it more towards the engine work once the fundamentals are better understood.

### **Reviewer 5:**

Funding seemed sufficient to the reviewer, who was surprised that the presenter did not comment on the significant cut in the funding of his DFI project. The reviewer could not imagine that budget cut did not have an impact on his activities.

### Presentation Number: ft057 Presentation Title: Co-Optima— Emissions, Emission Control, and Spray Research Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

Presenter Josh Pihl, Oak Ridge National Laboratory

**Reviewer Sample Size** A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer remarked that the project is a good blend of diverse analyses: Cold start/light-off, fuel composition, engine modes, PM and hydrocarbon (HC) considerations, engine variety, and others.

### Reviewer 2:

The reviewer commented that the approach to the overall characterization of the impact of fuels on engine performance and emissions is completely in line with the Co-Optima program.

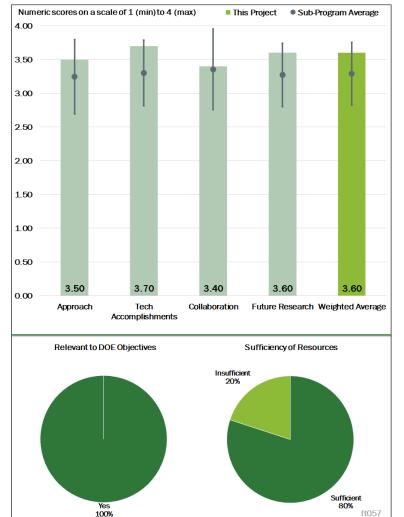


Figure 5-8 - Presentation Number: ft057 Presentation Title: Co-Optima— Emissions, Emission Control, and Spray Research Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

### Reviewer 3:

The reviewer said that the project is reasonably designed and planned.

### **Reviewer 4:**

The reviewer pointed out that the approach for the four issues addressed for particulates and gas phase HC species is very developed and being carried out very broadly as this is just a summary of several projects. The role of oxygenates is important to pursue as they appear to be constants for the future in fuels. And in general, one cannot sell a vehicle without meeting the emissions standards for that vehicle, so this research is very critical for looking at new fuel compositions.

### **Reviewer 5:**

The reviewer observed five projects gathered into one presentation, which is difficult to review in its present form. The reviewer stated that the approach is actually gathering a range of ideas and seeing which one hits a button. Nothing in these projects indicates the actual source of soot from various engine combustion technologies. The reviewer commented that the presentation is overflowing with initial speak, which shortens the presentation, but assumes that everyone knows the initial speak. That is not true.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

The reviewer noted that the project has made excellent progress and appears well on track. Slides 4 and 5 demonstrate the progress while highlighting the remaining steps further backed by the Future Work on Slide 14. Comparing accomplishments to the remaining (future) work, the reviewer noticed the marked project progress.

### Reviewer 2:

It seems early in this effort, but the reviewer saw notable results here, especially in the role of fuel alcohols. Excellent work has been done on particulate formation and the effort to see direct emissions impacts of fuel changes is closer.

### **Reviewer 3:**

The proposed tasks in each of the projects have been completed or are being completed.

### Reviewer 4:

The reviewer expressed concern about undervaluing the accomplishments of the five different projects crammed into this one presentation. The reviewer thought that the PI did an admirable job of speaking as fast as he could to give the reviewers a snapshot of each of the five elements, but the reviewer thought it is a mistake to try to incorporate this many projects into a single talk.

The only thing that such a setup did was to highlight the strong collaborative nature of the Co-Optima program, which is evident in the way the PI could seamlessly move through the projects. That indicated to the reviewer a high level of familiarity with all of the work, which can only come from regular communication. Kudos to the large team for that.

### **Reviewer 5:**

The reviewer said that it would be a very good idea to develop correlative models to link the yield sooting index (YSI) and PMI to make use of the benefits of both soot indicators. It would also be an excellent idea to expand YSI prediction to the prediction of thermo-physical properties, which are important data needed in the engine spray and combustion computations and optimization.

### Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

The reviewer saw evidence of excellent collaboration across the national laboratories and commented that it must be an amazing challenge to coordinate teleconferences and meetings. Kudos to the team.

### Reviewer 2:

The reviewer stated that collaboration exists; the partners are fairly well coordinated.

### Reviewer 3:

It was not clear to the reviewer how tightly integrated the projects actually are; however, much needed information exchange among the partners should actually be happening. The reviewer wished that presentations like this were made available to the "at large" community.

### **Reviewer 4:**

The reviewer found good to excellent collaboration among existing partners at national laboratories and universities. Including catalyst manufacturers is more important at this point in the project. The reviewer mentioned that the 2017 comments addressed this issue, but the evidence for more involvement in this

direction is not clear among the 145 individuals from 86 organizations mentioned as collaborators. A few examples would have been useful outside the national laboratory and university areas.

### **Reviewer 5:**

The reviewer indicated that there is no shortage of collaboration in this project: It integrates several national laboratories, various universities, and other organizations and stakeholders. Not much information, however, was made available on coordination, planning, and execution or allocation of roles and responsibilities. Given such a large mass of investigators across the many organizations involved, the reviewer wondered how effectively coordination and communication are structured. Information in Slide 27 is too basic to clarify such a picture.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

It seemed to the reviewer that there was some cross fertilization among the projects, which the reviewer strongly encouraged. The reviewer believed that the more cross fertilization, the higher likelihood of success.

### Reviewer 2:

The reviewer said that the proposed future research is in areas where needs exist that have been identified in the results thus far. The impact of the emissions work with LT catalysts may have the broadest impact.

### **Reviewer 3:**

The reviewer noted that clear and dynamic synergy appears to exist between the progress made to date and the listed future work. Future tasks are targeted at existing challenges or obstacles while they are aligned with the project's main goals and objectives.

#### **Reviewer 4:**

The plan seemed effective to the reviewer.

### **Reviewer 5:**

The reviewer asserted that a complete evaluation of the project was hard because there was so much crammed into this talk. The reviewer thought that it is completely unreasonable to cover five projects in a single talk; they should be separated, even if it extends the AMR. It was impossible to give valuable feedback when the PI zoomed through at a "drug commercial disclaimer" pace.

Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer indicated that this project clearly is aimed directly at fuel-economy improvements being identified from different fuel blends along with making sure that any results are evaluated from the point of view of the entire vehicle.

#### Reviewer 2:

Given its consistent focus on the program objective (e.g., PMI, developing predictive capabilities, impact on emissions, etc.), the reviewer noted that the project clearly continues to support DOE funding for this purpose.

### **Reviewer 3:**

Though the reviewer strongly questioned the rational design behind the Co-Optima effort, this project does indeed support DOE objectives.

Reviewer 4:

The project can potentially achieve the DOE goal of Co-Optima.

Reviewer 5:

The reviewer responded that the project probably supports DOE's objectives and wished that there was convincing information about the active communication among the projects.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

**Reviewer 1**: The reviewer stated that funding is insufficient if it is preventing collaborative work.

Reviewer 2:

The reviewer said that the breadth of research collaborations has provided the level of support that is sufficient.

Reviewer 3:

The reviewer pointed out that 9 DOE national laboratories and 13 universities ae involved; there is no shortage of resources.

Reviewer 4:

The team members have sufficient resources, according to the reviewer.

Reviewer 5:

Resources seemed sufficient to the reviewer.

### Presentation Number: ft062 Presentation Title: Characterization of Biomass-Based Fuels and Fuel Blends for Low-Emission, Advanced Compression Ignition Engines (Co-Optima) Principal Investigator: Ajay Agrawal

(University of Alabama)

**Presenter** Ajay Agrawal, University of Alabama

**Reviewer Sample Size** A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer remarked that the plan for addressing the technical barriers is sound. In particular, using simultaneous diagnostics, including the innovative rainbow schlieren technique, will provide unique data that will add value to the understanding of fuel sprays. While the current operating conditions are not representative of the entire engine operating range, they are in a relevant range.

### Reviewer 2:

For the last year, the reviewer noted that the PI set up the experimental and

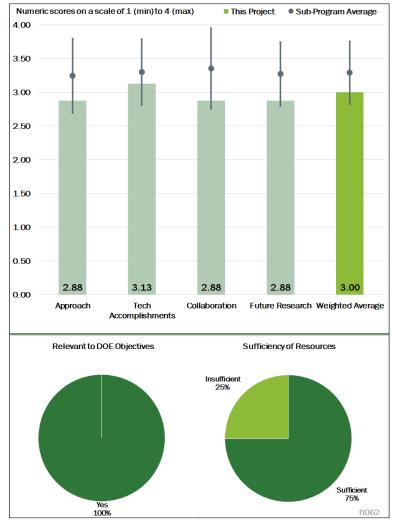


Figure 5-9 - Presentation Number: ft062 Presentation Title: Characterization of Biomass-Based Fuels and Fuel Blends for Low-Emission, Advanced Compression Ignition Engines (Co-Optima) Principal Investigator: Ajay Agrawal (University of Alabama)

modeling frame. The combination of several optical diagnostics, advanced statistics, and process modeling is feasible.

### **Reviewer 3:**

The reviewer opined that the rainbow schlieren deflectometry might be able to provide more information, but the reviewer was not sure what additional knowledge it can provide compared to conventional schlieren. The model developed by neural network is a black box. It really does not help better understand the physics of fuel spray and combustion.

### **Reviewer 4:**

The reviewer stated that the approach to this work is okay. The optical diagnostics seem good and understanding how the rainbow schlieren can be applied to combusting sprays will be interesting. According to the reviewer, an area that needs improvement is how the experiments are going to be relevant and linked to Leaner lifted flame combustion (LLFC). The connection between bio-based fuel blends and LLFC was not entirely clear to the reviewer, who suggested that that could be really laid out for better understanding of the

validity of the approach. It seemed to the reviewer that this connection relies on the impact of a bio-based fuel to the supercriticality of the spray. The reviewer wanted to know whether a supercritical fuel spray enables LLFC better. LLFC is mixing controlled, and in the limit, mixing-controlled combustion can be modeled or related to dense gas jets (which are therefore dense fluid mixing and "supercritical"). Additionally, the reviewer said that supercritical states are better achieved with higher pressures and temperatures. The new constant-flow vessel may not be able to achieve relevant pressure and temperatures (+100 bar, +950 K). The approach of the project may produce data and empirical models for irrelevant boundary conditions. The reviewer saw this as a major concern with the new vessel and project approach. An alternative approach may be to take the diagnostics to a different vessel that can achieve the relevant pressures and temperatures.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

The reviewer commented that the project has made significant progress to date. Establishing the rainbow schlieren technique has been completed and shown to provide insightful data for fuel sprays. Shake-down of the simultaneous diagnostics has provided good baseline data and looks almost ready for implementation in the spray chamber. Based on the original plan, the reviewer said that the program is progressing well.

### Reviewer 2:

The reviewer found that preliminary results show that the team is on track to achieving project goals. The rainbow schlieren method produced promising results. The reviewer looked forward to the next year to learning more about quantitative measurements.

### **Reviewer 3:**

The reviewer reported that there has been good progress in setting up the experiments to study fuel spray and combustion.

#### **Reviewer 4:**

The reviewer observed that progress on the project seemed to be good. Building a new vessel and setting up optical diagnostics is a fairly good-sized task. The concern the reviewer had is that the success criteria for the vessel and realistic capability may be poorly defined. Again, the reviewer questioned whether relevant temperatures and pressures can be achieved. Industry experience says that getting a flow-through vessel up to +100 bar and +950 K may take significant time and money.

Question 3: Collaboration and Coordination Across Project Team.

#### Reviewer 1:

The reviewer remarked that the results show good collaboration and coordination with the national laboratory partners.

#### Reviewer 2:

According to the reviewer, good collaboration has been established with the national laboratories.

#### **Reviewer 3:**

The reviewer indicated that the collaboration on this project is satisfactory, mainly because there could be significant leveraging from others working with flow-through vessels and optical diagnostics within Co-Optima. The reviewer urged reaching out to SNL more for their experiences with newly built flow-through vessels and continuing to coordinate with LLNL and ANL on the neural-net modeling.

### **Reviewer 4:**

The reviewer found collaboration with Sandia (Mueller and Pickett) to be a good start, and future coordination with modeling teams at Argonne will be good. In particular, it will be interesting to see if the rainbow

schlieren technique provides unique data for model comparison that other techniques that are currently used by the Engine Combustion Network (ECN) do not. The reviewer encouraged more engagement with simulation teams, as that is a clear plan for how to compare the experimental results and the simulation. Work with the ECN should partially facilitate this, but as the ECN is not focused on fuel blends, other ways of engaging should be considered for the Year 3 work in particular.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

The reviewer indicated that the planned future work is logical and builds on the preliminary results shown during the presentation. The research team showed awareness of the difficulties ahead for both the experimental and modeling tasks and planned for them.

### Reviewer 2:

The future work sounded okay to the reviewer. Being able to evaluate many bio-based fuels in the context of LLFC is good. Alignment to supercriticality, mixing, and LLFC needs further thought. The reviewer urged considering adding decision points about how the project will need to change if relevant pressures and temperatures cannot be achieved in this flow-through vessel.

### **Reviewer 3:**

The reviewer suggested stopping neural-network based modeling, which is trivial using the toolbox in MATLAB. The model is not going to help us better understand the correlations between fuel properties and combustion properties. The reviewer wanted to see more attention paid to understanding the fundamental physics of spray combustion and recommended that the PI develop a methodology to get valuable information out of rainbow schlieren deflectometry.

### **Reviewer 4:**

The reviewer indicated that the future experimental work plan is very strong and the PIs have laid out a clear path for the experiments. The future work with the modeling is slightly less clear to the reviewer; in particular, it was not exactly clear what value the neural-network modeling would add beyond analysis of a given dataset and how it could be used to either gain deeper understanding or advance the state of the art. This is particularly true given that no physics are built into the neural network as it currently stands. The reviewer urged that the PIs should strengthen the neural-network modeling component in future work and identify where this contribution can be unique as compared to other data-analysis and modeling approaches.

Question 5: Relevance—Does this project support the overall DOE objectives?

### Reviewer 1:

The reviewer commented that the project is part of DOE's effort to develop ACI ICEs. The novelty is the combination of three different optical diagnostics is better understanding of fuel-spray characteristics and fuel-composition effects.

#### Reviewer 2:

The reviewer remarked that the work on this project directly addresses DOE barriers in the areas of advanced combustion and fuel sprays. The Year 3 work will also address barriers related to co-optimization of fuels and engines.

#### **Reviewer 3:**

According to the reviewer, understanding spray and combustion of biomass-based fuels and fuel blends is important to co-optimize fuels and engines. It supports the overall DOE objectives.

### **Reviewer 4:**

The reviewer affirmed that this project supports the DOE goals of energy security and increased efficiency with bio-based fuels.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

In the reviewer's opinion, this project is vastly underfunded. Increasing the new flow-through vessel's pressure and temperature capability will take much more money and resources. The reviewer urged considering increasing funding or changing the approach

### Reviewer 2:

The reviewer asserted that the PI showed excellent results for the funding received until now. The reason seems to be that the project benefitted from the work previously done by the PIs on the topic and the good facilities at the University of Alabama.

### **Reviewer 3:**

The reviewer stated that there are sufficient resources to achieve the stated milestones.

### **Reviewer 4:**

The reviewer commented that the milestones to date have been met in a timely fashion and the PIs seem to have the required experimental resources to do the proposed work. The issue of a higher pressure facility was raised and the PIs are currently upgrading the facility; however, the resources to go beyond the current plan do not exist. The reviewer remarked that this does not, however, impede the PIs from obtaining new and useful data in the remainder of the project.

### Presentation Number: ft063 Presentation Title: Micro-Liter Fuel Characterization and Property Prediction (Co-Optima) Principal Investigator: Ingmar Schoegl (Louisiana State University)

Presenter Ingmar Schoegl, Louisiana State University

**Reviewer Sample Size** A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

With regard to screening fuels reasonably quickly and with consistency, the reviewer remarked that the micro-flow reactor appears advantageous as it enables measurement access. The team members and collaborators are quite strong.

### Reviewer 2:

If it can be successfully developed, the reviewer stated that this will be an important capability for Co-Optima. The researchers' approach to achieving this goal is well laid-out and is correctly focused on the most important

conditions for which engine-relevant data are needed.

### **Reviewer 3:**

The reviewer said that the project is using an innovative approach based on a micro-flow reactor to enable fuel characterization using micro-liter quantities. If successful, the technique would facilitate characterization of fuel components in early stages of development when only small quantities are available. Additionally, the reviewer suggested that the technique has the potential to enable automated testing for multiple samples, thereby allowing a high throughput.

As described, the reviewer opined that the technique should be able to generate data on laminar flame speed and impact of dilution (air/EGR) on combustion. However, it was not yet evident to the reviewer how ignition delay, RON, MON, and sensitivity will be determined. It was also unclear to the reviewer how any ignitiondelay measurements made using this technique will be compared to ignition-delay measurements from RCMs and shock tubes.

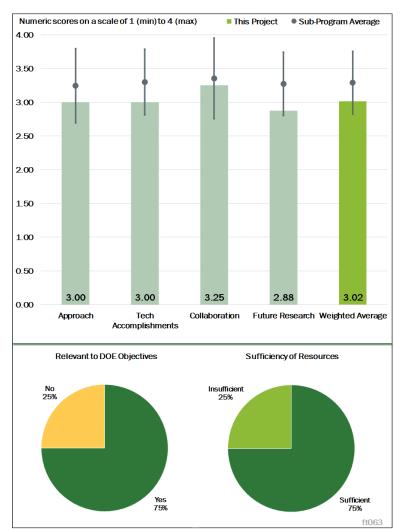


Figure 5-10 - Presentation Number: ft063 Presentation Title: Micro-Liter

Fuel Characterization and Property Prediction (Co-Optima) Principal

Investigator: Ingmar Schoegl (Louisiana State University)

Key technical barriers have been identified and are being actively pursued, which is critical for success. The reviewer expected that next year's update will provide a clearer picture of the capabilities and limitations of the proposed technique (e.g., low and high vapor-pressure fuels). While there are uncertainties and multiple technical barriers, the reviewer remarked that the proposed technique shows a lot of promise.

### Reviewer 4:

The reviewer remarked that this is an untested procedure and the chances of success seem just fair. The small size of the reactor maximizes contributions from surface reactions, which may lead to faster or slower burn rates than what actually occurs in engines. According to the reviewer, a key parameter is the surface-to-volume ratio. An appropriate test procedure should be carried out with different configurations for reactors.

The reviewer noticed another issue to be evaluated is to control the size of the droplets because the liquid has to evaporate completely before burning. Different droplet sizes should be experimentally tested. The reviewer inquired about how long complete burning takes under any given set of conditions (tube diameter, droplet size, temperature, pressure).

According to the reviewer, experimental conditions need to be clarified and specified, especially temperature and pressure, with the smallest possible uncertainty. These uncertainties have to be understood and quantified because they will be propagated during the simulation phase. Otherwise, the reviewer suspected that it will be challenging to make decisions based on the data that will be derived from these experiments. The 3-year period might not be long enough to develop a reliable and standardized methodology.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

While the project has only completed its first year, the reviewer summarized the good progress made in development of the proposed technique: apparatus modifications and upgrades to enable testing at 10 bar with work underway to extend the capability to 30 bar; implementation of thin-filament pyrometry to enable temperature measurements along the length of the tube; preliminary results from experiments investigating the impact of flow velocity, equivalence ratio, pressure, and fuel composition; and the successful demonstration of nanoliter fuel delivery. The project is making good progress and is currently on track.

### Reviewer 2:

The reviewer observed good progress for a project underway for little over a year: a number of key improvements to the experiment system have been made; pressure effects have been determined; and data generation on reference fuels has progressed

### **Reviewer 3:**

The reviewer said that the program is just completing its first year. The progress is good and is encouraging. There is a long way to go, but at this time, success appears likely.

### **Reviewer 4:**

The reviewer pointed out that on Slide 5 on the presentation, the milestone M1.2 should be covering the limits of pressure and temperature (range of pressures including lower and upper limits) at which combustion occurs inside the micro-reactor. At some point, the success and failure of this micro-reactor has to be fully understood when it comes to operating conditions. Milestone M1.2 seemed incomplete for the former reason to the reviewer. Consequently, the reviewer suggested that M1.4 should be re-explored for a set of test results that really cover the relevant metrics because these metrics have not been truly examined and specified.

Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

The reviewer said that the project is demonstrating progress because of its collaborative efforts.

### Reviewer 2:

The reviewer saw the project as a highly collaborative part of the Co-Optima team.

### Reviewer 3:

The reviewer commented that the PI is working closely with national laboratory collaborators as well as subcontractors.

### **Reviewer 4:**

The reviewer indicated that the team should have access to databases that cover engine testing and performance. The level of collaboration needs to be expanded, for example, to include work from the American Society of Testing Materials and the American Petroleum Institute.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

The reviewer pointed out that the principal focus of future work is to develop the capability to operate the measurement system at engine-relevant temperatures and pressures. The reviewer agreed that this is the most important objective to pursue.

### Reviewer 2:

According to the reviewer, the proposed research is in line with the goals of the project and aimed at addressing the technical barriers that have been identified.

### Reviewer 3:

The reviewer noted that the research plan is okay but it would appear to need to move more quickly to have significant impact and relevance in the overall Co-Optima fuel assessment.

### **Reviewer 4:**

The reviewer stated that the technical needs to make this project successful are underestimated. Ignition delay measurements from Texas A&M University were referenced out of nowhere on Slide 21 of the presentation, which prompted this reviewer to ask how these measurements overlap with the current micro-reactor program. The relationship between ignition delay and the rate constants is significantly more complex. This reviewer further requested that chemical reactions are properly written (i.e.,  $A+B \rightarrow C+D$ ). Initial qualitative results are uncertain and need estimates for error limits, according to this reviewer, who emphasized the need for effective experimental parameters and instrumentation design.

Question 5: Relevance—Does this project support the overall DOE objectives?

### Reviewer 1:

For effective assessment of potential new fuels or fuel components, the reviewer said that it will be important to be able to determine their engine relevant characteristics: RON and sensitivity, for example. If successfully developed, the reviewer stated that this system would allow such measurements to be made for very small test samples of candidate fuels.

### Reviewer 2:

At the current stage of the study, the reviewer commented that the results are very preliminary and have not been compared with other analogous measurements and procedures for validation purposes. On the other hand, the reviewer exclaimed that the idea of utilizing micro-liter reactors for fuel testing has interesting possibilities.

### **Reviewer 3:**

The reviewer noted that the development of micro-liter fuel characterization is not only relevant to Co-Optima but for fuel studies in general.

### Reviewer 4:

The reviewer commented that a couple of years ago, a high-throughput, small-sample assessment method appeared important and potentially useful in contrast to other types of fuel-screening combustion vessels. The number of fuel permutations does not seem all that many at this time. Other methods, including detailed chemical and structure analysis, may give more informative results on performance and emissions tendencies. The reviewer indicated that the best screening method for engines is to use the engine.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

According to the reviewer, experience shows that the development of a new standardized procedure will require much larger resources that those initially anticipated.

### Reviewer 2:

The reviewer reported that there are numerous contributors and advisors to the core team. This helps with the overall resource needs.

### **Reviewer 3:**

The reviewer mentioned that resources appear to be sufficient for the proposed scope of the project.

### **Reviewer 4:**

It appeared to the reviewer that the program has sufficient funding.

### Presentation Number: ft064 Presentation Title: The Development of Yield-Based Sooting Tendency Measurements and Modeling to Enable Advanced Combustion Fuels (Co-Optima) Principal Investigator: Charles McEnally (Yale University)

Presenter Charles McEnally, Yale University

Reviewer Sample Size A total of six reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The reviewer commented that the approach to do the two-dimensional simulation appears very appropriate and, with the interaction from other laboratories and universities, leads to useful results for other laboratories to use in their Co-Optima work. Providing a source of understanding to a range of people using these results is an excellent way to begin this work. The reviewer noted that having a database of over 400 compounds available is itself a major initial effort that is very beneficial to include.

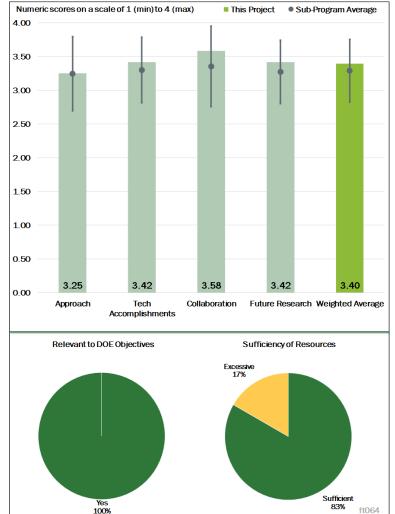


Figure 5-11 - Presentation Number: ft064 Presentation Title: The Development of Yield-Based Sooting Tendency Measurements and Modeling to Enable Advanced Combustion Fuels (Co-Optima) Principal Investigator: Charles McEnally (Yale University)

### Reviewer 2:

The reviewer remarked that the investigators used a first-principles approach, a blend of know-how from authentic published literature, expertise from national laboratories, experimentalists and computationalists, and fundamentals of diffusion-flame and fuel chemistry. The speaker also did an excellent job presenting the work and answering all of the questions with well-rounded answers.

### Reviewer 3:

The reviewer opined that YSI is likely going to be a more precise metric for screening fuels. The two main advantages are the ease of measurement and the low volumes required. Two things the reviewer perceived were missing from the approach was a strategy to deal with fuels beyond the "bookends" of n-heptane and toluene, and no discussion of blend effects. For example, the reviewer wanted to know what happens to YSI of a 50:50 blend of toluene:n-heptane. The reviewer asked if it is dominated by the high YSI component. There needs to be more investigation of the blend effects and core Co-Optima fuels, according to the reviewer.

### **Reviewer 4:**

For the experimental YSI approach, the reviewer referenced a great question raised by one of the reviewers, which inquired about using hydrogen  $(H_2)$  in a nitrogen gas  $(N_2)$  fuel for the flame so that all carbon would be from the doped fuel?" The reviewed commented that there was not a satisfactory answer given (lack of time, perhaps) and that it would have been nice to see this addressed. Additionally, the reviewer wanted to know why the values for equations 1 and 2 (Slide 7) are defined as such. The reviewer said the approach YSI simulations seem to be well done, and opined that considering the number of components in standard pump gasoline and diesel fuels, calling 400 compounds a "comprehensive" database (Slide 9) is a bit much.

### **Reviewer 5:**

The reviewed stated that the approach of the project is highly fundamental for application to engine work. It was unclear to the reviewer how the YSI evaluation for atmospheric-pressure laminar flames will be applicable to engine conditions that are highly turbulent and are at high pressures. Granted, the study is looking to understand fuel effects on soot formation; however, different ambient conditions give rise to different sooting tendencies for the same fuel. It was unclear to the reviewer if the percentage of monoaromatic and the percentage of polyaromatic HCs in fuel are considered in the machine-learning model for soot predictions. Also, when transitioning to LTC conditions, the reviewer inquired if YSI is a good indicator for PM as at LTC conditions, PM has low content of soot and high content of HCs.

### **Reviewer 6:**

After fighting through FT057, it was nice for this reviewer to have the detail on one of the projects. The reviewer warned that creating a YSI library is a wise, but a boring way to do the research. This library will carry this information forward and impact many other projects in the future.

However, over the years of Glassman and his students evaluating the behavior of lifted burn flames and their properties, the reviewer was disappointed not to see a more detailed description of the flame structure and what property, if there is one, gives the soot measurements reproducibility. The description of the modeling effort of the flames is encouraging; however, there are extraneous influences that change the results. The reviewer would like to have seen an uncertainty for the measurements.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

The reviewer found that good progress has been made on all of the milestones that are appropriate for this project. There is an ambitious timeline and the project team appears to be meeting it.

#### Reviewer 2:

The reviewer noted that the project started recently (May 2017) and technical progress is on track. The team has established the base methane flame and has validated the soot model for the base flame. It was unclear to the reviewer what soot model is being used and what inception and surface growth species are being used in the model.

#### **Reviewer 3:**

The reviewer stated that having a database of YSIs covering a range of two orders of magnitude for a various fuels, as well as studying the new molecular fuels is a good start. For these early stages, the team has completed an impressive number of relevant and useful results, especially highlighted by the oxygenated aromatics work. The reviewer offered that comparison with experiments in more realistic settings, of course, is yet to come.

### **Reviewer 4:**

The reviewer commented that Slides 11-12 are a great indication that there are simplifying concepts that can simplify the soot formation for this flame. The creation of a sooting reaction mechanism is a great way to impact research chronologically down the line.

The reviewer especially appreciated the publication of a comprehensive list of the sooting yields of a range of compounds. The reviewer pronounced the modeling to be very encouraging yet wondered if the reaction mechanism(s) is/are available somewhere. The reviewer asked why a flamelet-based model is needed for a flame that should have stability.

### Reviewer 5:

While the investigators had a noticeable focus on the objectives, the reviewer said that the work is said to target applications to engine combustion as clearly stated in the presentation title, "...to enable advanced combustion fuels." It would have been helpful to the reviewer if the work/presentation included, at a minimum, highlights on how such transition would be made: From focus on the fundamentals (which the investigators did an excellent work on) to applications in real-life (engine combustion), including impact of in-cylinder combustion and boundary conditions (geometry, air-fuel mixing mechanisms, turbulent effects, etc.). The reviewer indicated that this need not have been a detailed analysis, but painting the pathway for such real-world applications.

### **Reviewer 6:**

The reviewer stated that there was a very interesting result on the dependence of oxygen-bond type/species on the YSI measured. There were very nice modeling results of the methane-flame soot formation. The reviewer's main concern was not really seeing how any of these results relate to combustion in an engine. The reviewer also did not see any plan for relating these results to actual engine results.

Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

The reviewer stated that Yale University and Pennsylvania State University are working closely with key national laboratory and other academic participants in Co-Optima. There are very strong collaborations throughout.

### Reviewer 2:

The reviewer reported that the team has not shied away from utilizing any available expertise or information (published or available otherwise, such as the Harvard Dataverse, or within national laboratories) to broaden their understanding of the mechanisms involved or to build their know-how.

### **Reviewer 3:**

If the DOE paid for this work, the reviewer urged that at least a link to <u>https://doi.org/10.7910/DVN/7HGFT8</u> should be included on the Crosscut Lean Exhaust Emissions Reduction Simulations website. The reviewer opined that the entire "at large community" is a stakeholder in this project. The reviewer found the collaboration group to be of very high quality.

### **Reviewer 4:**

The reviewer said that collaboration with Co-Optima appears evident from the description. The publications do not yet reflect that, if that is appropriate at this point. At these early stages, Yale and Penn State are performing the work, but the team should find results from a broader base of researchers as time goes on.

### **Reviewer 5:**

The reviewer noticed that Slide 14 identified the wrong laboratory partner. ORNL is not a listed collaborator and NREL is called out later in the slide. Again, the reviewer would like to see some engine-relevant collaboration, with perhaps ORNL.

### **Reviewer 6:**

The reviewer commented that there is good national laboratory collaboration in the project but no industry collaboration. This project is at a very low TRL where industry may not see value, which concerned the reviewer. Having said that, the reviewer acknowledged that the work is very important in understanding the science behind soot formation for various fuels and hence it is important that the lessons from this study are applicable to engines, which is not clear at this point.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

According to the reviewer, the proposed future research is in line with work thus far and new results from other laboratories. The reviewer stated that including fuels for MCCI is important, as is also developing better simulations of YSIs.

### Reviewer 2:

The reviewer remarked that all three key areas of future work as stated in the presentation are well within the targeted objectives. Painting pathways to in-cylinder applications would be helpful and within the project's end-charter.

### **Reviewer 3:**

The reviewer stressed the need to relate this project to engine operation.

### **Reviewer 4:**

The reviewer asserted that developing a YSI table for compression-ignition engines is a must-do for this project to have the impact it should have.

#### **Reviewer 5:**

The reviewer pointed out that the project is only 30% complete so the proposed future work remains on target and appropriate for the objectives of the project. There is keen interest in how the YSI will relate to sooting behavior in a real engine. Although there is not work planned in GDI, there exists a great deal for information within Co-Optima both at steady state and transients for the sooting behavior of GDI engines with Co-Optima blends. The reviewer commented that it would be very interesting to know what the YSI of the Co-Optima core gasoline fuels are and how that relates to observed GDI soot behavior; that would take a relatively short time to do. In addition, NREL has engine soot data on several simpler blends that could be correlated with YSI.

#### **Reviewer 6:**

The reviewer said that evaluating sooting tendencies at atmospheric pressures with laminar flames may not be directly applicable to soot formation in engine conditions. If the reviewer had to give one suggestion, then it would be to perform the experiments at elevated pressures. (20 atmospheres [atm] or 40 atm). At least the effects of pressure on the flame and soot formation/oxidation mechanisms would be captured to some extent. The effect of turbulence is hard to capture in flames.

### Question 5: Relevance—Does this project support the overall DOE objectives?

#### Reviewer 1:

The reviewer exclaimed that a sooting index that is appropriate for a range of ICEs and a range of fuels would be wonderful.

### Reviewer 2:

Co-Optima projects are defined to support DOE objectives by lowering the cost and enhancing reliability of fuel usage and the meeting of emissions-control standards, according to the reviewer.

### **Reviewer 3:**

The reviewer said that this project, focused on "...enabling advanced combustion fuels," meets the DOE goal of optimizing fuel-engine sub-systems for Co-Optima.

### **Reviewer 4:**

The reviewer agreed that this project meets all of the criteria for being relevant both in the area of fuel screening and emissions assessment for new Co-Optima blends.

### **Reviewer 5:**

The reviewer affirmed that this project seems to achieve the objectives of Co-Optima and the Co-Optima university funding opportunity announcement.

### **Reviewer 6:**

The reviewer acknowledged that the project meshes well with the Co-Optima program of DOE and addresses the overall objectives of DOE.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

The reviewer commented that the team has done a good job filling in the project needs via reaching across to external resources (e.g., national laboratories) and to integrate various needs (expertise, data, etc.) into the project. The reviewer noticed no shortage of resources or observed excess resources.

### Reviewer 2:

The reviewer indicated that resources, especially with this array of potential collaborators, seem sufficient. No issues are raised about work at Yale and Penn State, except to assure that funding continues.

### **Reviewer 3:**

According to the reviewer, funding so far has certainly provided encouraging results.

### **Reviewer 4:**

The reviewer said that the project just completed 1 year and the resources seem to be sufficient for the successful completion of the project.

### Reviewer 5:

The reviewer found the budget to be appropriate for the work scope.

### **Reviewer 6:**

The reviewer suggested that the budget seems rather high for this work.

Presentation Number: ft065 Presentation Title: Dynamic Species Reduction for Multi-Cycle Computational Fluid Dynamics (CFD) Simulations (Co-Optima) Principal Investigator: George Lavole (University of Michigan)

### Presenter Rob Middleton, University of Michigan

Reviewer Sample Size

A total of five reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

The approach was reasonable to the reviewer

### Reviewer 2:

The reviewer said that the success of this work depends on the use of the proper chemical kinetics database.

### **Reviewer 3:**

The reviewer stated that the concept of the project is good. The investigators seem to be convincing in their arguments that "little" chemistry occurs during the non-valve overlap region. In general, the reviewer would agree with that conclusion, with the caveat that

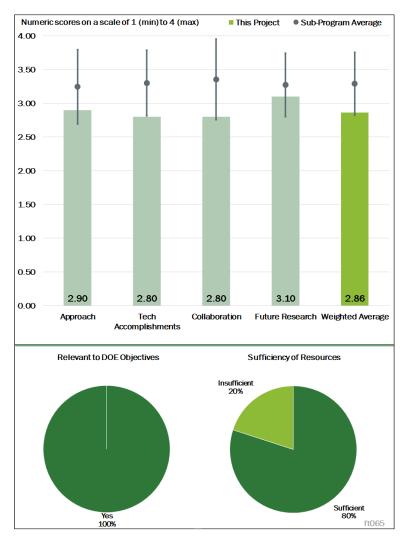


Figure 5-12 - Presentation Number: ft065 Presentation Title: Dynamic Species Reduction for Multi-Cycle Computational Fluid Dynamics (CFD) Simulations (Co-Optima) Principal Investigator: George Lavoie (University of Michigan)

very slow chemistry occurs and probably has very small impact on the overall combustion kinetic description. The reviewer proclaimed that the skip-species option in CONVERGE clearly misses appreciable chemistry. It changes combustion character. There is no clear reason given why the University of Michigan dynamic species reduction (DSR) approach "fixes" the problem. A common problem with dynamic species reduction is that the re-emergence of a species in a future step has no history; there are n. o derivatives in terms of growth and second-order behavior. The reviewer wanted evidence that the combustion process did not "wander" over longer times due to the approximations.

### **Reviewer 4:**

The reviewer remarked that this project presents a very important part that is missing in other Co-Optima projects because it looks into modeling multi-cycle simulations that will be essential for transient control and mode switching. The approach for dynamic species reduction is well-planned, building upon prior experience. Converting the codes from KIVA to CONVERGE is fine. The reviewer stated that that the major missing part is not having a detailed multi-cycle experimental validation beyond an in-cylinder pressure trace, which is not difficult to achieve. Validating other combustion metrics like cycle-to-cycle heat release and engine-out

emissions should be considered, assuming these data can become available to the PI from the ANL group. This reviewer agreed that if the selection of the ACI mode takes too long, the PI can start with prior HCCI data at the University of Michigan through previously funded DOE projects. So, the project can do proper, full-cycle, multi-cycle evaluations.

### **Reviewer 5:**

According to the reviewer, the overall project objectives are clear. The high-level approach and the tasks are also stated reasonably well. However, there is a lack of in-depth technical descriptions on the fundamentals of the DSR/re-mapping techniques employed in this project and in which areas they offer improvements over the dynamic mechanism reduction and multi-zone modeling approaches that are currently built in CONVERGE. Also, the reviewer indicated that the target size and components of the base detailed/semi-detailed kinetic mechanism need to be well defined such that the project benefit and impact can be properly evaluated.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

Considering the personnel change, the project has made reasonable progress on acquiring engine meshes, attaining baseline simulation results, and implementing the University of Michigan DSR routines into CONVERGE.

### Reviewer 2:

The progress seemed reasonable to the reviewer.

#### Reviewer 3:

The reviewer found not much progress at this stage of the project.

#### Reviewer 4:

The reviewer pointed out that the work seems to be subject to program management delays.

### **Reviewer 5:**

The reviewer commented that the project presents interesting results for the significance of considering species reaction during negative valve overlap. In addition, the findings for not needing to consider species reaction during gas exchange from exhaust valve opening to intake valve closure and during open valve is of great value for the research community. The project will not be able to fulfill the goal of 80% computation time reduction in CONVERGE with DSR.

**Question 3: Collaboration and Coordination Across Project Team.** 

### Reviewer 1:

This reviewer described the collaboration as a supplier collaboration, i.e., Convergent Sciences gets DOE/University of Michigan (UM) to develop a submodel for nothing. The reviewer asked what the give back is to UM, who gets license fees, and who gets public credit; this is a common problem. Having been in similar negotiations, this reviewer did not want UM and the students mined for free. Unfortunately, UM is in the submissive position. Strongly emphasizing that only licenses are not enough, the reviewer suggested marketing it as the Convergent Sciences/UM version of the code.

### Reviewer 2:

The collaboration seemed reasonable to the reviewer.

#### **Reviewer 3:**

The reviewer suggested that the authors take into consideration the work done on sensitivity analysis by Dr. Hai Wang from Stanford University for one-dimensional homogeneous systems.

### **Reviewer 4:**

The reviewer pointed out that the project includes collaborations among the University of Michigan, ANL, and Convergent Science. The collaboration with other Co-Optima members needs to be increased because other Co-Optima projects are lacking the parts that are studied in this project. Further collaboration provides avenues to receive further experimental data required for multi-cycle experimental data validation. This also creates opportunities to see the effect of the project outcomes on different ACI combustion regimes.

### **Reviewer 5:**

The reviewer noted that the project overall has good collaborations with ANL and Convergent Science. To better support the Co-Optima goals, establishing good coordination and collaboration among this project, the ANL CFD team, and the Co-Optima kinetics/simulation toolkit team would be beneficial.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

The reviewer commented that the future work is well planned to address the remaining technical challenges and barriers.

### Reviewer 2:

The reviewer stated that the future work includes logical next steps towards the goals of this project.

### **Reviewer 3:**

The next steps looked appropriate to the reviewer.

### **Reviewer 4:**

The reviewer found the future work to be reasonable.

### **Reviewer 5:**

The reviewer looked forward to seeing the success and completion of this first stage before considering the quality of the results.

Question 5: Relevance—Does this project support the overall DOE objectives?

### Reviewer 1:

The reviewer stated that the project is making progress towards the goal of developing a modeling tool to study cycle-to-cycle variability that can lead to robust, fuel-efficient ICEs that are commonly used in vehicles. This supports the goal of the Co-Optima program to reduce vehicular fuel consumption by 10% for LD vehicles.

### Reviewer 2:

By accelerating the computation time for multi-cycle, 3-D, CFD engine simulation, the reviewer indicated that this project provides good support towards achieving the Co-Optima goals and the overall DOE objectives.

### **Reviewer 3:**

The reviewer remarked that the work is very much relevant to DOE objectives because it is coupling fluid dynamics with chemistry.

### Reviewer 4:

The reviewer found the work to be reasonable.

### **Reviewer 5:**

The reviewer commented that faster is better.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

#### Reviewer 1:

The reviewer said that the resources are adequate to achieve the project milestones and address the technical barriers.

#### Reviewer 2:

The reviewer indicated that the outline of the project is aligned with funding.

### **Reviewer 3:**

The reviewer noted that resources are reasonable.

### Reviewer 4:

The reviewer reported that resources seem to be sufficient. Money from Convergence would move the project along better.

### **Reviewer 5:**

The reviewer suggested that the PI needs to recruit/find graduate student(s) in order to achieve the project goals on time. Computational resources are sufficient for this project.

Presentation Number: ft066 Presentation Title: Reduced Petroleum Use through Easily Reformed Fuels and Dedicated Exhaust Gas Recirculation Principal Investigator: Tom Briggs (Southwest Research Institute)

### Presenter

Tom Briggs, Southwest Research Institute

**Reviewer Sample Size** A total of four reviewers evaluated this project.

Question 1: Approach to performing the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

### Reviewer 1:

With respect to investigating fuel effects to enhance the  $H_2$  production and dedicated EGR technology, the reviewer stated that the approach being taken is very solid. The project appears highly dependent on experiment results. A stronger modeling component would be advantageous, according to the reviewer.

### Reviewer 2:

The reviewer noted that dedicated EGR has the potential to improve ICE efficiency. Understanding the fuel effect on  $H_2$  production and the approaches of

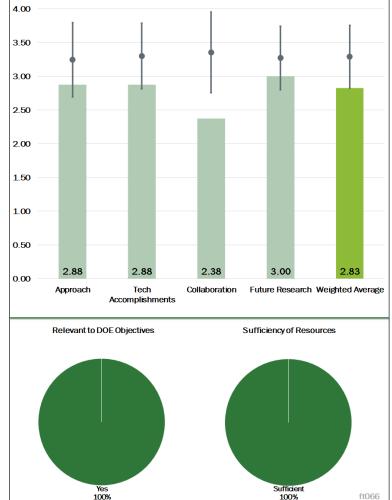
Figure 5-13 - Presentation Number: ft066 Presentation Title: Reduced Petroleum Use through Easily Reformed Fuels and Dedicated Exhaust Gas Recirculation Principal Investigator: Tom Briggs (Southwest Research Institute)

further improving dedicated exhaust gas recirculation (DEGR) efficiency is valuable. The reviewer suggested that the project can be improved by adding CFD modeling.

#### **Reviewer 3:**

The reviewer remarked that the approach is a compelling way to extend the lean/dilution limit and combustion stability of engines. The goal of operating a stoichiometric gasoline engine is also compelling as it eliminates the need for a complicated aftertreatment system.

According to the reviewer, the project team has studied internal EGR reformation for a number of years and has produced great results. An unanswered question is the commercial feasibility of a dedicated EGR system. Extending the lean limit even further requires additional  $H_2$  production and requires running the dedicated cylinder even richer (absent a better  $H_2$  producing fuel). The reviewer said that this will lead to higher HC and soot emissions, which will lead to EGR-cooler fouling. The presenter suggested that at a phi of 1.3, the EGR cooler did not foul; however,  $H_2$  production was around 3%. At a  $H_2$  generation of 8% and a phi of 1.6, the



This Project

Sub-Program Average

Numeric scores on a scale of 1 (min) to 4 (max)

presenter suggested the EGR cooler fouled and plugged. These results suggested to the reviewer that there is a limit to how much  $H_2$  is feasibly generated and the extent to how far the lean limit can be extended.

Beyond an improvement in the hydrogen-to-carbon (H:C) ratio in the fuel, it was unclear to the reviewer how a fuel can be biased to produce additional  $H_2$  without looking at the kinetic pathways. The reviewer commented that this does not appear to be in the project scope. The reviewer observed that this project is very similar to Co-Optima, with the creation of a special fuel that can bias  $H_2$  production and designing an engine that can take advantage of it (higher CR mainly). It was unclear to the reviewer why this project is a standalone and not part of the Co-Optima program.

### Reviewer 4:

The reviewer remarked that this project improves the potential of DEGR. The goal is to find a new chemistry via new fuel options to generate more  $H_2$  in the dedicated cylinder, for example, via an increased H:C ratio. The reviewer wanted to know whether this exploratory work of finding new chemistry with a new fuel could be done via simulation first to filter out several options and guide the experiments. According to the reviewer, DEGR itself has found challenges on its path to production implementation with current market fuel. The reviewer inquired if it is prudent to think that adding the complexity of a new fuel will help that situation.

Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

### Reviewer 1:

The reviewer commented that the investigations of how to increase  $H_2$  production via injection controls and valve timing produced important results. Confirming key features of fuels for  $H_2$  generation was an important finding.

### Reviewer 2:

The reviewer found the project to be on track to achieve its objectives.

### **Reviewer 3:**

The reviewer indicated that progress has been very slow, with paperwork being blamed.

### **Reviewer 4:**

The reviewer posited that the work using H<sub>2</sub> enrichment is extremely compelling. The ability to shorten combustion duration with H<sub>2</sub> enrichment can extend the load limit of high-dilution engines and also lead to higher CR engines by mitigating knock. According to the reviewer, the results presented showed a H<sub>2</sub> generation of almost 8%, however, at the cost of EGR-cooler fouling. A 3%-enrichment was theorized to increase the CR by 1-2 points, which would ideally increase the ideal cycle efficiency by a similar number of points. It was unclear to the reviewer how much of the efficiency advantage gained by H<sub>2</sub> enrichment in the main cylinders is negated by rich operating conditions in the dedicated cylinder. The HC, CO, and H<sub>2</sub> would be oxidized in the engine so overall combustion efficiency is still high (minus what condenses out in the EGR cooler). The reviewer requested information on overall engine efficiency as well as per-cylinder efficiencies in future presentations. Additionally, the reviewer said that the durability of the additional hardware responsible for circulating the DEGR is not addressed. The goal of increasing the CR with H<sub>2</sub> enrichment would decrease ignition delay and stretch out burn rates. The effect of this on overall efficiency and minimum enrichment levels to avoid knock was not clear to the reviewer.

The reviewer commented that the ability to modulate injection strategy to extend robust combustion in the dedicated cylinder is a good idea; however, no coefficient of variation (COV) of IMEP values was presented. For future presentation, the reviewer requested information on COV of IMEP.

### Question 3: Collaboration and Coordination Across Project Team.

### Reviewer 1:

According to the reviewer, there is collaboration with Fiat Chrysler Automobiles (FCA) and an energy company. It could be ideal to link this project to Co-Optima program.

### Reviewer 2:

The reviewer stated that the technical engagement by Total and FCA does not appear very strong. Eventually, this project should be more engaged with the fuel strategies in Co-Optima. The reviewer wanted to know how this effort is leveraged or independent of the High-Efficiency Dilute Gasoline Engine (HEDGE) program.

### **Reviewer 3:**

The reviewer said that the project incurred a significant delay, and as such, there does not appear to be significant interaction among the partners. There is future work identified to procure a higher CR engine from one of the partners; however, the future plans are vague for the fuel supplier.

### **Reviewer 4:**

The reviewer stressed that it is very critical that either a petroleum or biofuel-based fuel supplier be part of this project, not just to supply test fuels but to collaborate at a higher level to guide it in selecting fuel options that have viable commercial pathways.

Question 4: Proposed Future Research—the degree to which the project has effectively planned its future work in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways.

### Reviewer 1:

The reviewer stated that the right areas have been identified for the remaining work.

### Reviewer 2:

According to the reviewer, the project is planned in a logical manner and there is no major risk. The reviewer encouraged the PI to put more effort into understanding the fundamentals of fuel impacts on  $H_2$  production and DEGR combustion.

### **Reviewer 3:**

The reviewer remarked that the future work would appear stronger if the relationship to the Co-Optima fuels matrix were made clearer. Co-Optima does not seem to have a fuel path for DEGR-type engines.

### **Reviewer 4:**

The reviewer pointed out that this project incurred a significant pause which likely affected the current status and future work of the project. The future work identified is basic in nature, but a higher CR engine to utilize the  $H_2$  enrichment is important to understand the efficiency benefits of the engine. Tailoring a fuel with a higher H:C ratio will also help  $H_2$  production; however, biasing the production of  $H_2$  in the DEGR cylinder requires kinetic modeling, which the reviewer recommended. Achieving a richer than 1.3 phi in a durable configuration (i.e., EGR-cooler fouling) will be challenging and thus additional insights in the reformation process are required. The reviewer suggested this as future work.

Question 5: Relevance—Does this project support the overall DOE objectives?

### Reviewer 1:

According to the reviewer, DEGR is a novel ICE technology, potentially achieving better engine efficiency. It is worth studying the fuel impact on DEGR combustion.

### Reviewer 2:

The reviewer said that this project aims to increase engine efficiency and hence petroleum-use reduction.

### **Reviewer 3:**

The reviewer remarked that DEGR-type technology is a fundamentally, directionally sound path to higher engine efficiency. It is one of the more innovative approaches though not simple to implement.

### **Reviewer 4:**

The reviewer indicated that this work strongly supports DOE's vision of energy security, higher efficiency engines, lower emissions engines, and lower cost technologies. The reviewer questioned whether it should be a standalone project or if it should be incorporated into the Co-Optima program as the objectives are similar.

Question 6: Resources—How sufficient are the resources for the project to achieve the stated milestones in a timely fashion?

### Reviewer 1:

The reviewer indicated that there are sufficient resources to achieve the stated milestones.

### Reviewer 2:

The reviewer observed that Initial exploratory work can be done with the provided resources.

### **Reviewer 3:**

The reviewer stated that the budget is appropriate for the project scope and goals. Kinetic modeling may require a slight increase in the budget, but should be manageable.

### **Reviewer 4:**

The reviewer found the resources to be at least sufficient. Companion work under the HEDGE consortium is significant. A few words about the interface are needed in the presentation.

## Acronyms and Abbreviations

| 3-D                                       | Three-dimension   |
|---|---|
| ACI                                       | Advanced compression ignition   |
| ACI-F                                     | Advanced compression ignition: fuel effects   |
| AFIDA                                     | Advanced fuel ignition delay analyzer   |
| AMR                                       | Annual Merit Review   |
| ANL                                       | Argonne National Laboratory   |
| atm                                       | Atmosphere  |
| BAU                                       | Business as usual   |
| CFD                                       | Computational fluid dynamics  |
| CFR                                       | Constant-pressure flow rig  |
| СО  | Carbon monoxide   |
| COV                                       | Coefficient of variation  |
| CR  | Compression ratio   |
| CRADA                                     | Cooperative research and development agreements   |
| DEGR                                      | Dedicated exhaust gas recirculation   |
| DFI                                       | Ducted fuel injection   |
| DOE                                       | U.C. Department of Energy   |
|   | U.S. Department of Energy   |
| DSR                                       | Dynamic species reduction   |
| DSR<br>dT                                 |   |
|   | Dynamic species reduction   |
| dT  | Dynamic species reduction<br>Change in temperature  |
| dT<br>ECN                                 | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network   |
| dT<br>ECN<br>EGR                          | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network<br>Exhaust-gas recirculation  |
| dT<br>ECN<br>EGR<br>FCA                   | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network<br>Exhaust-gas recirculation<br>Fiat Chrysler Automobiles   |
| dT<br>ECN<br>EGR<br>FCA<br>FE             | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network<br>Exhaust-gas recirculation<br>Fiat Chrysler Automobiles<br>Fuel economy   |
| dT<br>ECN<br>EGR<br>FCA<br>FE<br>FT       | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network<br>Exhaust-gas recirculation<br>Fiat Chrysler Automobiles<br>Fuel economy<br>Fuel and Lubricant Technologies                |
| dT<br>ECN<br>EGR<br>FCA<br>FE<br>FT<br>FY | Dynamic species reduction<br>Change in temperature<br>Engine Combustion Network<br>Exhaust-gas recirculation<br>Fiat Chrysler Automobiles<br>Fuel economy<br>Fuel and Lubricant Technologies<br>Fiscal Year |

| H <sub>2</sub>  | Hydrogen gas                            |
|-----------------|---|
| НС              | Hydrocarbon                             |
| HDV             | Heavy-duty vehicle                      |
| HCCI            | Homogeneous-charge compression ignition |
| HD              | Heavy-duty                              |
| HEDGE           | High-Efficiency Dilute Gasoline Engine  |
| HOV             | Heat of vaporization                    |
| ICE             | Internal combustion engine              |
| IMEP            | Indicated mean effective pressure       |
| КС              | Kinetically controlled                  |
| LD              | Light-duty                              |
| LLFC            | Leaner lifted flame combustion          |
| LLNL            | Lawrence Livermore National Laboratory  |
| LT              | Low temperature                         |
| LTC             | Low-temperature combustion              |
| MCCI            | Mixed-mode compression ignition         |
| MD              | Medium-duty                             |
| ml              | Milliliter                              |
| MON             | Motor octane number                     |
| MS              | Mass spectroscopy                       |
| NA              | Naturally aspirated                     |
| NO <sub>x</sub> | Oxides of nitrogen                      |
| OEM             | Original equipment manufacturer         |
| OS              | Octane sensitivity                      |
| РАН             | Polycyclic aromatic hydrocarbon         |
| PI              | Principal Investigator                  |
| PM              | Particulate matter                      |
| PMI             | Particulate matter index                |
|                 |   |

| R&D        | Research and development  |
|------------|---|
| RCEM       | Rapid compression expansion machine   |
| RCM        | Rapid compression machine   |
| RON        | Research octane number  |
| SCO        | Spray/combustion—optical imaging  |
| SI         | Spark ignition  |
| SNL        | Sandia National Laboratories  |
| SS         | Sprays—simulation   |
| SX         | Sprays—X-ray imaging  |
| TRL        | Technology readiness level  |
| UM         | University of Michigan  |
| U.S. DRIVE | U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability |
| VCR        | Variable compression ratio  |
| VTO        | Vehicle Technologies Office   |
| YSI        | Yield sooting index   |