5. Fuel and Lubricant Technologies

The Vehicle Technologies Office (VTO) has a comprehensive portfolio of early-stage research to enable industry to accelerate the development and widespread use of a variety of promising sustainable transportation technologies. The research pathways focus on fuel diversification, vehicle efficiency, energy storage, and mobility energy productivity that can improve the overall energy efficiency and efficacy of the transportation or mobility system. VTO leverages the unique capabilities and world-class expertise of the National Laboratory system to develop innovations in electrification, including advanced battery technologies; advanced combustion engines and fuels, including co-optimized systems; advanced materials for lighter-weight vehicle structures; and energy efficient mobility systems. VTO is uniquely positioned to address early-stage challenges due to strategic public-private research partnerships with industry (e.g., U.S. DRIVE, 21st Century Truck Partnership) that leverage relevant expertise. These partnerships prevent duplication of effort, focus DOE research on critical R&D barriers, and accelerate progress. VTO focuses on research that industry does not have the technical capability to undertake on its own, usually due to a high degree of scientific or technical uncertainty, or that is too far from market realization to merit industry 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, generating 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 combustion engines, fuels, and emission control catalysts. The FT subprogram will apply the 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.

Project Feedback

In this merit review activity, each reviewer was asked to respond to a series of questions, involving multiple-choice 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 ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ft037	Co-Optimization of Fuels and Engines (Co-Optima)	Robert Wagner (ORNL/NREL)	5-4	3.30	3.30	3.70	3.30	**3.35**
ft067	Multi-Mode/Multi-Mode Compression Ignition : Fuel-Property Characterization and Prediction	Tim Bays (NREL/PNNL)	5-10	3.19	3.44	3.50	3.31	**3.37**
ft069	Multi-Mode: Fuel-Property Impacts and Limitations on Combustion–Spark Ignition Focus	Derek Splitter (ORNL)	5-17	3.43	3.29	3.36	3.43	**3.35**
ft070	Multi-Mode: From In-Cylinder Combustion Diagnostics to Drive-Cycle Fuel Economy	Magnus Sjoberg (SNL)	5-23	3.00	3.10	3.40	3.00	**3.10**
ft071	Multi-Mode Operation in Gasoline Direct-Injection Engines: Fuel-Property Effects and Approaches to Expand the Advanced Compression-Ignition Range	Toby Rockstroh (ORNL)	5-28	3.00	3.33	3.67	3.25	**3.28**
ft072	Multi-Mode: Desired Fuel Properties for Advanced Compression-Ignition and Spark-Ignition Engine Performance	Chris Kolodziej (ANL)	5-33	3.40	3.50	3.20	3.20	**3.40**

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ft073	Co-Optima Emissions and Emissions Control for Spark Ignition and Advanced Compression Ignition Multi-Mode Combustion	Sreshtha Sinha-Majumdar (ORNL)	5-38	3.50	3.43	3.36	3.21	**3.41**
ft074	Multi-Mode: Gasoline Direct-Injection Sprays	Lyle Pickett (SNL)	5-44	3.60	3.90	3.60	3.50	**3.74**
ft075	Multi-Mode: Fuel Kinetics	Bill Pitz (ANL/LLNL)	5-48	3.71	3.50	3.86	3.50	**3.60**
ft076	Model-Based Fuel and Engine Optimization	Juliane Mueller (LBNL)	5-53	3.10	3.50	3.30	3.20	**3.34**
ft077	Heavy-Duty Mixed-Controlled Compression Ignition: Fuel Effects and Ducted Fuel Injection	Charles Mueller (SNL)	5-57	3.63	3.88	3.38	3.75	**3.73**
ft078	Heavy-Duty Mixed-Controlled Compression Ignition: Impacts of Fuel Properties on Combustion, Injection Characteristics, and Emissions Controls	Martin Wissink (ANL/ORNL)	5-60	3.25	3.25	3.42	3.33	**3.28**
ft087	Multimode, Co-Optimized, Light-Duty Vehicle Engine	Phil Zoldak (Hyundai-Kia North America)	5-65	3.30	3.40	3.20	2.90	**3.29**
ft088	Fuel Property Experimental Kinetics	Gina Fioroni (NREL)	5-69	3.70	3.70	3.60	3.30	**3.64**
ft089	Heavy-Duty Advanced Compression Ignition	John Dec (SNL)	5-73	3.30	3.40	3.40	3.50	**3.39**
Overall Average				**3.36**	**3.45**	**3.47**	**3.31**	**3.41**

Presentation Number: ft037
Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima)
Principal Investigator: Robert Wagner (Oak Ridge National Laboratory)

Presenter

Robert Wagner, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

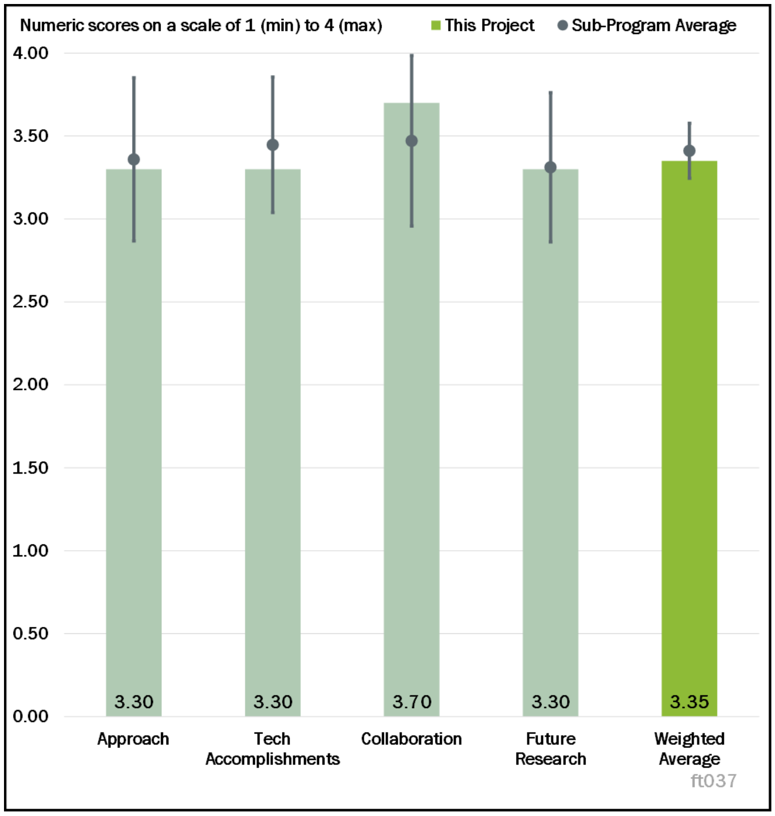

Figure 5-1 - Presentation Number: ft037 Presentation Title: Co-Optimization of Fuels and Engines (Co-Optima) Principal Investigator: Robert Wagner (Oak Ridge National Laboratory)

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

Reviewer 1:

The encompassing approach of Co-Optimization of Fuels and Engines (Co-Optima) is very good. It is a multi-laboratory effort, working in experimental and simulation space, both for light-duty (LD) and heavy-duty (HD) engines. The project is looking at costs of fuels, understanding of combustion, and fundamental understanding of how fuel properties influence ignition and combustion. All of these aspects are very important. One item that was conspicuous by its absence is the potential for this project to leverage critical fuels technologies and economics to enable United States (U.S.) companies to meet upcoming greenhouse gas (GHG) regulations while maintaining and improving efficiency and meeting ever-tightening toxic air emissions standards. The ability to be a major lever in helping original equipment manufacturers (OEMs) to achieve GHG regulatory compliance needs to be a more important focus to this project.

Reviewer 2:

The approach is very strong and is continuing to get better. The collaboration continues to get stronger and with it the identification of the research on critical barriers is becoming more sharply focused.

Reviewer 3:

The team has done a great job setting up the program over the past years.

Reviewer 4:

Historically, the overall Co-Optima program approach has been solid, drawing in the strengths of laboratories across the U.S. Department of Energy (DOE) complex to align on topics surrounding fuels and engine research. The highest value results from the program focus on fundamental fuel property understanding, with engine-fuel interactions a close second. Within the scope of the program, however, there are some projects that look to be rolled into the effort even though they are not centrally aligned with the Co-Optima mission. In addition, there are activities that appear focused on increasing the scope of a specific laboratory's capabilities, in some cases duplicating capabilities that already exist in other labs. These are of lower value.

This reviewer would have liked to see more high-level alignment with the SuperTruck 2 (ST2) program, because this DOE-funded program represents the cutting edge of high-efficiency, HD line-haul truck development. As Co-Optima morphs to a stronger focus on the HD space, ensuring the research goals and efforts are aligned with the needs identified by the SuperTruck 2 program is important. As an example, many of the SuperTruck projects, both SuperTruck 1 (ST1) and SuperTruck 2, included some level of work on an advanced compression ignition (ACI) concept. ACI technology packages were down-selected out of all projects as they moved forward, reflecting that a mixing-controlled combustion solution was the most promising for delivering the efficiency targets. The Co-Optima shift in focus seems to run counter to this knowledge, raising the question on what is driving the shift in focus. Is this an industry pull, like it was for LD mixed-mode combustion, or a DOE laboratory push? As efforts move forward, ensuring a close connection to the SuperTruck 2 projects is critical to ensure Co-Optima is both utilizing knowledge gained in their projects and responding to the barriers and opportunities they identify.

This reviewer would have liked to see more focused and concrete deliverables for the computational fluid dynamics (CFD) and simulation activities and additional clarity of what is being delivered on the simulation side. How to effectively incorporate fuel properties into CFD simulations is still an open question and area for development, but it is critical to have robust governance on the project outputs. The newly formed Partnership for Advanced Combustion Engines (PACE) program has a strong focus on delivering useful open-source sub-model outputs from the simulation work, which would be a good model for Co-Optima to adopt to ensure the simulation projects are delivering useful results.

The LD focus on mixed-mode combustion is still a strong topic and it would be good to bring this effort to a strong finish. Decisions on when to move on from this topic should be dictated by the research progress and state of conclusions rather than artificial external timelines. This reviewer was encouraged by the decision to extend the mixed-mode effort. Taking the time necessary to have a definitive result and outcome is far more valuable than quickly pivoting to chase after new topics of the day. In many cases, it beggars belief that the projects that quickly churn out a result and are ready to move on to the next topic are truly delivering high-impact work. The reviewer recommended letting the transition to new areas be driven by the impact of the work, the results to answering key questions, and the resolution of technology barriers and not just the first to "complete" a task.

The reviewer suggested that Co-Optima to consider dialing the focus of the program into more narrowly tailored areas and to give the program the time to deliver high-impact work. The reviewer recommended the program not be too driven to cover all possible fuel-engine research questions and transition to the next flashy topic based on a timeline external to whether work is truly complete and impactful in a given area.

One of the challenges and barriers listed is the mismatch between engine and blendstock development research. This is a very clear issue in the program, and there is a clear need to spend more effort to bring alignment between the blendstock development and the combustion development programs. No paths forward were highlighted, however. The reviewer believes co-optimization cannot occur if the two programs are not in sync.

Reviewer 5:

The approach focuses on finding a new fuel, blending agent to gasoline, or expanding the understanding of existing gasoline fuel properties to enable low-temperature combustion (LTC) or ACI modes. While this work is needed, it is focused largely on increasing engine efficiency. There seems to be far less effort on overcoming the following barriers to LTC/ACI combustion, which must be overcome before commercialization can be considered; not to mention, that if a new fuel blend is needed, commercialization of that new fuel has its own challenges:

- Expanded speed and load range of LTC regime
- Reduced engine-out hydrocarbon (HC) and carbon monoxide (CO) emissions
- Lower combustion noise
- Simpler transient control/combustion mode switching
- Improved cold operation
- Lower boost pressure
- Higher specific power
- Crank angle at 50% mass fraction burned (CA50) control and tolerance to boundary condition perturbations:
    - Ambient temperature
    - Humidity
    - Market fuel variability
- Low-cost lean-oxides of nitrogen (NO_x) aftertreatment system.

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 technical accomplishments are excellent.

Reviewer 2:
There has been substantial progress in this project over the last year. Fuel properties, advanced combustion, and more precise and accurate measurement and prediction of fuel properties—all of these are critically important as we head to a more sustainable future for liquid fuel powered vehicles. One aspect that might be worth more pursuit is the ability of these fuel components or blendstocks to be an enabler for a practical LTC engine.

Reviewer 3:
The reviewer observed great progress to date and some of the more exciting projects in fuels since gasoline blended with 10.5%-15% ethanol (E15).

Reviewer 4:
Progress had been good but more work in the right areas, namely, spark-assisted homogeneous charge compression ignition (HCCI) type mixed mode, is needed to help overcome the challenges in mixed-mode combustion for LD application.

Reviewer 5:
The program seems to have lost some focus in the transition from Co-Optima 1.0 to 2.0. The boosted spark ignition (SI) efforts in Phase I had clear engagement and strong partnerships across the DOE laboratories. The ability of the group to come together and develop a merit function for boosted SI engines with a strong technical backing was a good result. The 2.0 effort appears significantly less focused and more prone to uncoordinated efforts with multiple research probing vastly different topics. The concern here is that the final result from Co-Optima 2.0 may have very low impact on the key questions and opportunities it was designed to explore.

There is a clear need to identify the high-level arc of a specific research topic, so that it is possible to understand how the project is measurably progressing along the path to deliver a solution or understanding in a given area. As an example, what is the key challenge or barrier for mixed-mode combustion? How are projects aligned to deliver understanding against that barrier? What are the key steps along that path? This is only one example, but this approach is needed broadly across all of the topics across the effort. Understanding the arc of the program is important to understanding the scale of progress being made.

There is no doubt that the program is delivering high quality work across a broad range of topic areas. The significant volume of technical publications delivered is to be lauded.

The program logs completion of many milestones, and a few highlighted go/no-go decisions, across the different projects that are a part of the overall effort. Moving forward, there should be a focus to ensure milestones are meaningful measures of progress of the effort and less process-based check boxes that are easily achieved. The go/no-go milestones should also be explained in the context of significant program decisions. Identifying key break points in the effort, and developing go/no-go milestones or decision points, is far more instructive than a process check, such as the ducted fuel injection (DFI) go/no-go highlighted this year. This reviewer proposed using the go/no-go as higher-level project management tools.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The collaboration and coordination in Co-Optima is outstanding. There is a coherent, integrated work plan, and it appears that each team member does a good job of communicating and ensuring that their work fits into the overall goals. The inter-lab cooperation is impressive because that is very difficult to establish and maintain. The integration between experiment and simulation is also impressive from a global point of view.

Reviewer 2:
Since its inception, Co-Optima has progressed from essentially disparate projects to a closely coordinated program with well-focused projects. The reviewer sent kudos to the leadership.

Reviewer 3:
There is excellent collaboration across many partners.

Reviewer 4:
The Co-Optima team is to be congratulated on achieving excellent collaboration among the various National Laboratories. The program has paved the way and set the example for collaboration in future DOE programs like PACE.

Reviewer 5:
Under the broad heading of Co-Optima, there is coordination across the overall team driven by the program structure. On a more local level, it is less clear that the coordination and collaboration exists across all project teams. There are examples of programs with clear cross-laboratory collaboration and others with very limited connectivity.

With the shift to Co-Optima 2.0, and the new research program areas, the targeting and alignment of teams around central project objectives become increasingly muddied. The work seems more scattered, and it is clear some of the long-standing DOE lab siloes are starting to reappear within certain project scopes. Moving forward, the program needs to focus on pressing for more multi-laboratory initiatives and closer collaborations to deliver on a common goal. Focusing on narrowing the breadth of the projects, with an increase in technical depth on a reduced number of subjects, could help increase the coordination and collaboration across efforts.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
Proposed future work in ACI is probably the right pathway from a combustion point of view, while finishing up work on mixing-controlled compression ignition (MCCI) combustion. One thing this reviewer would like to have seen is an overall goal toward reducing the well-to-wheels (WTW) carbon dioxide (CO_2) footprint between combustion system (including engine efficiency) and fuel choice (low carbon/high performance fuels). The combination of efficiency and low carbon fuel will directly impact the WTW compliance for GHG. It would be nice to see this presented more prominently.

Reviewer 2:
It was not clear to this reviewer the extent to which the future work on multi-mode engine combustion will contribute to the current understanding in industry of what is required to overcome the challenges of implementation. Demonstration vehicles have been built and Mazda has announced market introduction.

The barriers identified for medium-duty (MD) and HD vehicles seem reasonable.

It seemed to this reviewer that testing the central fuel and central engine hypotheses is an important task. It also seems that it will be challenging and perhaps involve a significant effort. How is this going to be integrated into your future plans?

Reviewer 3:
The proposed near-term research efforts look reasonable and are solid, next-step progressions of the ongoing work. The reviewer noted that inclusion of a specific principal investigator (PI) name to the planned outcomes in fiscal year (FY) 2021, on Slide 25 highlights again the question of coordination and collaboration across the laboratory space. If individual PIs are responsible for key future deliverables, that makes the project appear less of a cohesive effort and more a collection of independent projects. Are all PIs driving work to these central outcomes?

A focus of later stage effort on reduction of overall transportation CO_2 is a good target, but with a few clear caveats:

- Scale is a critical factor, and analysis will need to be targeted on what fuels can be delivered, and consumed, at a meaningful scale. A narrow range of specialized applications at low volumes is not impactful. A focus on impact to the whole transportation system could be impactful.
- There are a lot of ongoing efforts globally, both commercial and in the research and development (R&D) space, focused on this topic, so the effort will have to be carefully defined to ensure that it builds upon these efforts, not just repeating them from the start.
- How this effort fits within the central concept of Co-Optima, that optimizing fuels and engines in concert will enable high system-level gains, will need to be clear.
- Need to ensure that the current work is complete and has delivered meaningful outcomes.

Reviewer 4:
There is limited room to improve MD and HD engines via fuel properties and engine design. The reviewer recommended taking a wider view and including some future electrification in the mix. This will allow Co-Optima to downsize the engine, where the fuel and engine design could really allow a novel engine to significantly improve efficiency. Running a 9 liter (L) versus 15 L may be possible with some hybridization, for example. This would require running the 9 L engine at a much higher load on typical drive cycles. It also

changes the operating points for mixed-mode combustion regimes and may result in disqualifying certain fuels/regimes due to high NO_x.

Reviewer 5:
It is suggested that the LD portion of Co-Optima 2.0 on mixed-mode combustion be brought to a crisp end and focus shifted to programs like PACE.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
This is exactly the type of program that DOE should be funding—improving efficiency and reducing GHG footprint to help American companies better compete and to meet upcoming regulatory constraints at the same time.

Reviewer 2:
This work is very relevant. To reduce the CO_2 footprint of our mobility system to a level necessary for sustainability will require the optimization of the entire fuel, engine, etc., system. This is the focus of Co-Optima.

Reviewer 3:
The Co-Optima program has strong alignment with DOE focus areas on increasing vehicle efficiency and increasing fuel diversity.

Reviewer 4:
Co-Optima supports the DOE goals.

Reviewer 5:
The program all along has sought to reduce petroleum consumption and address GHG emissions.

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

Reviewer 1:
The scope and resources of this program are appropriate for the targets and goals that it seeks to achieve.

Reviewer 2:
Resources seem sufficient.

Reviewer 3:
The resources are at a healthy level without being excessive.

Reviewer 4:
The assigned resources have been used well.

Reviewer 5:
Overall program funding is reasonable, given the broad scope of the effort. On an individual program basis, there are some broad disparities in funding level that are not fully accounted for or explained. Some project funding levels may be insufficient, while others appear notably excessive.

Presentation Number: ft067
Presentation Title: Multi-Mode/Multi-Mode Compression Ignition: Fuel-Property Characterization and Prediction
Principal Investigator: Tim Bays (Pacific Northwest National Laboratory)

Presenter

Tim Bays, Pacific Northwest National Laboratory; Gina Fioroni, National Renewable Energy Laboratory; Matt McNenly, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of eight reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 88% of reviewers indicated that the resources were sufficient, 13% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

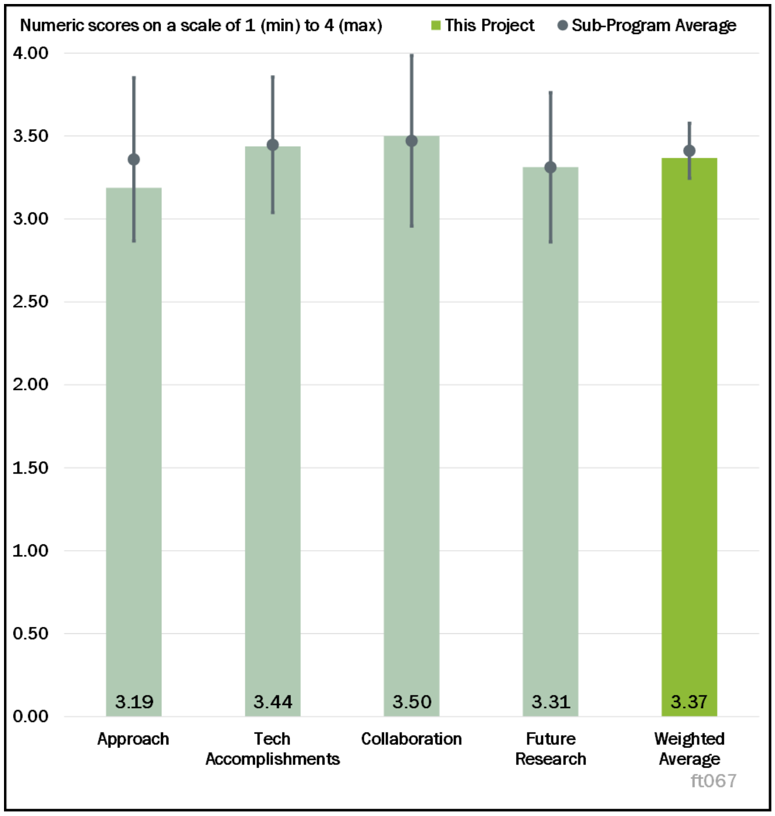

Figure 5-2 - Presentation Number: ft067 Presentation Title: Multi-Mode/Multi-Mode Compression Ignition: Fuel-Property Characterization and Prediction Principal Investigator: Tim Bays (Pacific Northwest National Laboratory)

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

Reviewer 1:

Pacific Northwest National Laboratory's (PNNL) (Bays) approach to understanding of the influence of oxygenate clustering on fuel properties affected by distillation is the well-planned and thought-out research expected from a National Laboratory. This research is important in understanding combustion and more importantly LTC. which may be sensitive to certain fuel property effects. Dr. Bay's approach using nuclear magnetic resonance (NMR) is unique.

National Renewable Energy Laboratory's (NREL) (Fioroni) research into the impact of azeotropes on heat of vaporization (HOV) and species evolution uses a unique tool and approach to develop HOV information that will be useful for engine designers and researchers in the future.

Reviewer 2:

The project is well focused and planned to deliver underlying knowledge and data on fuel effects in engine combustion and fuel-blending phenomena. Coordination with the Vehicle Technologies Office (VTO) and the Bioenergy Technologies Office (BETO) participants appears good.

Reviewer 3:
This project aims to improve the measurement of critical fuel properties relevant to engine efficiency, including gasoline volatility and evaporation, relationships to azeotropic behavior, and predictive modeling of properties that blend non-linearly. The project also focuses on advancing the underlying science needed to develop biomass-derived fuel and advanced engine technologies. The scope and the tools available to this project team all are well suited to making significant progress on improving our understanding of the objectives above.

Reviewer 4:
This fundamental work will be very powerful if and when it can be more closely associated with modeling for sprays, combustion, and emissions. The team does now have that work planned for 2021, and it will be the critical link for ultimate utilization of the fundamental work.

It is surprising that the Aspen model can correctly predict spikes in instantaneous heat of vaporization (iHOV) behavior for gasoline-alcohol blends during evaporation, and yet we know so little about the causality. Detailed analysis of the modeling architecture could suggest the route to further experimental campaigns for full comprehension of these effects. Spikes in the iHOV like this will have a substantial impact on eventual spray and evaporation modeling.

Reviewer 5:
The point of some of this fundamental work is not really clear to this reviewer. The molecular modeling to predict evaporation behavior is interesting in and of itself, but has no tie to any physical measurements that show there is a significant impact of the variables considered on the spray evaporation and resulting engine behavior. This reviewer had no doubt that there are differences, but the significance factor is key. If this does not help an OEM make its engine better or a fuel company make its fuel better, then the work does not really accomplish much of engineering value (scientific value, yes, but that is a different program). The work to predict research octane number (RON) and motor octane number (MON) is useful, especially in the context of blend studies. As previous reviewers noted, this does not cover everything that we need to understand about the fuel, but it is a good first step.

Reviewer 6:
Investigations into the impacts of molecular clustering on vapor pressure (Task F.1.2.2a) and investigations into the instantaneous heat flux of evaporating mixtures (Task F.1.3.2) are both technically sound and have the potential to shed light on fundamental processes influencing how fuels move from the liquid to the gas phase. However, particularly in the case of the instantaneous heat flux measurements (Task F.1.3.2), a key question is whether the phenomena observed in the benchtop experiment will be relevant to practical engines, in which liquid fuel evaporation timescales are presumably much shorter, reducing the time available for diffusion within the liquid during evaporation.

The neural-network approach (Task G.1.1a) to fuel blending models being developed by Lawrence Livermore National Laboratory (LLNL) is offering high-accuracy predictions of fuel properties and beginning to exceed predictions of existing, well-regarded blending models while offering the ability to utilize more precise descriptions of mixtures.

Reviewer 7:
In general, all sub-projects under FT067 are addressing the objective of the project to characterize and predict fuel properties relevant to engine combustion (MM or otherwise). There is a disconnect between the stated barriers on Slide 2, which emphasize fuel kinetics and LTC, and the sub-projects included in the presentation. None of the sub-projects is directly addressing fuel kinetics or LTC. However, the fuel property characterization and prediction being targeted by the sub-projects—including fuel volatility (vapor pressure), evaporation, and knock resistance (octane)—are critical for improving the modeling capabilities of current engine simulation tools, and the associated teams are encouraged to continue their fundamental research.

Reviewer 8:
The order of operations in this project seems out of order for efficiency. For example, the reviewer suggested starting with the actual measurements of fuel evaporation and only going on to the very complex work with the molecular dynamics simulations. It looked to the reviewer that this is an awful lot of work to undertake when there is not much difference.

Additionally, this presentation often failed the “so-what?” test (made famous by another reviewer, who encapsulated this comment in a question during the presentation)—the reviewer spent quite a lot of time reading and re-reading the yellow bar take-away messages on each slide (for example, Slide 8) to try to figure out what is the real conclusion in terms of the application of the new fundamental knowledge gained in this work.

The reviewer indicated that the overall work done in this project is solid, but that the significance of the work is not well described in the presentation. For example, the reviewer was able to learn from some fuel industry colleagues that this work relates well to the refinery models, but that was never made clear in the presentation. In addition, the reviewer thought there was a missed opportunity to point out (from what could be seen in the slide) that the error analysis showed that the model has better results than an octane engine.

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:
Although many projects have been slowed due to the COVID-19 pandemic this year, important findings have been produced on the effects of oxygenate clusters and better prediction of octane numbers in blends that have non-linear characteristics. The overall record of publications is strong.

Reviewer 2:
The team made significant progress in understanding how oxygenate clusters and networks contribute to vapor pressure, finding the dominating interactions of gasoline-alcohol blend evaporation, and developing a neural network model for the predictions of fuel properties.

Reviewer 3:
The reviewer stated these are great fundamental efforts, for which the community is impatiently clamoring for the eventual utilization of these efforts to enhance the predictive spray and combustion modeling tools.

Reviewer 4:
This project has made very good progress over the past year. Some of the notable accomplishments include:

- Better understanding of the impact of oxygenate clusters on fuel volatility and evaporation
- Improved characterization of the HOV
- Development and refinement of a neural network-based model to identify fuel blends with desirable properties.

The ability of the blending model to accurately estimate fuel RON and MON is quite impressive. The neural network based model seems to be a promising tool for optimizing fuel blends with targeted properties.

The aforementioned accomplishments, along with others, demonstrate progress toward DOE’s higher-level goals. However, the absence of well-defined performance indicators makes it difficult to quantify the progress toward DOE’s goals. Considering that DOE’s guidelines require progress to be evaluated against well-defined performance indicators, the project team should consider making a concerted effort to show such information in the Annual Merit Review (AMR) presentation.

Reviewer 5:
By furthering the understanding of clustering, azeotropes, and HOV, the researchers are enabling a better understanding of non-linear blending effects such as octane and distillation. The researchers are making great technical progress.

Reviewer 6:
The technical results presented here are of high quality, providing fundamental insights into the phase change of fuels and demonstrating the robustness of the approach to fuel-blending models.

Reviewer 7:
The progress on the tasks under execution has been good. Again, that is with the proviso that some of the tasks seem divorced from the ultimate engine needs.

Reviewer 8:
The project is clearly on track, even with the COVID-19 pandemic. The reviewer thought the technical accomplishments are sound, but again, struggled to understand how this fundamental knowledge will be impactful to the application.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
There is outstanding collaboration between participating National Laboratories and universities. This was also evident during the periodic stakeholder conference calls.

Reviewer 2:
The efforts by the team members are using complementary characterization methods. Members appear to be sharing and co-analyzing results and are working across the VTO and BETO sponsor organizations. The blend octane number predictions via neural net are very interesting and potentially valuable.

Reviewer 3:
The reviewer observed strong collaborations across National Laboratories. Based on the slides presented, it seems that there are some universities that participated in this project. However, it is not very clear what their roles are. The reviewer hoped their contributions can be included in the “Technical Accomplishment” slide to be clear.

Reviewer 4:
The team coordinates work between nine National Laboratories and university laboratories to perform this work. There is outstanding coordination within the team to get the work done. In the future, when LLNL wishes to validate its blending models, there is enough expertise in the team to do so.

Reviewer 5:
It appears that the partners are well connected and collaborating appropriately.

Reviewer 6:
The various moving pieces do seem well coordinated within the teams. The reviewer would like to see significantly more teaming with some of the experimental groups that can show the significance of this work. The Engine Combustion Network (ECN) groups are studying sprays; can this team link with them to show that the fundamental work here is relevant to the experimental results that they see? The engine combustion groups have the ultimate test: to find out if the engine cared about some of the things this team is studying. This team needs to link with the ECN to show impact potential.

Reviewer 7:
Collaborators include nine National Laboratories, and four universities, but the reviewer did not see any collaboration with industry. The reviewer thought that having some industrial feedback would greatly help this project remain relevant to VTO and BETO goals for deployment.

Reviewer 8:
Each task has a number of external collaborations listed, primarily with universities, but there appears to be less coordination among the three tasks presented here.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The reviewer was glad to see that the work is planned to move toward linking the fundamental work to real spray and combustion phenomena. The reviewer thought that the quicker the projects can show links to spray and combustion behavior, the better; that will focus the further fundamental studies toward the right questions.

Reviewer 2:
The future work appears coordinated with the overall Co-Optima effort. The team responded well to reviewer comments from last year.

Reviewer 3:
The team very clearly identified the challenges, barriers, and limitations of the research at the current stage. Future research areas are well planned and aimed at solving the remaining challenges.

Reviewer 4:
The future research direction is crucial to the applicability of these fundamental studies. The team recognizes this and has planned 2021 work accordingly.

Reviewer 5:
The team proposes fundamental research to understand reaction species that explain phi-sensitivity and non-linear octane blending. This will be done by using machine learning to cluster simulated chemistry features to uncover hidden correlations between engine models and engine performance; conducting droplet vaporization simulations to realize the effect of HOV of alcohol blends on mixture stratification due to evaporation; and quantifying the effect of dilution properties on autoignition. This is the type of work National Laboratories should be working on, ones where they take on complex problems with unique research and expertise.

Reviewer 6:
The identified challenges, barriers, and proposed future research appear to lay a lot of emphasis on phi-sensitivity. While phi-sensitivity may be important for a particular combustion mode, some of the fundamental fuel property characterization being investigated by the sub-projects in this report can be significantly more impactful. For example, the reviewer suggested that improving fuel vaporization and spray development capabilities of engine simulation tools stands to have a much more substantial impact on automotive engines currently under development than phi-sensitivity. Improved spray modeling is critical not only for improving simulation of engine combustion but also soot formation, with the latter being a significant challenge that the automotive industry is currently working on addressing regardless of the type of combustion system. The team is encouraged to apply the fundamental understanding of fuel properties presented in the current report to improve the spray modeling and engine combustion capabilities of engine simulation tools.

Reviewer 7:
Based on what has been postponed due to COVID-19, it seems that the future work plans are solid, but the reviewer thought the impact of this work could be greatly improved by bringing in some more formal collaboration with the Coordinating Research Council (CRC) companies.

Reviewer 8:
NREL's (Task F.1.3.2) proposed future work—using simulations of evaporation, which have now been shown to predict the relevant azeotropic behavior to interrogate the impact of said phenomena on droplet evaporation in engine-relevant situations—is a great way to potentially transfer the fundamental knowledge gained through benchtop experiments.

LLNL's (Task G.1.1a) future work—using kinetic models to investigate phi-sensitivity and machine learning to search for correlations—is both a highly relevant and valuable endeavor. Particularly, the machine learning task addresses a shortcoming in current research the challenges of distilling complex multi-physics problems to controlling variables.

It is unclear how investigations into the relationships between distillation behavior and fuel octane ratings (Task F.1.2.5) will be conducted without significant partnerships with organizations that have been working on this topic for years (Argonne National Laboratory [ANL]).

The proposed work, "Develop methods to control and optimize fuel component vapor-liquid partitioning, through modification of distillation azeotropes…" does not provide enough detail, while the concept of tailoring autoignition properties through the tuning of azeotropic behavior is interesting but academic.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
This research to provide fundamental understanding will aid future biofuel formulations for maximum utilization effectiveness.

Reviewer 2:
These efforts clearly support the overall DOE objectives. The reviewer believed that DOE should sponsor more fundamental research, like this project.

Reviewer 3:
Once the planned 2021 work is complete, the relevance will be very clear to the community. The reviewer encouraged the project team to keep up the good work.

Reviewer 4:
Improved fuel property characterization is essential for enhancing the capabilities of engine simulation tools and, in the process, helps accomplish the DOE's goal of improving engine and vehicle efficiency.

Reviewer 5:
Without understanding the effects on non-linear octane blending and how it changes phi-sensitivity, it will be extremely difficult to operate engines using LTC regimes.

Reviewer 6:
The reviewer believed that the work is relevant to the more fundamental goals of Co-Optima.

Reviewer 7:
The tasks presented here are relevant to overall DOE objectives of delivering knowledge to industry that supports improving the efficiency of internal combustion engines and reducing the consumption of petroleum. Both the fundamental phase-change phenomena and the prediction of fuel properties support these goals.

Reviewer 8:
Within the context of the Co-Optima program and its support of DOE objectives, this project does play a role. The reviewer tended to think it is biased a little too far to the fundamental, or, at the very least, it is not well communicated how it ties to the engine engineering side of the program. As the teams can show how this work impacts real engine behavior, then the project can be more and more relevant toward DOE objectives.

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

Reviewer 1:
For the work being done, the budgets seem quite reasonable for the work plan and output.

Reviewer 2:
The team has sufficient resources to achieve the stated milestones in a timely fashion.

Reviewer 3:
The team appears to have resources appropriate to the tasks.

Reviewer 4:
The funding is sufficient for the proposed work.

Reviewer 5:
Based on the progress of the team and the extensive research capabilities of the team, the resources appear to be satisfactory.

Reviewer 6:
The resources seem sufficient.

Reviewer 7:
The funding appears on the low end of sufficient, considering the team size and progress.

Reviewer 8:
The project ambitions, indicated by the goals and proposed future work, are not fully supported by the resources devoted to the project.

Presentation Number: ft069
Presentation Title: Multi-Mode: Fuel-Property Impacts and Limitations on Combustion–Spark Ignition Focus
Principal Investigator: Derek Splitter (Oak Ridge National Laboratory)

Presenter

Derek Splitter, Oak Ridge National Laboratory

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 86% of reviewers indicated that the resources were sufficient, 14% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

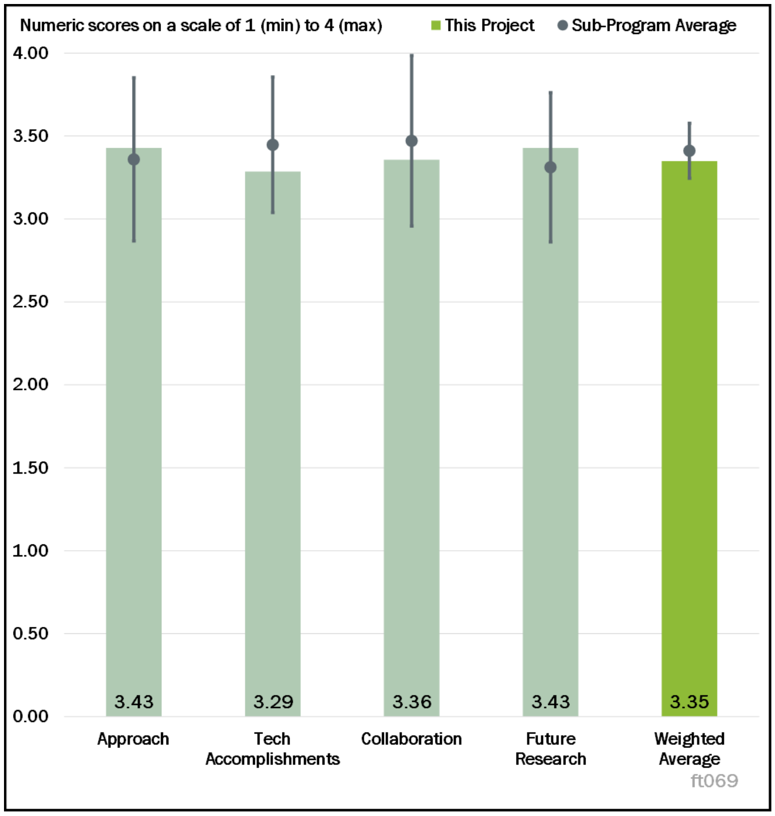

Figure 5-3 - Presentation Number: ft069 Presentation Title: Multi-Mode: Fuel-Property Impacts and Limitations on Combustion–Spark Ignition Focus Principal Investigator: Derek Splitter (Oak Ridge National Laboratory)

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

Reviewer 1:

The approach is excellent. The researchers are covering a considerable number of factors that could affect the limitations of MM combustion in SI engines. The engine and spray work is impressive.

Reviewer 2:

The team leverages multi-cylinder engine (MCE) experiments, CFD modeling, and single-cylinder engine (SCE) work to explore advanced strategies to mitigate knock and increase fuel tolerance of ACI MM combustion. Overall, the project is well scoped. The goal of the CFD work should be better explained, especially how it will support the SCE and MCE work.

Reviewer 3:

The combination of knock mitigation work with ACI fuel tolerance is logical and drives well at the technical barriers.

Reviewer 4:

It is very encouraging to see that the project team is directly trying to address barriers identified by the automotive stakeholders. Doing so increases the likelihood of the ongoing and proposed research to contribute to development of production engines and thus be implemented in mass market applications. The topics being investigated in this project (impact of MON, low-temperature heat release [LTHR], spray modeling, and low-speed pre-ignition [LSPI]) are very relevant for current and near future engines, and continued research in these areas is strongly encouraged. The MON/octane sensitivity (OS) investigation should consider exploring higher engine speeds at elevated intake air temperatures, as these conditions are relevant for both peak power and heat rejection. As none of the other questions cover this, the reviewer is including this feedback as part of this response. The current presentation has insufficient description of operating conditions on most plots, which makes it harder to assess/appreciate the significance of the data being presented. Kindly consider specifying the operating conditions either on the plots or in backup for future presentations.

Reviewer 5:
The primarily experimental approach outlined here, with kinetic modeling support, will deliver highly relevant data on the impacts of fuel properties on the range of operation of conventional SI and ACI operating modes, as limited by knock (or ringing), as well as other unidentified phenomena that may be challenging to predict through modeling. In particular, the upgrade to the General Motors (GM) SG2 head will improve the relevance of the ACI results.

Reviewer 6:
There are lots of different tasks here, but they are broadly very well tied to end impacts of Co-Optima. The work is providing valuable insights into the impact of fuel chemistry as well as gross properties. Simulation comparisons to the experiments also bring value to validate the simulation quality and demonstrate how to effectively use the simulations. The reviewer is less enthused with the stochastic pre-ignition (SPI) studies as presented here. There are some new details to be sure, but the broad results are more or less covered in the current literature on the phenomenon. It would be helpful to see what the end goal of the SPI work is, and how it is distinct from all the work done to date in that area.

Reviewer 7:
First, the reviewer found it really important to note and emphasize that it is really difficult to do a comprehensive review of the projects in this presentation because there were just too many included to allow for time to go into any depth of description. The reviewer strongly disliked this approach to reviewing these projects. When you are talking about large amounts of money and complex science, this “mash up” approach does not do justice to the work.

The approach to this work is based in experimental evaluation of the Co-Optima core fuels under real engine (not just SCE) operating conditions. Due to this realistic evaluation of the fuels, the reviewer knew that simple fuel properties are insufficient for determining their performance (no easy answer) (regarding the ORNL engine projects.

The ANL sprays work is really too young to review yet if it started late in 2019.

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’s comments here are similar to those for Question A. The investigation of MON effects on power density is of high value; if fuels were to change to accommodate ACI, there still needs to be consideration of the fallback to more conventional operation. And separating the details of fuel chemistry and octane is of high value. This is work that both supports future ACI efforts, but also supports current industry efforts to increase conventional SI combustion. There could also be value to the general aviation community and the ongoing efforts to get rid of 100 Low Lead (100LL) fuel from the market, but the failure to date is in finding a good alternative. If some of the chemistry work here were communicated to those in the aviation world, there could be some nice knock-on benefits.

Reviewer 2:
The team has made very nice progress. The work related to CFD should be accelerated to catch up to the other activities.

Reviewer 3:
The technical accomplishments seem on pace for this investigation. However, it can be difficult to assess due to the wealth of parallel avenues presented at once. There is usually only a couple of minutes discussing the technical content and singular slides representing the congruous contributions from all other portions of the project.

Reviewer 4:
This project has made excellent progress over the past year. Some of the notable accomplishments of the project include:

- Impact of MON on knock resistance
- Impact of fuel composition on LTHR under different operating conditions
- Improved spray modeling and combustion simulation to help investigate LTHR
- Better understanding of the impact of fuel volatility on LSPI/SPI.

The excellent match between experiments and simulations for spray pattern and penetration and the combustion process/pressure profile is quite impressive. It is unfortunate that the PI was limited by resources, as the SPI response of low volatility fuel under different operating conditions (higher load) would have provided further insight into the impact of volatility and oil additives (Calcium [Ca]) on the likelihood of SPI occurrence. The PIs are encouraged to include quantifiable performance indicators in future reports in accordance with DOE guidance to reviewers for evaluating projects.

Reviewer 5:
This reviewer really liked the work that is being done here. The reviewer would have given the projects a higher mark; however, the SPI chart on Slide 17 shows that there is no statistical significance between the data. From the looks of it, the data could have used a larger data set. There is significant clustering of the data to show trends, but the whiskers in the box and whisker-plot overlap are indicating a need for more data to reduce the error. The reviewer wished the rating would allow more granularity, as the lack of data looks to be from insufficient funding of the engine testing.

Reviewer 6:
There is clearly significant progress being made in the engine projects; however, it is clear that the barriers are significant and there are persistent issues that are difficult to overcome. Additional work is clearly needed.

Reviewer 7:
Investigations into the effects of a fuel’s MON rating on high-speed high-load operation are promising, but have not yet covered a range of fuels and compression ratios such that this question can be put to rest. The results shown from SCE investigations into autoignition behavior provide a baseline for future work in this engine platform, however, the results shown here replicate prior results and have not progressed to providing new insights.

Engine modeling results demonstrate reasonable agreement with the experiment in two of the three validation cases shown, but the “Strong pre-spark heat release (PSHR)” case exhibits significant differences in flame propagation between the experiment and the model that will need to be addressed before investigations into fuel-specific phenomena can begin.

LSPI investigations hold promise but the results shown here have not yet advanced the state of understanding beyond what is available in the literature.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer sees excellent collaboration and coordination with other laboratories and universities, and very strong ties to industry. The strong participation in the Advanced Engine Combustion (ACE) Memorandum of Understanding (MOU) and the strong corporate support is excellent.

Reviewer 2:
This reviewer is impressed with the level of collaboration that has been going on during the entire AMR. This specific project has an impressive list of experts in the engine and modeling fields.

Reviewer 3:
Excellent collaboration between participating National Laboratories and industry stakeholders.

Reviewer 4:
The collaboration across the project teams appears to be fine. The reviewer wonders the reason that it took so long of making the engine data available to ANL for the CFD work. The project gained support directly from auto and oil industries, showing excellent relationship and collaboration.

Reviewer 5:
The apparent level of collaboration and coordination varies across the project team. Demonstrated examples of collaboration include the engine modeling task, which combines experimental data from multiple sources (engine data from ORNL and spray data from Sandia National Laboratories [SNL]) to support the task. Another positive example is the connection between experimental autoignition studies in engines and the kinetic-modeling task.

Reviewer 6:
In general, the team is appropriately collaborating amongst the working group. However, it was unclear if a distinct collaboration between the ACI autoignition sensitivity changes and the other groups working on fuel chemistry/kinetics impacts exists.

Reviewer 7:
This is an odd assemblage of projects to look for collaboration. They are generally on separate engine platforms and investigating different topics within the broad topic area. The reviewer was sure the PIs are coordinating well since most of them are at one lab, but did not see any meta-narrative that says how the findings from the various tasks come together.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The project team very clearly identified the challenges, barriers, and limitations of the research at the current stage. Future research areas are well planned and aimed at solving the remaining challenges. The team should consider how the results of this work can be better transferred for future engine development.

Reviewer 2:
The future work plan seems appropriate based on the barriers to be addressed.

Reviewer 3:
The project has made excellent progress thus far, and continuation of several of the ongoing efforts is encouraged. For example, there is growing evidence that fuel particulate matter index (PMI) is not only important for engine-out particulate emissions but also the propensity of SPI occurrence. Investigation of the

impact of PMI on SPI occurrence is strongly encouraged. Improving the CFD capabilities to model fuel spray, evaporation, and combustion (including LTHR) is also strongly encouraged.

Reviewer 4:
The proposed future research appears to be comprehensive. The reviewer would only suggest that the SPI testing have more data points and that follow-up with the engine testing be performed.

Reviewer 5:
This reviewer particularly looked forward to the multi-cylinder SI work, as it will become more translational to the application.

Reviewer 6:
The proposed future research collectively addresses a number of particular challenges identified by the United States Council for Automotive Research (USCAR) and Co-Optima, including the applicability of fuel properties such as PMI to LSPI, and the response of fuel-dependent, low-temperature autoignition reactions to lean operation.

Other proposed work seems duplicative; for instance, "Extension of the pressure-temperature (P-T) analysis framework to consider in-cylinder…" already exists within the literature and within the DOE national laboratory complex.

Reviewer 7:
Again, the different tasks end up with different grades here. The study of LTHR and SI versus ACI operation is great; this is foundational stuff that will be required for any future engine development. The CFD work is also well tailored to future R&D needs. The P-T analysis is fascinating stuff, though the reviewer still struggled to follow it well when watching a fast presentation. On the other hand, the SPI work is less valuable looking to this reviewer's eyes. The industry has spent some time looking at fuel effects on SPI, and there are publications looking at some of those effects. The biggest challenges to SPI with respect to fuel are generally that the OEM will not have any knowledge of or control over the fuel that goes into the engine (particularly when the industry talks about global fuel markets). Therefore, OEMs will remain constrained to hardware designs that are tolerant to worst-case fuel scenarios. This reviewer was not sure exactly what to recommend instead, but did not think the plans as stated are all that valuable, especially within the context of ACI.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
Broadly, these tasks are well aligned with DOE objectives to demonstrate technologies for improved fuel economy.

Reviewer 2:
This project aligns with DOE objectives and Co-Optima goals.

Reviewer 3:
The project is well aligned with overall DOE objectives to advance the efficiency of vehicle engines.

Reviewer 4:
The research topics undertaken as part of this project are extremely relevant, not just for MM combustion but for conventional SI engines as well.

Reviewer 5:
The issues being investigated by the research team are significant barriers to the impact of MM combustion. By understanding the effects of fuel properties on MM combustion efficiency, improvements can be made.

Reviewer 6:
Knock mitigation is probably one of the most key issues to internal combustion (IC) engine efficiency—so this project is highly relevant.

Reviewer 7:
The projects and tasks shown here directly contribute to the understanding needed to design the next generation of engines and fuels, leading to reduced fuel consumption and greater utilization of resources.

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

Reviewer 1:
The budget seems adequate for the work performed and work proposed.

Reviewer 2:
The team seemed to have adequate resources.

Reviewer 3:
The project funding appears well aligned with the project scope and milestones.

Reviewer 4:
The funding is sufficient for the proposed work.

Reviewer 5:
Resources appear sufficient.

Reviewer 6:
The projects are adequately resourced, allowing significant effort to be devoted to the tasks, which is in alignment with their importance.

Reviewer 7:
On Slide 17 the data appear to be statistically insignificant. From the reviewer's experience, this is an effect of too few data points. This can be eliminated by running more tests because a clear trend can be drawn from the data.

Presentation Number: ft070
Presentation Title: Multi-Mode: From In-Cylinder Combustion Diagnostics to Drive-Cycle Fuel Economy
Principal Investigator: Magnus Sjoberg (Sandia National Laboratories)

Presenter

Magnus Sjoberg, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 80% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 20% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

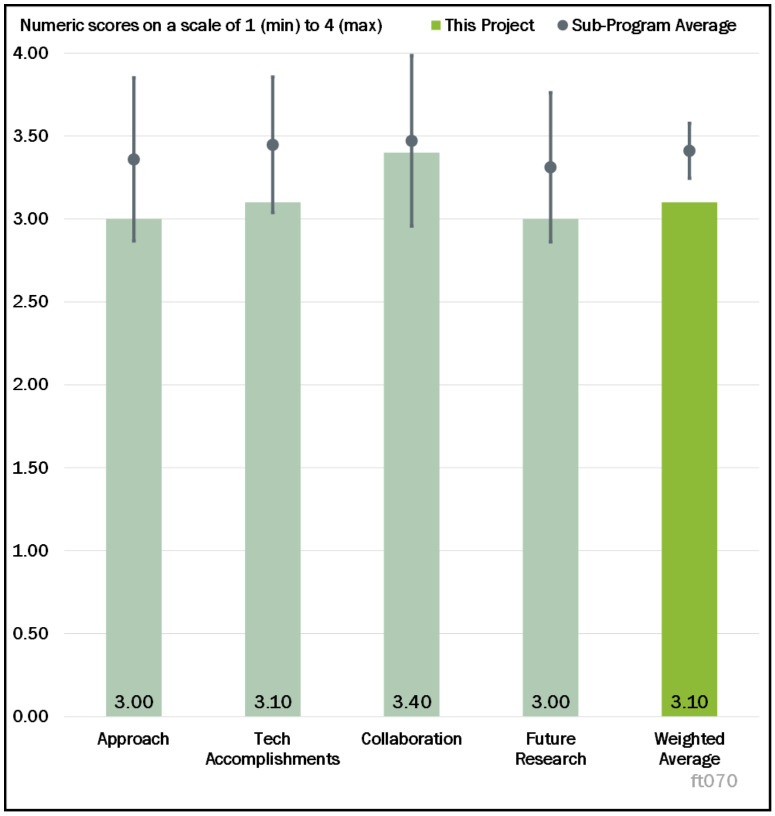

Figure 5-4 - Presentation Number: ft070 Presentation Title: Multi-Mode: From In-Cylinder Combustion Diagnostics to Drive-Cycle Fuel Economy Principal Investigator: Magnus Sjoberg (Sandia National Laboratories)

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

Reviewer 1:

The team has an outstanding approach using both metal and optical engines along with computational analysis.

Reviewer 2:

The approach in this project is pretty good—there is experimental and simulation work that appears to support each other nicely—but the overall goal of the project seems a bit unclear. If the intent is to explore MM combustion systems for an LD engine, there needs to be a determination made about whether the overall engine will be stoichiometric or lean. The aftertreatment requirements are quite disparate, and there is no way that any potential benefits of a part-time stoichiometric/part-time lean system will not be consumed by the horrific cost and complexity of two aftertreatment systems. As mentioned in one of the questions, the target needs to be ultra-low nitrogen oxides (ULNO$_x$) compliance, not current NO$_x$ compliance. There needs to be a better case made for why this MM approach is going to provide benefits in efficiency or operational use compared to simply hybridization or electrification.

Reviewer 3:

The reviewer was not sure how, or if, the knowledge from these research efforts is advancing the knowledge of MM combustion relative to what industry already knows. The reviewer would happily change this comment if the research questions being investigated here were shown to have been developed in collaboration with an industry group like USCAR, for example.

Reviewer 4:
The connection between yield sooting index (YSI) study and piston top fuel film formation to mixed-mode ACI combustion is unclear.

There is also a range of different combustion approaches explored in the work, and understanding fuel effects on the specific mode is a focus and clear outcome. However, the reviewer highlighted the following key challenges with mixed-mode operation:

- Optimal fuel properties for the advanced combustion portion of the cycle may differ vastly from those being used in the conventional portion, and understanding this impact is critical to the success of a mixed-mode concept.
- Multiple combustion modes require a transition between operating strategies, and operation through that transition may compromise performance and ultimate capabilities of the advanced combustion mode.

These are the central challenges of mixed-mode, but seem to be largely absent from the direction of the work. For any concept to be practical for commercial adoption requires that its operation meets relevant emissions targets. Including required aftertreatment considerations should be fundamental to any advanced combustion strategy evaluation.

Reviewer 5:
The approach taken at SNL is mostly sound, with the investigations of YSI as an alternative to PMI to understand sooting and particulate matter emissions from lean stratified charge engines with oxygenated fuels. However, pursuing the prediction of fuel economy with Gamma Technologies Power (GT-Power) and Autonomie with the results obtained from the SCE, with no rigorous engine-out NO_x control, may have very little value. This task is best left to the OEMs, which is their strength.

The purpose of efforts at ANL and LLNL is not clear. Is there any indication of what fuel property enables spark-assisted compression ignition (SACI) type combustion? Other than the OS of the fuel, the reviewer asked whether the fuel properties for SI boosted operation and HCCI combustion conflict with each other. LLNL’s finding—via 80,000 fuel simulations—that high RON and high OS enable high load operation has been known for a long time.

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 team has made great progress to date.

Reviewer 2:
The progress in this project has been noticeable and has merit. In particular, the model improvement for speed and accuracy and the optical diagnostics that identify soot formation characteristics based upon fuel properties is impressive. But, the challenge of MM is to determine when the engine should be operating in which mode and under which conditions. The work done here should help define that approach, but it appears to be a bit incomplete. The project has made substantial progress in understanding soot formation but cannot decide whether it is stoichiometric, lean, or dilute, or how large the operating range should be for each combustion mode. When this reviewer looked at potentially using this MM approach, it appears that the challenges are greater than the potential improvement can overcome. Idle reduction, low load cycle, $ULNO_x$, and GHG regulations all combine into forcing OEMs to adhere to a coherent strategy for operating the engine. This work has made some progress toward that goal, but the project needs to re-define what the desired outcome should look like.

Reviewer 3:
Overall, the work is very good. The sensitivity analysis being done at ANL has the potential to be very useful, but would carry much more impact if it could be verified experimentally.

The work at LLNL on fuel robustness includes an adjustable parameter in K, an empirical "constant," which is part of the octane index (OI). K changes with engine operating conditions, and even such things as differences in the fuels' HOV can bring about changes in K. As a result, the reviewer did not know how to interpret the results of this effort.

The observation that the PMI has a dependence on vapor pressure of the fuel is not all that surprising. However, trying to include this in any correlation for calculating the PMI of the fuel will now make the modified-PMI a function of the engine in which the fuel is being used, as the fuel's vapor pressure, in combination with the engine hardware, geometry, and operating condition, will impact the distribution of the fuel vapor within the cylinder and the propensity for the formation of liquid films in the cylinder.

Reviewer 4:
The project is delivering significant research output, for which it is to be commended, and is in line with the level of funding received. However, it is not obvious that the work is making quantifiable progress forward to enabling mixed-mode combustion in LD vehicle applications. The project needs to be clearer about how the simulation work will ultimately support the effort. Validation of CFD models is a required baseline step in the development process, but it is important to highlight how these will be used to enable, and further understand, fuel property impact on mixed-mode operation. The reviewer noted that the two CFD-related milestones, model validation and data transfer, are process milestones. Moving forward, these milestones should be prescribed in a way to demonstrate progress against key barriers in understanding mixed-mode operation.

Additionally, CFD results for parameter sweeps were indicated as not having been fully validated with experiments. This is something critical to resolve to ensure that results being generated have value.

Finally, modeling of the fuel economy gain with MM operation needs to include a real penalty associated with both the transition between operating strategies and the emissions control required to deliver tailpipe emissions meeting regulatory standards. For advanced combustion concepts, this is an absolutely essential part of the equation. Results that do not include this, especially the emissions control factor, are meaningless.

Reviewer 5:
Lots of work has been done, however, as mentioned above, the value or impact of the work may be less than desirable. For example, in the work at ANL, partial fuel stratification (PFS) has been added to the recipe of SACI. This has made the combustion more complex and dependent on more control parameters. Was the injection quantity and timing of the late pilot injection varied to test the effect of phi stratification on end-gas autoignition? When does soot become an issue with the late injection?

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
This is an excellent example of how to run a collaborative effort. They have brought in excellent industrial partners as well as laboratory partners.

Reviewer 2:
As is typical of most Co-Optima teams, this project appears to be fairly well coordinated among team members and among different aspects of work—engine experiments, benchtop experiments, and simulation. Communication and coordination appear to be rather good.

Reviewer 3:
The collaboration with this project is excellent. The reviewer hoped that there was close interaction with industry stakeholders as to what they believe are the technology and fundamental barriers that, if solved, would facilitate moving MM operation into the market. It was not clear in the presentation if this is the case.

Reviewer 4:
Good collaboration exists among SNL, ANL, and LLNL.

Reviewer 5:
There appears to be reasonable coordination across the project team, with transfer of information between simulation and experimental activities. There is significant collaboration in areas of fundamental science between project members and other parties. The reviewer encouraged more connectivity with other advanced combustion researchers and automotive R&D organizations to ensure the approach to the project aligns with the key barriers and requirements for mixed-mode operation. Some of the shortfalls highlighted in this year's results could have been avoided with the right connectivity and input earlier in the process.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
Within the stated goals and established projects for this program, the future research is well laid out.

Reviewer 2:
The approach is outstanding, but there is one particular missing aspect that this reviewer hoped can be addressed. For the vehicle simulation work, the reviewer expressed interest in the team doing two things: run the simulations with some emissions constraints given an engineering estimate of how much NO_x and particulate matter (PM) you could tolerate in a production engine; and run the simulations as well with some hybrid powertrains to avoid some of the problematic regions and with even more heavily downsized engines.

Reviewer 3:
There is significant variation and scatter in the LLNL work, but it is focused on low-component-number surrogate fuels. If possible, this should expand to look at more market representative fuels. The reviewer noted that the CFD simulation activity should have an increased focus on delivering results and an increased understanding of fuel property effects rather than further refinement of the models. Overall, the project needs to sharpen its focus onto the key challenges with mixed-mode combustion, and how fuel properties can be used to reduce those barriers, enable operation, and improve overall operating efficiency across all operating regimes.

Reviewer 4:
In the time remaining for Co-Optima 2.0, work at all three labs should concentrate on how the results and findings so far change when engine-out NO_x emissions are constrained (with exhaust gas recirculation [EGR] or other techniques) to make the lean aftertreatment cost effective.

Reviewer 5:
The most important question to be addressed is whether this will be a lean or stoichiometric combustion system in MM. They are fundamentally different and will require OEMs to utilize them in fundamentally different ways. Any future work that relies upon stoichiometric operation at high load and lean LTC operation at lower load is essentially a non-starter. The aftertreatment disaster alone will disqualify this approach; in particular, having enough exhaust energy at low load to keep selective catalytic reduction (SCR) functional in a lean environment to meet $ULNO_x$. The rest of the future work appears to be reasonable insofar as following

up with current success, but the overall intent of the project has a major flaw that must be addressed and is not explicitly addressed in the future work slide.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
Yes, this project does support overall DOE objectives.

Reviewer 2:
Establishing the simulation capabilities for fuel characteristic optimization to identify potential enhancements to MM operation is a relevant objective for DOE.

Reviewer 3:
The project, if focused on the key challenges of mixed-mode operation, does support the DOE objectives for increasing efficiency of, and reducing emissions from, vehicle transportation.

Reviewer 4:
The project fits the DOE goals to improve engine efficiency.

Reviewer 5:
This project aims to reduce petroleum usage and GHG emissions.

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

Reviewer 1:
Resources are sufficient.

Reviewer 2:
There was one statement in Slide 4 that resources were not sufficient to complete the task. No explanation was given. Other than this, it seems that the resources are sufficient.

Reviewer 3:
The scale of this effort is larger than other, similar projects. The combined scale of SNL funding is significant.

Reviewer 4:
The resources are sufficient.

Reviewer 5:
The resources are sufficient and can be focused more on high-impact issues.

Presentation Number: ft071
Presentation Title: Multi-Mode Operation in Gasoline Direct-Injection Engines: Fuel-Property Effects and Approaches to Expand the Advanced Compression-Ignition Range
Principal Investigator: Toby Rockstroh (Argonne National Laboratory)

Presenter

Toby Rockstroh, Argonne National Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 83% of reviewers indicated that the resources were sufficient, 17% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

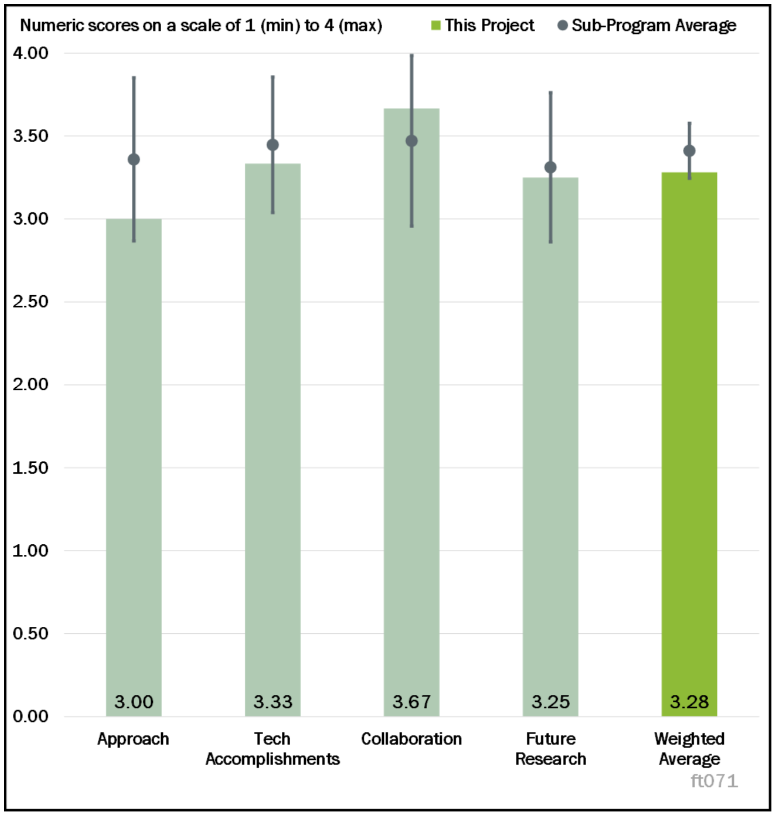

Figure 5-5 - Presentation Number: ft071 Presentation Title: Multi-Mode Operation in Gasoline Direct-Injection Engines: Fuel-Property Effects and Approaches to Expand the Advanced Compression-Ignition Range Principal Investigator: Toby Rockstroh (Argonne National Laboratory)

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

Reviewer 1:

LD MM engine operation offers practical, near-term fuel economy gains over a significant operating map. MM operation consists of low-load ACI and high-load boosted SI. Challenges for MM operation include ACI operating-range combustion and control strategy challenge; strategies needed to enable SI/SACI transition; and maintaining high-load boosted SI operation. This project utilizes engine experiments and high-fidelity CFD modeling approaches to characterize fuel property effects and operating strategies to enable MM engine operation. The researchers’ approach to the work is outstanding.

Reviewer 2:

The technical approaches used are good and linked nicely across the tasks to address the barriers to ACI combustion. Particularly of value is the effort to understand the mode-switching operation between ACI and conventional combustion. The work to develop methods for control schemes is also valuable, as combustion control remains one of the biggest challenges for implementing ACI.

Reviewer 3:

The combined modeling and experimental approach appears well aligned and feasible. There are several good investigations crammed into this 20-minute presentation. It is difficult to assess the details of the approach for several collaborative thrust areas in such a condensed format. This was clear during the question and answer (Q&A) immediately following the presentation. The questions asked would have been clearly explained by the presenter if given enough time to provide an overview of the underlying science and methodology when presenting the accomplishments.

Reviewer 4:
While the presentation identifies the technical barriers that the project tries to address, the link between the described work and the technical barriers is not established very well. For instance, it is not clear how the work focusing on estimating start of combustion will be used to develop methods to extend the limits of LTC. Also, a lot of effort seems to have been spent on correlating the rapid compression machine (RCM) ignition delay data and the chemical-kinetics-based ignition delay estimated using the Livengood-Wu (LW) integral. It may be convenient to use, but is the LW integral the appropriate tool/correlation for this task? There seems to be a lot of effort trying to account for the relatively large errors in the LW based ignition delays. Perhaps the errors are a consequence of the limitations of the LW integral.

The graphic on Slide 9 seems to indicate that the plan is to implement an active pre-chamber in the SCE. However, the material presented corresponds to a passive pre-chamber. The distinction between the planned work and work that has been conducted is not very clear. Additionally, it is not clear if/how the CFD models for MM/ACI combustion will be validated against experimental data. While some evidence has been provided of the ANL model being validated against engine data, there is no mention of corresponding engine data for the ORNL model. While both models appear to be very promising tools for evaluating MM/ACI combustion, it is critical to ensure they are validated against engine measurements.

Reviewer 5:
While it is technically and academically interesting to investigate SACI performance with pre-chamber hardware (Task E.1.2.5), it is unclear how the technical approach used in these experiments will lead to advances in achieving ACI and mode-switching strategies.

The approach of using CFD models (Task G.5.5) to run sensitivity studies can be useful. However, it requires intelligent design of the tested conditions with control over key parameters (combustion phasing, knock, emission) rather than a randomized or parametric approach, which previous research programs have shown to mainly result in exploring irrelevant engine operating conditions. Further, for a model to be useful over a wide range of conditions (e.g., the various combustion modes and conditions that are intended to be tested here), it must be shown to capture the key trends and associated conditions, which are currently the state of the art for CFD models. Therefore, that raises doubt as to whether the approach taken here will truly be able to contribute understanding of the wide range of fuel-property and engine interactions that are envisioned here.

Reviewer 6:
The industry focus areas are fuel economy and emissions and a specific look at CO_2 reduction. It is unclear where the project team thinks this is headed. “Panning for gold” was indicated by this reviewer, who explained that, basically, the project is developing an engine concept and seems to be using the Co-Optima fuel set to determine how well it works. Did this reviewer miss the part where the project team did a fuel property sensitivity study? It is not clear what the learnings provide to help implement the combustion system and mode switching. It would help if the team could show how the modeling work predicted an improvement, and then verify with an engine 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 team has had significant breakthroughs in both modeling the ignition and engine performance in MM operation as well as modeling the transition from ACI to SI.

Reviewer 2:
It appears that a lot of progress has been made in all of the tasks. Other than the COVID-19 delays, the team appears to be well set for achieving the project goals.

Reviewer 3:
All thrust areas of the project appear to be operating at pace for successful project completion.

Reviewer 4:
A significant amount of work has been conducted in each of the covered sub-projects. However, it appears a majority of the work thus far has been in establishing the tools/experimental setups that will be used for work to be conducted over the next year. This reviewer looked forward to observations and conclusions drawn from the work proposed for these projects. Based on the data presented, it appears the passive pre-chamber investigated did not help extend the operation limits for MM combustion. It will be interesting to see if the active pre-chamber enables MM operation over a broader operating regime.

The PIs are encouraged to include quantifiable performance indicators in future reports in accordance with DOE guidance to reviewers for evaluating projects.

Reviewer 5:
The technical accomplishments were solid, but the reviewer just struggled with understanding their relevance. The reviewer thought this was a casualty of the number of projects that were crammed into a single presentation. It made it difficult for the presenters to go into any kind of detail to set the scope of the impact of the work.

Reviewer 6:
The investigations into the predictive power of the LW integral under ACI conditions shed insight into the challenges of using this technique for quantitative predictions, particularly under lower-temperature, higher-pressure conditions where the autoignition event is influenced by first-stage and negative-temperature coefficient (NTC) chemistry. The use of a pre-chamber for ACI/SACI ignition is interesting and an appropriate way to generate relevant in-cylinder thermodynamic conditions for ignition studies with novel and high-performance fuels. However, the use of an unfueled pre-chamber has significant limitations, as shown in the results presented here, and makes achieving relevant conditions challenging.

Additionally, the CFD results from Task G.1.1.1 show surprisingly good agreement with experimental results. What has been learned from the work so far?

This reviewer opined that presented results from Task G.5.5 are worrying. When studying fuel-engine interactions, it is important that relevant engine platforms, combustion modes, and fuels are used in conjunction. When they are not, the results may not reflect the controlling physics found in practical/optimized combinations of hardware and fuels. The results show that a Ford 1.6-L SI engine was used for investigations, which is certainly appropriate for SI, lean SI, and perhaps HCCI with light stratification. However, extending the investigations all the way to MCCI combustion does not make sense, as the PI realized. While this poor pairing of hardware and combustion modes has been halted, even the partially premixed compression ignition (PPCI) mode is questionable, unless the model of the 1.6-L platform has been modified with a new injection system that delivers fuel appropriately under late-injection into hot and high-density conditions. Examining the results on Slide 16, the contour plots highlight a common problem with CFD explorations of operating conditions: most of the conditions shown here are irrelevant, either due to high-pressure rise rates (as can be expected for the overly advanced combustion phasing shown in the right-hand side figure) or low efficiency (likely due to incomplete combustion). What would be insightful would be to show the space of conditions that yield both high efficiency and low-pressure rise rate. Unless algorithms are used to ensure that the majority of investigated operating conditions are relevant (complete combustion, low-knock, low criteria pollutants), large explorations of input parameters will be a poor use of resources.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
Excellent collaboration between National Laboratories, industry, and academia.

Reviewer 2:
The researchers are coordinating well between National Laboratories and within their labs.

Reviewer 3:
All three projects had strong and well-coordinated collaborations.

Reviewer 4:
These tasks are closely linked, and it does appear that the team members are coordinating well to have the experiments and simulations proceeding efficiently.

Reviewer 5:
While there was not time for the team to fully detail the collaboration between investigators within this study, the level of collaboration became increasingly clear during the Q&A discussing the LW modeling setup.

Reviewer 6:
Tasks E.1.2.5 and G.1.1.1 seem to have strong coordination with one another. Task G.5.5 does not seem coordinated with the other two tasks but does seem to have strong coordination across Co-Optima.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The future plans look effective to continue addressing the barriers associated with this program.

Reviewer 2:
The future work scope and timing appears appropriate to successful project completion.

Reviewer 3:
The proposed research is in line with the goals of the project and aimed at addressing the technical barriers that have been identified. The CFD modeling efforts are encouraged to validate the project team's results against experimental data to the extent possible.

Reviewer 4:
While the research into MM combustion is excellent, recent research suggests that when using the pre-chamber, if the nozzle hole is small enough, the combustion in the nozzle might be quenched and radicals that may better enable LTC combustion in the combustion chamber will be formed. Engine and modeling efforts may be directed toward this.

Reviewer 5:
There are significant remaining challenges for each project to continue to attack.

Reviewer 6:
The proposed fuel-property impact studies (Task E.1.2.5) are too broad, and it is unlikely that all of the properties listed will be able to be thoroughly investigated during the project duration. The proposed investigations of tradeoffs between lean- and EGR-diluted MM operation are highly relevant as the pre-chamber will allow relevant thermodynamic conditions to be created in-cylinder. Task G.1.1.1 modeling work

is on point and with a validated model will hopefully lead to practical insights. Task G.5.5 modeling work needs to be targeted at relevant conditions in order to deliver relevant results.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
The tasks are well configured to support fundamental development of ACI engines.

Reviewer 2:
This project is clearly aligned with the DOE objective toward enhanced vehicle engine efficiency.

Reviewer 3:
This project is relevant in advancing the performance of MM engines that will further DOE's objectives.

Reviewer 4:
The investigations of interactions between modern engines and fuel properties will facilitate the design of new, high performance fuels (HPFs) that will improve LD vehicle efficiency by enabling advanced combustion modes.

Reviewer 5:
The proposed research is relevant for DOE's objectives of developing MM and ACI combustion. However, the included research projects are unlikely to result in near-term (less than 5 years) fuel economy gains as Slide 3 may be interpreted to suggest.

Reviewer 6:
It was difficult to understand this presentation and its impact. The reviewer thought the relevance bullet on the summary slide (Slide 21) is a blanket statement that could be put on every presentation at Annual Merit Review (AMR). The relevance on Slide 3 is much better.

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

Reviewer 1:
The budget looks good for the work being performed.

Reviewer 2:
The level of resources appear sufficient and appropriate for the scale of activities in this project.

Reviewer 3:
Resources appear to be sufficient for the proposed scope of the project.

Reviewer 4:
The team has sufficient resources to complete its work.

Reviewer 5:
Resources seem sufficient.

Reviewer 6:
Tasks G.5.5 and E.1.2.5 are resourced appropriately. Task G.1.1.1 is under-resourced and should see more resources devoted to build on the well-validated model that has been developed.

Presentation Number: ft072
Presentation Title: Multi-Mode: Desired Fuel Properties for Advanced Compression-Ignition and Spark-Ignition Engine Performance
Principal Investigator: Chris Kolodziej (Argonne National Laboratory)

Presenter

Chris Kolodziej, Argonne National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 80% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 20% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

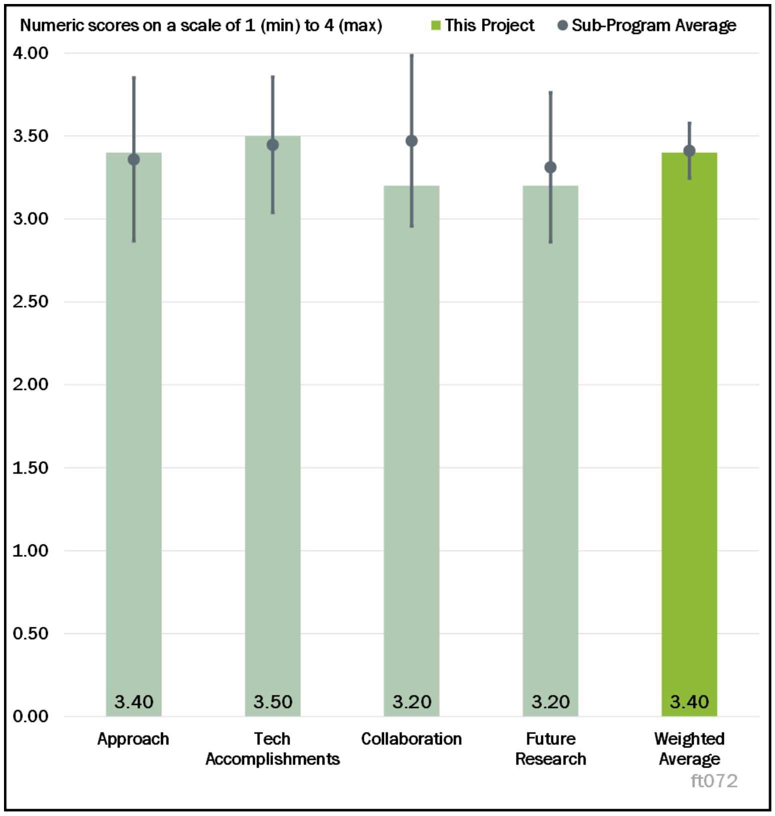

Figure 5-6 - Presentation Number: ft072 Presentation Title: Multi-Mode: Desired Fuel Properties for Advanced Compression-Ignition and Spark-Ignition Engine Performance Principal Investigator: Chris Kolodziej (Argonne National Laboratory)

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

Reviewer 1:

The approach to utilize a Cooperative Fuel Research (CFR) engine and a MD SCE, combined with simulation, makes a lot of sense. The CFR engine can provide very controlled engine conditions to study the fuel autoignition effects and the MD SCE should be able to expand upon those CFR engine results for more practical information. If zero-dimensional (0-D) modeling can be used effectively, this will aid greatly in technology transfer. This project also does a good job in understanding that lean/dilute combustion is likely the system of choice for MD/HD engines, and autoignition will likely be the only realistic choice for this class of engines in the future.

Reviewer 2:

The research is very thorough and being carefully carried out. It follows a systematic progression in attempting to answer the questions at hand.

Reviewer 3:

The team has already recognized that it needs to run additional gasoline-range fuels on the beyond-MON CFR engine.

Reviewer 4:

The approach is sound, and most of the work is directed at finding fuel properties that enable both boosted SI combustion as well as LTC at light loads.

Reviewer 5:
This combined set of projects is a very dichotomous effort. On one side, the ANL activity shows a clear path forward to understand and characterize fuels and their impact on operational barriers. On the other side, the NREL effort looks like it primarily used project funding to build a new engine test cell and has not made much progress toward evaluating fuel effects. This has also limited the effectiveness of the NREL modeling efforts. The NREL work is at a point where delivering the overall project results does not look feasible. The project timeline is more than 50% complete and slated to end at the conclusion of FY 2021. Yet, demonstration of ACI in the NREL SCE is not expected to be achieved until FY 2021. If ACI is not demonstrated until then, it is very unlikely that there will be any meaningful progress on delivering understanding of fuel properties or defining real optimal properties for MD and HD ACI in the remaining time available within this phase of the project.

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 team has made great progress to date considering how COVID-19 resulted in lab shutdowns for months.

Reviewer 2:
A substantial amount of progress has been made. The CFR engine has produced very impressive results in understanding the autoignition properties of various fuels and fuel components. The correlation with other engines in other locations is also impressive. It would also be helpful if this project were to incorporate some of the other groups' work in phi-sensitivity and incorporate that into the results shown here, along with the HCCI number or the proposed "supercharged octane number (SON)" number.

Reviewer 3:
The work at ANL particularly has made good progress with the quest for a new OI correlation with the CFR engine. It is not clear if the addition of another K (K_B) factor and octane number (SON) will help in the quest for a fuel that enables both modes of combustion. The effects of RON, MON, OS, and flame speed—work going on at NREL—is on target.

Reviewer 4:
The researchers have been very productive and bring the appropriate techniques and tools to bear in acquiring the data and doing the analysis. This reviewer believed that the fundamental explanations of the project's results are more complex than what the project team is proposing, as per statements made during the presentation. The use of the OI is an appropriate idea because it acknowledges that there is a link between the engine's temperature, pressure, and concentration-time histories and a given fuel's autoignition characteristics—through the competing kinetic pathways during the autoignition chemistry of the different fuels. The OI uses an empirical factor, K, to account for this. K was originally determined by a regression analysis, so it is, in essence, an empirical "constant." The reviewer thought this has led to confusion and sloppy use of K; there is not agreement within the field on what K really embodies. It is often treated as a constant when applied to a range of experimental data, such as in merit function calculations, for example. Slide 7 in this presentation may be an example of this sloppy use. The compression ratio is changed for each of the fuels in order to maintain a constant CA50. At the same engine speed, this will change the time rate of change for the temperature and pressure for each of the different fuels. The reviewer believed that it is a mistake to then state that the OI for each of the fuels in these tests is the same. The reviewer interpreted the statement that the Ks were equal, so fuels with the same RON and MON would have the same OI, ergo, a different assessment criterion for ranking fuels relative to ACI suitability was needed. This may be the case, but the reviewer did not believe these data specifically point to that. The data are interesting and important, but care needs to be taken in discussing its implication relative to the development of indices that will inevitably have implicit empiricisms.

Reviewer 5:
There are no real technical accomplishments or progress from the NREL efforts despite significant funding levels. The engine installation is in progress and the modeling development is in progress, but there are no clear fuel research outcomes. Validation of CFD models also needs further refinement if the results shown are representative of the current state. The simulations leave much to be desired in terms of replicating experiments since it does not look to be a very close fit, or accurately represents combustion details. The ANL work looks to be somewhat behind, but there are clear deliverables highlighted and significant progress along the two pathways focused on developing metrics for the ACI and conventional operation side of the mixed-mode strategy. Moving forward, the reviewer would encourage work toward seeing whether these two parameters could be incorporated into a single expression. A first step could be to visualize them as an x-y plot and see where different classes of fuels fit within the broader space.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The reviewer described the team as outstanding and reported nine labs and more than 20 partners.

Reviewer 2:
This project appears to have excellent collaboration and coordination among project team members. There is a sensible progression from CFR engine to Ford SCE and simulation work in between. This reviewer would have liked to see a bit more communication with the project working on phi-sensitivity; both sides would likely benefit from this. It is difficult to talk to everyone and also focus upon specific tasks; this is where effective project management and communication become critical. This is a strength of most of the Co-Optima teams, including this one.

Reviewer 3:
Based on one of the questions from another reviewer, this reviewer wondered if more communication with industry stakeholders, like USCAR, would be an additional collaboration worth considering.

Reviewer 4:
Little collaboration seems to exist across the project team. Given the lack of progress of one project, meaningful collaboration may not have been possible. However, external collaboration and coordination with outside parties appears fairly minimal and, on the surface, not overly significant. This subject area seems ripe for cross-laboratory collaboration, connecting the results from the CFR experiments to other mixed-mode projects running engines, as well as screening method development tasks and fundamental fuel-property analysis tasks at various outside laboratories.

Reviewer 5:
The details of the collaboration were not clear, but it looks like most of it occurs behind the scenes by industry and university 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. Note: if the project has ended, please state project ended.

Reviewer 1:
Most of the proposed future research is very relevant and natural extensions of current successes. One question is whether a gasoline direct injection (GDI) injector is the optimal way to study fuel stratification in a compression ignition (CI) engine? Is there a reason why a modified diesel injector was not chosen for the Ford SCE? Under boosted, high compression ratio operating conditions, there may not be much stratification possible with a relatively low-pressure GDI injector.

Reviewer 2:
The reviewer suggested considering a re-evaluation of the data discussion on Slide 7. Overall, future plans are good.

Reviewer 3:
It is concerning that remaining challenges and barriers appear much the same as they were at the start of this effort; that raises the question of how much closer the project is to resolving the project barriers. The ANL effort is on a good track to delivering meaningful results. The reviewer recommended to consider building from that project, drawing in other Laboratories and increasing the scale of focus on this task, which could help mitigate risk and increase the potential for impactful results in this area. This reviewer had very low confidence that the NREL effort will deliver meaningful results in the remaining project timeline, given that NREL has not demonstrated ACI operation in the engine yet and is not slated to do so until FY 2021. This effort needs robust controls and go/no-go milestones to ensure it can deliver progress, or reroute funding to other laboratories to deliver on a refocused effort.

Reviewer 4:
Going forward, other than the known conclusion that high RON and OS fuels enable boosted CI combustion, work should be concentrated on finding the kinetic behavior and fuel property(ies) that enable mixed-mode combustion.

Reviewer 5:
The reviewer questioned the results using the 6.7-L diesel Ford engine for a variety of fuels and making many conclusions. Gasoline-like fuels in CI are very sensitive to injector and piston design and engine calibration strategies. Is there any risk that the project team might make some false conclusions given a fixed hardware? How will the project team account for differences in fuel volatility affecting PM and NO_x if the team gets some localized rich regions due to poor hardware design?

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
Better understanding the autoignition characteristics and which fuel properties are influential is critical to making advanced combustion systems possible for MD and HD engines. This project definitely supports overall DOE objectives.

Reviewer 2:
Understanding the details of a fuel's structure and how it interacts with the thermodynamic time-histories the fuel experiences in the engine cylinder as it traverses through its autoignition chemistry is very important and relevant for DOE.

Reviewer 3:
The work is very relevant to DOE objectives.

Reviewer 4:
This project is aimed at reducing petroleum usage and GHG emissions.

Reviewer 5:
The ANL effort is aligned with the Co-Optima focus on understanding mixed-mode combustion, contributing to a larger program focus on improving vehicle efficiency and decreasing emissions. The NREL effort, appearing to be focused on acquiring new laboratory capabilities, has not demonstrated alignment with DOE objectives.

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

Reviewer 1:
This project appears to have sufficient resources to make the necessary progress.

Reviewer 2:
There was no indication that the funding level was not sufficient.

Reviewer 3:
The resources seem sufficient to perform the tasks.

Reviewer 4:
Resources should be focused efficiently on identifying the fuel properties that enable LTC at light load, without deteriorating boosted SI combustion at high load.

Reviewer 5:
There has been significant funding for the NREL effort, markedly more than other activities, but very little results or forward progress on the specific research topic area. The focus appears to be developing a new engine test cell, and there already exist significant capabilities across the DOE lab space in this area. Although the ANL project has a proportionately small budget, it is demonstrating good progress. The reviewer suggested broadening the scope to include other laboratories, enabled by increased funding levels.

Presentation Number: ft073
Presentation Title: Co-Optima Emissions and Emissions Control for Spark Ignition and Advanced Compression Ignition Multi-Mode Combustion
Principal Investigator: Sreshtha Sinha-Majumdar (Oak Ridge National Laboratory)

Presenter

Sreshtha Sinha Majumdar, Oak Ridge National Laboratory

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

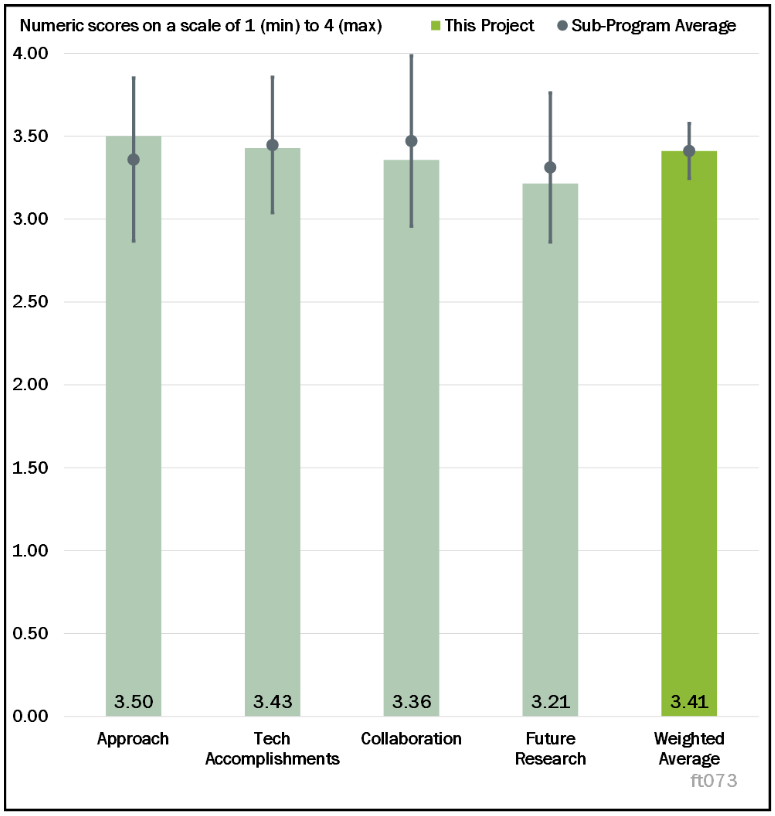

Figure 5-7 - Presentation Number: ft073 Presentation Title: Co-Optima Emissions and Emissions Control for Spark Ignition and Advanced Compression Ignition Multi-Mode Combustion Principal Investigator: Sreshtha Sinha-Majumdar (Oak Ridge National Laboratory)

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

Reviewer 1:

Emissions control for ACI engines is a critical barrier to commercial use; as criteria pollutant regulations become tighter, the low engine-out emissions from ACI will still be far too high for certification. These studies are well crafted to characterize the emissions as a function of fuel properties, chemistry, and engine operation. The tie to catalyst improvements then completes the picture for trying to address this critical barrier.

Reviewer 2:

The approach to evaluate the chemical and physical fuel impacts on emissions is logical.

Reviewer 3:

The approach to each of the sub-projects discussed this year, (1) Task E.2.2.7 (ORNL), (2) Task E.1.3.1 (ORNL), and (3) Task E.1.3.2 (PNNL), was well designed and described this year. Realizing that there are many Co-Optima projects, it is still unfair to put three in one time slot, as was done this year. The reviewer believed in 2019, there were only two. The experiments had access and used appropriate equipment.

Reviewer 4:

Overall, there was a strong approach in the majority of the projects covered in this presentation. Again, it is difficult on reviewers to make really in-depth comments on the work when so many projects are covered in a single talk. Twenty minutes is barely long enough to include any kind of depth with regard to just one of the projects, much less for three (or more in some cases). Therefore, if the review quality is lacking this year, this reviewer believed it is due to the project mashups presented (as in 2019) and not due to the online presentation style made necessary by COVID-19.

The reviewer thought it is particularly important to isolate the fuel property impact, and that the approach taken—to vary aromatic content and distillation range while limiting the changes in fuel sensitivity and RON—is a smart way to accomplish that. The reviewer really appreciated all of the synthetic gas reactor work at ORNL; this three-way catalytic converter (TWC) work yet again highlights the importance of bench reactors running realistic exhaust conditions (including water) with a less complex gas profile. It was not clear to this reviewer that the PNNL reactor work includes water in its synthetic gas.

Reviewer 5:
The scope of this work seems focused and somewhat limited. The representation of the fuel variance is interesting, but it is understandable that the effort keeps the variation limited. Are the conclusions drawn from one condition sufficient to represent a "normal" operating envelope? Looking at performance of commercially available TWCs is understandable. Looking at variations expands the degrees of freedom substantially.

Reviewer 6:
This effort focuses on the effects of fuel on engine-out speciation as well as tailpipe emissions. Although the engine-out speciation work is well thought out and inclusive of all the criteria emissions species, the tailpipe emissions results and approach are not as definitive. Those results are highly reliant on the catalyst formulation chosen.

Reviewer 7:
Emissions compliance is arguably the biggest challenge that needs to be addressed for MM/ACI combustion concepts to be production viable. This makes the research undertaken as part of this project perhaps the most critical for the success of MM/ACI combustion. All the sub-projects covered under FT073 are addressing key challenges associated with emissions aftertreatment. As automotive stakeholders have repeatedly stated, it is essential that the fuels for conventional SI combustion and MM/ACI combustion concepts need to be common. MM/ACI combustion concepts have virtually no chance of succeeding if they rely on a different set of fuels. Thus, the PIs are strongly encouraged to use fuels more representative of market fuels. For instance, the fuels used for the investigation of ACI combustion emissions are nominally 87 anti-knock index (AKI), but the RON is lower than the market average (approximately 91.5-92). Additionally, the "High" aromatic case is more representative of the average for the U.S. market. The higher range for aromatics in market fuels tends to be around 35%, instead of 25%.

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 evaluation of fuels and the catalyst performance influence were interesting. The investigation utilizing a reactor to characterize species will set expectations, but it will be interesting to see if quantification will be complicated once an engine is used for feed gas.

Reviewer 2:
The Accomplishments of the projects were excellent. For this reviewer, the first one presented was excellent, but harder for this reviewer to evaluate. The findings in the two aftertreatment projects were important, first evaluating the activity of a wide range of HCs that may be used in a Co-Optima fuel and, next, evaluating the activity of nanoparticle versus single-atom catalysts under equivalent conditions was very revealing. However, with only 6minutes per project, further extensions of this work could not be discussed, such as the impact of HCs on the activity of other reactants in the experimental feed in number two.

Reviewer 3:
There was a wealth of information presented from the various thrust areas without a time allotment for extensive background/setup explanation, making it difficult to assess the technical merit. Many of the results presented are already generally accepted as fact. However, these appear to be baseline assessments as the fuel recommendations get passed to the team.

It seems counterintuitive that the particulate mass and particle number (PN) are much lower for the fully stratified (0/100) case relative to the partially stratified (70/30). Even the elemental carbon emissions are higher for the 70/30 case than the 0/100. A major goal of incorporating partial charge premixing is to help lower particulate counts/mass from that of fully stratified operation. The start of injection (SOI) for the late injections is very different for the 70/30 and 0/100 cases. The investigators state that the injection timings were designed to hold CA50 constant for all combustion types, which is a solid strategy. The community looks for a greater host of operating conditions in the SCE testing phase.

Reviewer 4:
Excellent progress has been made over the past year on multiple fronts. The emissions data presented provide valuable insight into the impact of fuel composition on engine-out emissions for various ACI combustion modes. The PI is encouraged to continue this investigation under multiple operating conditions—first steady-state and then transient. Additionally, the investigation of light-down temperatures provides critical information for aftertreatment requirements of MM combustion concepts. It helps underscore the challenge of emissions compliance when operating on current market fuels as it indicates that highly paraffinic fuels will be more difficult to deal with under lean light-down conditions. Low-temperature oxidation using platinum (Pt)/ceric oxide (CeO_2) nanoparticles shows some encouraging results, but more work is needed to aid the development of low-temperature aftertreatment solutions. The PIs are encouraged to include quantifiable performance indicators in future reports in accordance with DOE guidance to reviewers for evaluating projects.

Reviewer 5:
There are strong findings from the past year with regard to defining the fuel chemical properties impact PM mass, whereas the fuel mixing and charge stratification impact the particle size and PN. Also, the tradeoff between NO_x and HCs was identified for ACI modes, with those HC emissions being a strong function of the fuel chemical properties. The ORNL gas bench work demonstrated that HC emissions will be a significant challenge for ACI operating strategies. If the project team cannot make it work under idealized, steady-state synthetic gas conditions, the reviewer struggled to believe that the community will be able to accomplish it on the vehicle.

PNNL work is too early for technical review.

Reviewer 6:
From the standpoint of aftertreatment, the presenter relies heavily on the chosen catalyst to be representative of all catalysts. This is definitely not the case. Unless the catalyst used in this work is an appropriately aged super ultra-low emissions vehicle (SULEV) catalyst, it would not be appropriate to draw strong conclusions from the light-off experiments. Additionally, palladium (Pd), Pd plus rhodium (Rh), and Rh-only formulations react HC differently. All three are used in current aftertreatment systems. Similarly, using the temperature at which 50% of the distillate fuel is recovered in a distillation experiment (T50) as a benchmark for U.S. Environmental Protection Agency (EPA) Tier 3 and California Air Resources Board Low-Emission Vehicle (LEV) III systems is not sufficient. Catalyst systems must work at 99.5% efficiency to achieve these emissions standards. Therefore, the temperature at which 90% of the distillate fuel is recovered in a distillation experiment (T90) performance is also very important. Finally, when comparing the performance of single-atom and nanoparticle catalysts, ensuring that they are aged under the same conditions is important. As a further note, engine calibration can also have an impact on both tailpipe and engine-out emissions and speciation. Finally, the fuel work related to combustion modes is appropriate and provides useful information.

Reviewer 7:
There has clearly been a lot of work done in all of the task areas. Not all seems to have the same value in terms of progress toward the goal. The engine emissions response to fuel chemistry, operating condition, and fuel property is really nice work. The results are not all that surprising, as it seems that a lot of these directional responses were already known. The reviewer would like to have seen more explanation of how these results have expanded our understanding. The light-off/light-down study is valuable, but is an area where it really needs to be linked to engine testing in parallel so that the bench testing can fully replicate what the engine will be doing to the catalyst. The reviewer would have also liked to see more than just HC oxidation but also NO_x reduction, because that is frequently the most difficult pollutant to deal with from a regulatory sense. It will also be useful to consider how the HC/NO_x ratio coming into the catalyst impacts the process, because that is an easy calibration knob. The reviewer questioned how valuable the work in low-temperature catalysis of unburned fuel is; the reviewer would have expected that most of the fuel would be partially combusted, and so again the low-temperature HC/NO_x combined reactivity would be of more significance.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
This project does a good job of leveraging the expertise of other Co-Optima teams and industry stakeholders through the Advanced Combustion and Emission Control (ACEC) Low Temperature Aftertreatment working group.

Reviewer 2:
There are strong collaborative efforts, particularly leveraging the Crosscut Lean Exhaust Emissions Reduction Simulations (CLEERS) organization.

Reviewer 3:
The fuels selection is based on Co-Optima identified fuel blendstocks. The efforts, to this point, are fairly distributed. Reactor experiments and fuel characterizations seem to be lumped into a single site effort. The coordination between contributors seems well conducted.

Reviewer 4:
The range of collaborators from various National Laboratories and other organizations means that these projects receive a large degree of comment and discussion during the year.

Reviewer 5:
A significant amount of data was obtained from this fuel work. However, the results would be strengthened if an OEM were a member of this project. There is good inter-laboratory collaboration.

Reviewer 6:
The team does have good internal collaboration. The reviewer thought there needs to be more collaboration with engine teams, though, to ensure that the bench testing is fully relevant to engine operation.

Reviewer 7:
The project team appears to be interacting well with the fuel development teams. However, the counterintuitive PN/PM results from the stratification comparison study call to question the collaboration and communication with the combustion teams. Are they collaborating with Lyle Pickett’s FT074 team, who is studying the sooting tendencies of injection events during the intake?

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The future work is appropriate for addressing the selected barriers. The community anxiously awaits the results from different aromatic content and distillation curves in ACI modes.

Reviewer 2:
All the future work identified in the report is very relevant and should be continued. It is critical that the engine experiments should explore a wide range of operating conditions, both steady state and transient. The work on emissions control architectures should include solutions for cold-start emissions as well as particulate emissions.

Reviewer 3:
The future work plans are strong. The reviewer definitely hoped this project is funded at a level to allow for the future work described in the presentation.

Reviewer 4:
The choices for future research appear excellent. For the stoichiometric conditions in projects 2 and 3, it could be useful to examine the impact of dithering the feed around the stoichiometric point, which the reviewer did not recall being discussed. In some systems this can have a large effect. The choice in project 3 to look at bi-metallic nanoparticles is an excellent idea. There are known synergies from studies over the past decades, e.g., Pt/Rh, that could have great interest in today's high-priced environment for platinum group metals (PGMs).

Reviewer 5:
The proposed engine-related work is appropriate and will be informative. The bench reactor and tailpipe emissions results will be less conclusive due to the highly variable nature of catalyst PGM composition and washcoat technology. The engine calibration will also have a significant effect on emissions results.

Reviewer 6:
Moving the work from the surrogates and micro-reactors to MCEs will be interesting. The work to date is focused on one operating condition but attempts to make claims of general applicability. Using more conditions or clarifying specific combustion regimes, if applicable, could be added.

Reviewer 7:
The proposed work is generally good, but does not fully capture this reviewer's comments from previous questions; looking at transient catalysis that is duplicating what we see with engine-mode switching would be highly valuable.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
Emissions control will truly be the enabler or death sentence for the Co-Optima fuels and combustion strategies; therefore, this reviewer thought that this presentation represents some of the most important work in the program.

Reviewer 2:
Without the research work covered under FT073, MM and ACI combustion concepts being explored by Co-Optima have no chance of being viable for mass production. Thus, this project is extremely critical for accomplishing the overall DOE objectives.

Reviewer 3:
Emissions compliance may be the biggest challenge for adoption of ACI, so this is a very relevant topic.

Reviewer 4:
To fully evaluate optimized fuels for fuel economy, their emissions control must also be evaluated and optimized, as these projects are providing the data for those optimizations.

Reviewer 5:
The project directly contributes to the DOE goals of reducing vehicle air pollution.

Reviewer 6:
Understanding the fuel composition's influence on catalyst performance is very useful, as is expanding work to include a range of fuels that has a greater or lesser PM production. The combination of fuels with related efficiencies and emissions influences, plus a consideration of the resulting catalyst reactions, is applicable.

Reviewer 7:
Optimizing fuel blends for engine and aftertreatment performance is highly desirable and could help increase fuel economy without sacrificing performance. However, it was noted that a reviewer's statement in the presentation suggested that this work will guide supplier and OEM development activities. That will most likely not be the case. OEMs and their catalyst suppliers develop catalyst systems for currently required Tier 3 fuels. They will not develop a separate catalyst system for another fuel. The onus is on the new fuel to be compatible with the aftertreatment system.

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

Reviewer 1:
The budget seems fine for the work being done.

Reviewer 2:
The resources used between National Laboratories seems focused and not overly expansive or overreaching.

Reviewer 3:
The reviewer had no issue with resources.

Reviewer 4:
The groups doing each of these sub-projects have the correct equipment for doing the initial evaluations needed and access to other tools to follow up on any surprising results.

Reviewer 5:
The team appears to have appropriate resources for project completion.

Reviewer 6:
The funding is sufficient for the proposed work.

Reviewer 7:
Resources seem sufficient.

Presentation Number: ft074
Presentation Title: Multi-Mode: Gasoline Direct-Injection Sprays
Principal Investigator: Lyle Pickett (Sandia National Laboratories)

Presenter

Lyle Pickett, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

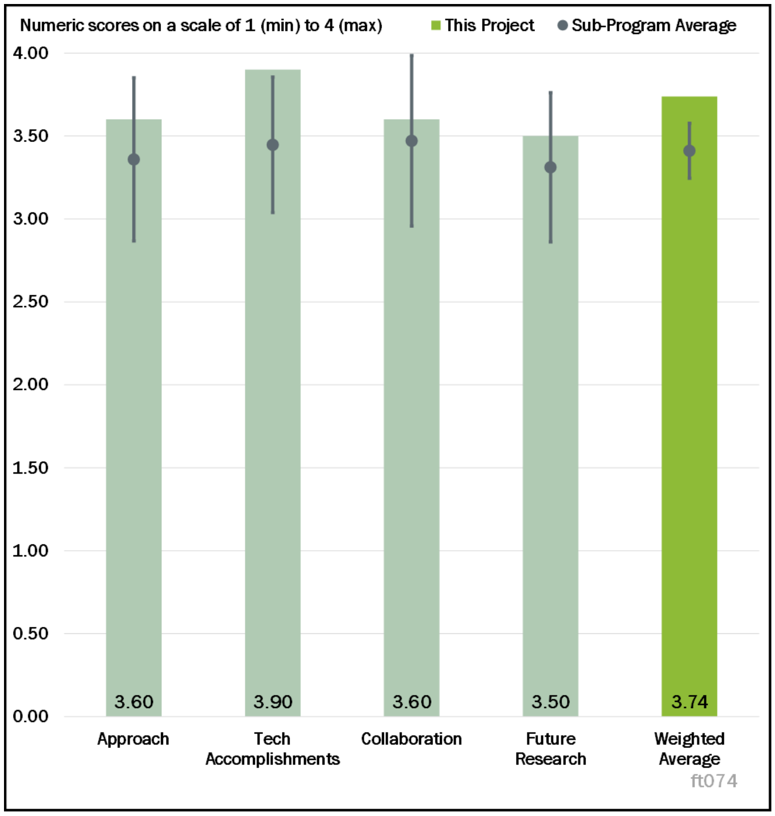

Figure 5-8 - Presentation Number: ft074 Presentation Title: Multi-Mode: Gasoline Direct-Injection Sprays Principal Investigator: Lyle Pickett (Sandia National Laboratories)

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

Reviewer 1:
This is outstanding work. Detailed fundamental understanding of in-cylinder spray behavior is being uncovered in extreme detail.

Reviewer 2:
The approach brings to bear the excellent experimental strengths of SNL in spray visualization and measurements. This is supported very well with appropriate CFD modeling of the data.

Reviewer 3:
The combination of experimental and computational aspects makes this an excellent project.

Reviewer 4:
The approach to this project is sound. The work uses spray vessels and high-fidelity simulation to study the spray characteristics of a GDI injector and the impacts of fuel property changes upon those spray characteristics. The work uses a battery of experimental techniques, among several partners, to help develop advanced predictive models for these sprays.

Reviewer 5:
The project approach is tuned to exploit the capabilities of the experimental setup being used. The project explores an aspect of injector performance connecting to mixed-mode work by viewing changes in injector performance at different conditions, including normal SI conditions versus the near top dead center (TDC)

injections that could be used in ACI portions of a mixed-mode strategy. The results of this work are applicable to both ACI concepts and conventional SI engines, which will increase the value of the results.

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 technical detail and progress of this work are impressive. Substantial insight has been gained into the influence of spray and fuel property characteristics upon soot formation, ignition, and flame propagation. The experiments helped to highlight shortcomings in the Reynolds-averaged Navier-Stokes (RANS) model and led to a substantial improvement in the simulation approaches used to examine these spray conditions, including cavitation and flashboiling.

Reviewer 2:
Very detailed measurements and associated analysis are uncovering new details of the impact of fuel characteristics of spray phenomena.

Reviewer 3:
Measurements and simulations of injector dribble from GDI sprays are a high value output from the last year's effort. A cohesive program to establish some clear results in this area is viewed as valuable.

Reviewer 4:
The new homogenous relaxation model (HRM) that was implemented is a great advancement for CFD that industry users can take advantage of. The team has made great progress to date, given delays due to COVID-19.

Reviewer 5:
Several new and interesting accomplishments have been made. Examples are the growth of the spray plume angle with flash boiling, spray collapse with increasing spray plume angle, wetting of the nozzle face during flash boiling conditions, and modeling work with the HRM of the flash-boiling process. The transparent fuel injector experiments complement the understanding gained with the other tools and modeling. Shortcomings of the RANS model in predicting burning rates have also been noted. The team is congratulated for the good progress and findings.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
There are a large number of collaborators in this work, even though only the direct SNL research results were explicitly shown. The ECN work is a major underpinning to this project, and those results are highly leveraged for this project. A large mix of National Laboratories and universities are contributing to this work.

Reviewer 2:
Through Co-Optima, PACE, and the ECN, the collaborations are extensive and contributory.

Reviewer 3:
The team has great partners to collaborate with.

Reviewer 4:
Several appropriate collaborations have been established with other researchers at SNL, ANL, and universities.

Reviewer 5:
There is a good list of collaborations across the different National Laboratories and with outside universities and research groups. Looking at the results discussion, it is less clear how these collaborations supported the results generated within the program.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
It is very important to move toward CI fuels, whether MCCI or ACI combustion systems. Bringing these tools and approaches to the challenges of autoignition—in particular, the autoignition of Co-Optima fuels and fuel components—will be necessary for success.

Reviewer 2:
Through the project team's insightful analysis, it has been able to identify appropriate next steps.

Reviewer 3:
One of the future tasks, "Determine if advanced hardware (high injection pressure GDI) can alter mixtures, dribble, and ignition characteristics," is very interesting and critical since the industry is testing much higher pressure injection for advanced combustion, such as done for gasoline direct injection compression ignition (GDCI) (Delphi) and gasoline compression ignition (GCI) (Aramco).

Reviewer 4:
Going forward, experiments and modeling of real multicomponent fuels will be of use to industry.

Reviewer 5:
From a purely technical standpoint, the proposed future work is solid and represents an opportunity for new knowledge gain that is useful to the engine combustion development community. The impact and connection to the Co-Optima effort as a whole, however, is less clear, and even more so to the Mixed-Mode task. It is important to connect more closely to the Co-Optima Mixed-Mode task objectives. Focus on what this effort can deliver to address a key barrier in mixed-mode concepts, or identify new, key fuel property effects relevant to that area. GDI sprays are relevant, but the alignment between the knowledge from this project and the higher level Mixed-Mode program barriers and objectives could be improved. Moving forward, this reviewer would like to have seen a concentration on using more fuels. Since this is a high-throughput chamber, the project team should evaluate a wider swath of fuels to generate new understanding. Additionally, an increased focus on the impact of specific fuel properties, for example distillation as noted, could be more valuable than focusing on the core Co-Optima fuels. Exploring how big shifts in properties—such as distillation, reactivity, or paraffins, iso-paraffins, olefins, naphthenes, and aromatics (PIONA) classes—would be a valuable addition to the effort.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
This project is essential to achieving DOE goals in a variety of projects. This type of fundamental work is needed.

Reviewer 2:
Understanding the detailed phenomena that occur in sprays is critical to improving engine performance.

Reviewer 3:
The project develops greater understanding of GDI sprays, which supports the overall Co-Optima program goals and ties to DOE targets to increase vehicle efficiency and reduce emissions.

Reviewer 4:
Characterizing injectors is a necessary and critical step to improve engines, thereby meeting DOE objectives.

Reviewer 5:
This project provides the necessary understanding of fuel sprays and mixing processes needed to enable high efficiency engines to reduce petroleum consumption and GHGs.

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

Reviewer 1:
The resources allocated appear to be consistent with a project of this size and scope.

Reviewer 2:
There is great value for the current funding.

Reviewer 3:
Project resources are sufficient and in proportion to the scale of activity.

Reviewer 4:
Resources are sufficient and not excessive.

Reviewer 5:
The resources are being used extremely effectively to accomplish the stated objectives.

Presentation Number: ft075
Presentation Title: Multi-Mode: Fuel Kinetics
Principal Investigator: Bill Pitz (Lawrence Livermore National Laboratory)

Presenter

Bill Pitz, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 71% of reviewers indicated that the resources were sufficient, 14% of reviewers indicated that the resources were insufficient, 14% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

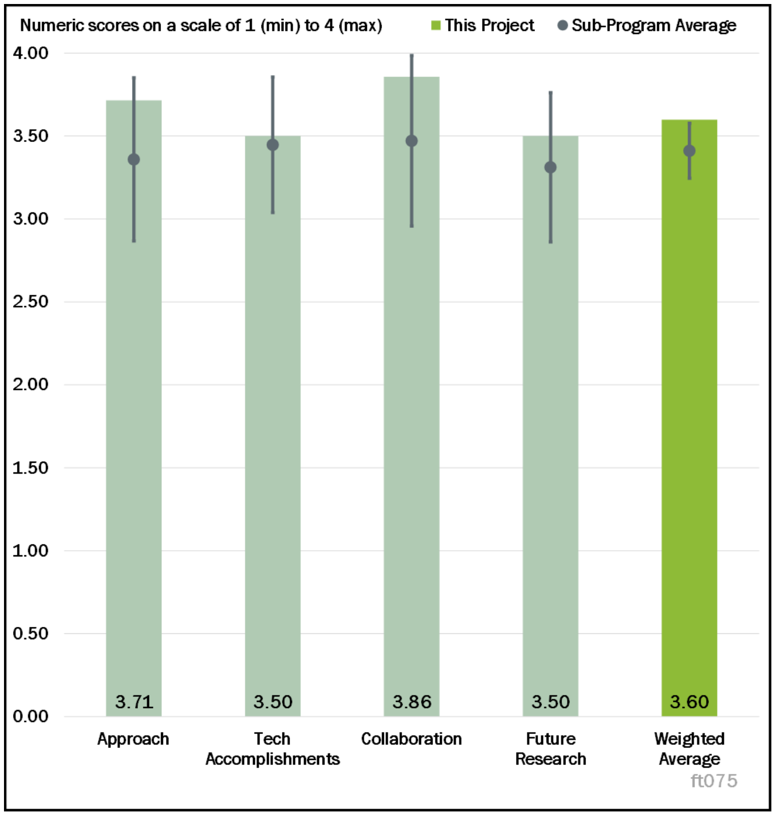

Figure 5-9 - Presentation Number: ft075 Presentation Title: Multi-Mode: Fuel Kinetics Principal Investigator: Bill Pitz (Lawrence Livermore National Laboratory)

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

Reviewer 1:

This project is well integrated with Co-Optima and is intended to fill gaps in kinetic models for a range of combustion modes. It is well focused on barriers and is likely to produce useful results.

Reviewer 2:

Reaction mechanisms and kinetic models are crucial for in-depth understanding of the combustion process as well as pollutant formation. This requires combined efforts of rate calculation, mechanism development, experiments for model validation, and mechanism reduction for real engine simulation. The project is very well designed to cover all areas listed above.

Reviewer 3:

This type of project provides exactly the type of tools the community needs to advance vehicle efficiency and reduce emissions.

Reviewer 4:

Improved chemical kinetic models are essential for enhancing the combustion and emissions modeling capabilities of engine simulation tools. The work presented in this report covers new Co-Optima blending components, the impact of NO_x on autoignition, and polycyclic aromatic hydrocarbon (PAH)/soot formation, all of which address critical needs for improved modeling of various combustion modes, including conventional SI.

Reviewer 5:
The project's overall approach to developing models for soot and PAHs occurring in MM, MCCI, and ACI engine modes is impressive. The project's development of kinetic models that accurately predict the promotion effect of nitric oxide (NO) to ensure accurate simulation of autoignition occurring in MM, ACI (MD/HD), and MCCI engine combustion is also impressive. This program is well thought out.

Reviewer 6:
The approach used in this project has been honed over decades of research into the study of fuel combustion kinetics and has consistently delivered results that have driven the field of combustion research. The further development and refinement of kinetic mechanisms for new fuel molecules, the work on kinetic mechanisms for PAHs (soot precursors), and the influences of NO_x on autoignition kinetics are foundational to the work carried out throughout Co-Optima.

Reviewer 7:
The approach to develop chemical kinetic mechanisms for HPFs just seems like a little bit of cart before the horse. These mechanisms take significant human and capital resources to develop, and it seems like this should be done after more promising candidates are identified in the engine experiments.

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:
Looking at the results in the presentation and thinking back not that many years ago, kinetic models did not have such nice agreement with experimental results. The comparisons between the models and the RCM data are impressive. There is still work that can be done in this space, but just 5 years ago, the difference between models and experimental results was considerably larger. The understanding of chemical kinetics is important in understanding ignition delay, emissions, and, especially, soot formation. This project shows great progress in that understanding.

Reviewer 2:
The model development that has come out of this project is impressive (seven new kinetic models) and led to numerous publications.

Reviewer 3:
This year's presentation notes development of seven new or updated kinetic models for a variety of fuels of interest. It is interesting to see that the results help explain some of the particle emission trends of fuels and blends. It would be interesting to catalogue how industry is using the developments and findings.

Reviewer 4:
The team made very good progress in advancing mechanisms for HPFs and soot formation, as well as the promotion effect of NO_x on autoignition.

Reviewer 5:
The team has made widespread progress on many of the objectives. As with any scenario modeling experimental phenomena, some of the models fit experimental data with various degrees of accuracy. The reviewer had only a couple of areas of concern with the results:

- The n-butanol and iso-butanol ignition delay results on Slide 11 do not appear to capture the correct trend shape. The trend does change from the original model, but caution is advised owing to this perceived trend shape mismatch.

- The allene and propyne models on Slide 13 predict a much narrower distribution than the experiments. The investigators fielded questions on this during the presentation period and cited the intrusive nature of the experimental apparatus as a potential for broadening the experimental distribution. Are there sensitivity studies that can quantify this impact? What are the critical parameters influencing this potential error source (aspect ratio of the probe to some critical length in the experiment?)? Are the investigators certain that this mismatch is created by experimental shortcomings?

Reviewer 6:
Reducing particulate emissions is one of the biggest aftertreatment challenges being tackled by the automotive industry. Thus, it is encouraging to see progress on this front. This work stream needs to be continued further. Improving the ability to model the impact of NO on autoignition will benefit combustion modeling of operating conditions with higher levels of residuals/internal EGR, regardless of combustion mode. Multiple Co-Optima and PACE projects present data on engine combustion simulations which directly and indirectly utilize the kinetic mechanisms developed as part of the current effort. For future presentations, it would be helpful for the audience and reviewers if the report included a slide or two highlighting efforts where the improved kinetic mechanisms have been used. Specifically, it would help to see a comparison of engine combustion simulation with old and improved kinetic mechanisms, as ultimately the motivation for improving kinetic mechanisms is to increase the accuracy of combustion and aftertreatment simulations.

Reviewer 7:
The kinetic sub-models developed for new HPFs consistently perform within the experimental error of fundamental combustion experiments, indicating performance that cannot realistically be substantially improved. The continued integration of new sub-models with the base gasoline model allow the modeling of complex fuel blends and mixtures of Co-Optima HPFs.

One area of potential improvement would be the more rapid transfer of the developed models to the public and stakeholders. The current practice of waiting for key publications to be written, submitted, and reviewed is slowing the utilization of these important tools.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The project includes a number of collaborators who are well integrated with the project team's efforts. This reviewer saw numerous high-impact publications from this collaboration.

Reviewer 2:
The project team collaborates extensively. No deficiencies were identified.

Reviewer 3:
There is outstanding collaboration between National Laboratories, academia (global), and industry.

Reviewer 4:
This is the largest collaborative group this reviewer had seen so far. There are 9 National Laboratories, 10 universities, as well as industry involvement. All of the researchers who are named are considered tops in their field. It is no wonder the results are as good as they are.

Reviewer 5:
Collaboration is strong with five university partners, National Laboratories, international institutions, and interactions with industry.

Reviewer 6:
The collaborations between the LLNL kinetics team and Co-Optima, as well as outside Co-Optima and with the broader community, are so numerous that they are challenging to list on a single page. Specifically, collaborations with engine researchers have driven significant insights into interactions between fuel kinetics

and engine performance/limitations/physics and are an important source of knowledge transfer and sharing throughout Co-Optima.

Reviewer 7:
Collaborations across the team were noted and adequately explained.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The planned objectives and approach for the next years are adequately explained and are focused on the goals and barriers.

Reviewer 2:
The future research is well planned to continue developing and improving kinetic models for gasoline-range and diesel-range fuel candidates, blendstocks for oxygenate blending (BOBs) and their blends, PAH/soot formation, and NO_x effect on combustion. Meanwhile, the reviewer suggested the team should focus more on the phi-sensitivity of fuels, given the potential of lean gasoline combustion.

Reviewer 3:
The future research is very ambitious and very useful. The community eagerly awaits these new/updated models/tools.

Reviewer 4:
The proposed future research is well thought out and should be considered in the future.

Reviewer 5:
As appropriately identified in the report, future efforts should including expanding the range of pressure, equivalence ratio, EGR, and dilution levels over which the kinetic mechanisms are validated. Additionally, the PIs are encouraged to prioritize improving PAH/soot modeling capabilities.

Reviewer 6:
The proposed future research maintains the course of this project and will likely deliver advancements in the key areas listed here (improved BOB kinetics, PAHs, NO_x, and autoignition interactions).

Reviewer 7:
The reviewer called for more model development, which will hopefully become more accurate.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
The outputs of this task are foundational to Co-Optima and the DOE VTO engine-research portfolio. The kinetic models developed here continue to shed light on processes occurring inside engines, including modern SI engines, advanced combustion engines, and canonical/academic engine experiments. Further, without the development of accurate kinetic models for novel HPFs, it will be challenging to understand the behavior of these fuels well enough to assess their performance across a range of engines and combustion systems without exhaustive experimental work.

Reviewer 2:
Fundamental fuel combustion research is the foundation of developing advanced clean and high-efficiency engines, and its contribution to support the overall DOE objectives should not be underestimated.

Reviewer 3:
This project is crucial for widespread utilization of Co-Optima results from many groups.

Reviewer 4:
Improved kinetic mechanisms are essential for increasing the accuracy of engine combustion and aftertreatment modeling.

Reviewer 5:
This project will enable engine developers and researchers to use accurate kinetic models to improve MM combustion engines.

Reviewer 6:
This work is relevant to DOE objectives and important for linking the fundamentals to the application.

Reviewer 7:
The research addresses the overall goals of Co-Optima in providing the underpinning science and data for fuel-engine co-development.

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

Reviewer 1:
The resources devoted to this project are not sufficient, based on the objectives and promise of this work. Examples of demonstrated need for funding include the University of Connecticut subcontract work, which allows fundamental experimental data to be obtained so that the modeling process can proceed with appropriate validation data.

Reviewer 2:
The project team seems to have enough resources to achieve the stated milestone. The overall budget should be increased to enhance the fundamental research in fuel combustion kinetics.

Reviewer 3:
The resources appear appropriate for the project scope and effort.

Reviewer 4:
Resources appear to be sufficient for the proposed scope of the project.

Reviewer 5:
There is no indication that this group is lacking in resources.

Reviewer 6:
Progress in the tasks has been fine and resources appear adequate. Evaluate this question again in consideration of COVID-19.

Reviewer 7:
The resources seem excessive based on how likely this work is to impact implementation of the Co-Optima fuels or engine combustion strategies. Fundamental work is very important, but the luxury of a wealthy portfolio.

Presentation Number: ft076
Presentation Title: Model-Based Fuel and Engine Optimization
Principal Investigator: Juliane Mueller (Lawrence Berkeley National Laboratory)

Presenter

Juliane Mueller, Lawrence Berkeley National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

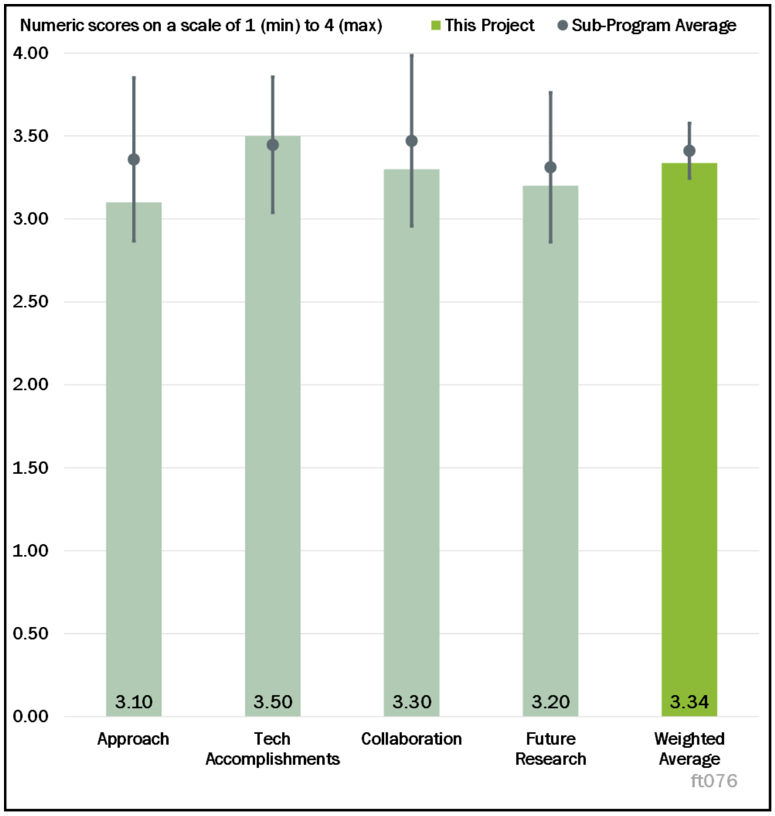

Figure 5-10 - Presentation Number: ft076 Presentation Title: Model-Based Fuel and Engine Optimization Principal Investigator: Juliane Mueller (Lawrence Berkeley National Laboratory)

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

Reviewer 1:

This approach is really interesting for automating the search for fuels that can match to a combustion approach. That is useful for addressing the technical barriers that prevent ACI adoption within the context of Co-Optima. The project does seem to lack a feedback loop closure though. This reviewer did not see any way to experimentally validate the results of the model search, and there are many ways that kinetic and CFD models can still provide wrong predictions when researchers go away from known regimes.

Reviewer 2:

The approach is unique and combines the existing capabilities of several modeling tools and artificial intelligence (AI) and machine learning (ML) techniques to computationally explore an exhaustive number of possibilities in fuel composition, thus exploring RON and MON ranges that result in expanding the MM load range as well as providing the control parameters like a fuel injection recipe to maximize load. The approach has the potential of being very powerful in narrowing down parameters for experimental validation.

This work has a lot of different thrusts, although the overall theme of speeding up computations and simultaneously improving simulation accuracy is an important one to support the overall Co-Optima program. Some of the pieces of the project seem a bit disjointed to be under a single heading, but the individual projects themselves are using an interesting approach to address important problems. The reinforcement and transfer learning strategies, in particular, are very interesting and will hopefully yield useful results. The approach on this part of the project is unique and was very well explained in the AMR. The reviewer is looking forward to the results next year.

Reviewer 3:
New approaches for characterization and quantification are novel. Identifying a process to select candidate fuels for experimentation is helpful for the sake of analysis, but expanding this technique beyond simple compound fuels increases complexity beyond the ability of the process to efficiently provide insight. Should the process work for more realistic combinations of constituents?

Reviewer 4:
The computational tools developed in this work are very powerful; however, there should be a better way to reconcile the "final" fuel for an architecture and duty cycle. In other words, if a high aromatic fuel is applicable at high load operation and a high olefin fuel is appropriate for robustness, a middle ground needs to be reached depending on the most commonly occurring duty cycle for the engine. The synthesis of that is unclear. One chief piece of information missing is the HOV or the vapor pressure of the fuel. Together with OS, the HOV will govern knocking. So, when a new fuel is concocted, it would be good to get a sense of the HOV as the chemistry models are all gas phase. Finally, many of the fuels have more than 20% aromatic content and some even 40%. Is this violating fuel standards?

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 implementation of new approaches to reduce computation time and effort would be extremely helpful in co-optimization of fuel and engine definition. The new approaches shown are very promising.

The accomplishments are on track with their proposed progress; it is good to see that the COVID-19 shutdown has not impeded the work. The PIs have used work-arounds and already available data sets to continue their comparisons and make progress on the method development. The Zero-order Reaction Kinetics (Zero-RK) work is a particularly nice accomplishment as it has been continually improving over the years and still remains an accessible and rapid tool for screening fuels, combustion concepts, and operating conditions. It is good to see the transfer of information from the higher fidelity simulation making an impact on a tool like Zero-RK that could have an impact at an industry level as well. The outcomes of the load range study were very interesting, and the optimization process was quite nice. One open question is the issue of transient operation: load range is not just a range of static loads but also getting from one load to the next. It would be interesting for the PIs to consider how to capture that in an optimization framework or if there is a reduced-order modeling way of considering the effects of fuel composition on transient performance, particularly transient emissions. Finally, the injection strategy optimization with reinforcement and transfer learning is very promising, and there are good initial results.

Reviewer 2:
Technical accomplishments achieved so far seem to be good. The reviewer is very intrigued in the future work on soot formation, especially with greater than 20% aromatic content in the fuel for improving load range. A way to quantify knocking should be established.

Reviewer 3:
While more work remains to realize the full potential of the approach, the results shown thus far for various fuels highlights the power of the approach.

Reviewer 4:
Within the context of the task as it stands, there has been good progress on the model development and application.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The interaction between National Laboratories appears exemplary in this effort. The use of Co-Optima directions is also incorporated well.

Reviewer 2:
Coordination among the laboratory teams is excellent, and there seems to be much progress as a result. There is some coordination with universities, but more is always good. Additionally, the PIs mentioned collaboration plans with software developers like Converge, which is good to see as this will translate these advanced methods to a wider audience. It would be good to see more collaborations with the engine tests and industry, although it seems like that will inherently increase as there is more progress on these tools. Some sort of engine validation exercise on the injection schedule optimization, for example, would be really interesting and maybe not too complicated to accomplish. This would be a great collaboration with a university if the National Laboratory engine research facilities did not have the bandwidth to participate.

Reviewer 3:
The collaboration among LLNL, Lawrence Berkeley National Laboratory (LBNL), NREL, and a couple of universities seems to be working very well.

Reviewer 4:
The collaboration among the modelers looks quite good. This reviewer thought there needs to be a lot more collaboration with the experimental teams, though, to validate the models and make sure that the team is predicting useful results.

Reviewer 5:
The collaboration is sorely missing a fuels company, such as Aramco, Exxon, Shell, or other. Inclusion of a fuels company will help mitigate some of the potentially unrealistic solutions obtained by ML and will help in level-setting the results.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The future research plans in all areas look great. It is also really nice to see a continual transition of updates from Zero-RK to the public domain. This is a major impact of this project on the research and engineering community.

Reviewer 2:
The listed future work on narrowing the RON range, identifying fuel blends, etc., while maximizing ACI load range and minimizing soot are right on the mark. Going forward, the MON and the relationship between RON and MON of the fuel blends should be included in the methodology to address the whole problem. As a byproduct, the fuel injection strategy behavior relative to the optimal results should also be reported.

Reviewer 3:
The proposed work looks fine, though it does not really seem to be working toward some actionable conclusions.

Reviewer 4:
The next steps in process validation are straightforward, though some more practical checkpoints would be useful in maintaining the relevance to the ability to use these techniques in practice.

Reviewer 5:
The soot modeling work is very important and needs to be quantified sooner than later. The HOV effect needs to be quantified in this work, and some parameters for predicting knocking should be introduced.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
Faster methods of designing the fuels will be a big boon to Co-Optima.

Reviewer 2:
This project supports DOE objectives on three important fronts. First, it is directly testing the central fuels hypothesis for Co-Optima and making significant advancements toward improving prediction of fuel blends and chemistries. Second, it is translating that learning to the broader community, particularly through tractable models like Zero-RK. Finally, the advanced computing and ML portion of the program is meeting broader DOE goals of advancing supercomputing capabilities and outcomes.

Reviewer 3:
This project aims to identify fuel composition blends that maximize engine ACI load range, thus increasing the potential of mixed-mode combustion engines to reduce petroleum usage and GHGs.

Reviewer 4:
Yes, it supports the Co-Optima effort.

Reviewer 5:
The presentation was delivered well. The explanation of the interaction of the National Laboratory efforts and progress was encouraging to see from an OEM perspective. The reviewer's concern is that the assumptions made, including the homogeneity of the charge, the simplification of the fuel into more discrete compounds and species, and zoned approach to the analysis, will limit the process transfer to more practical use cases.

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

Reviewer 1:
The team working on this project is a great group of people, and the financial and computational resources seem to be sufficient.

Reviewer 2:
Resources are being used very effectively.

Reviewer 3:
Budgets seem fine for what is being done.

Reviewer 4:
The contribution from each laboratory, and the apparent cooperation with individual efforts, looked to be very functional and key to the progress of the project.

Reviewer 5:
Funding seems to be sufficient for modeling and simulations work.

Presentation Number: ft077
Presentation Title: Heavy-Duty Mixed-Controlled Compression Ignition: Fuel Effects and Ducted Fuel Injection
Principal Investigator: Charles Mueller (Sandia National Laboratories)

Presenter

Charles Mueller, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 75% of reviewers indicated that the resources were sufficient, 25% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

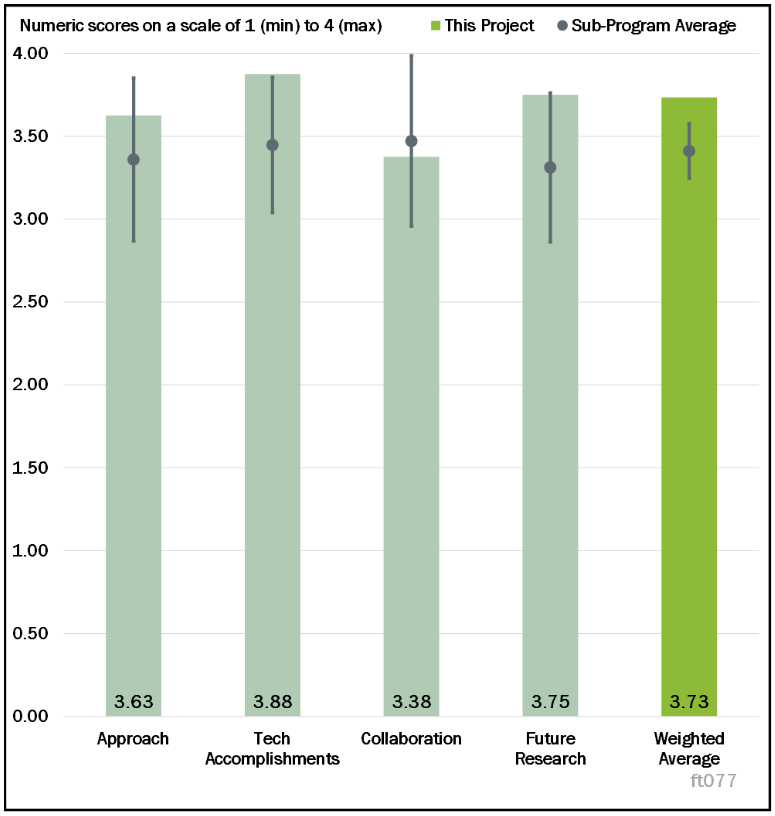

Figure 5-11 - Presentation Number: ft077 Presentation Title: Heavy-Duty Mixed-Controlled Compression Ignition: Fuel Effects and Ducted Fuel Injection Principal Investigator: Charles Mueller (Sandia National Laboratories)

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

Reviewer 1:

The potential for DFI is exciting. The work on surrogate fuels and soot is important, interesting, and being addressed in a systematic way.

Reviewer 2:

The team is employing unique experimental capabilities and optical diagnostics together to develop an enhanced understanding of the soot and NOx tradeoff. The approach is working very well.

Reviewer 3:

The approach of this project is effective. The optical engine work is extremely effective in displaying the mechanisms behind why DFI works as a highly effective soot reduction technique. One concern is the very slight reduction in efficiency. With the upcoming GHG and ULNO$_x$ regulations, any emissions reduction approach cannot be accompanied by an efficiency reduction, or the approach will not meet the GHG regulations. It would be helpful to see these constraints included in the approach for the work going forward. It is unclear how the efficiency deficit is going to be addressed.

Reviewer 4:

The optical engine at SNL is used to conduct a systematic, staged investigation of the potential of DFI. The only part missing is CFD modeling to further enhance understanding of the concept.

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:
There is tremendous progress on the DFI. The insight gained relative to the potential for a relatively simple, low number of component surrogate fuel is good news. And, important questions regarding soot formation have been uncovered.

Reviewer 2:
The team has made excellent progress, given the COVID-19 pandemic.

Reviewer 3:
Outstanding progress has been made in the quantity and quality of experimental work.

Reviewer 4:
This project has made substantial progress toward the goals by moving to a four-hole injector and operating the engine at higher speeds and loads. It is moving beyond proof of concept and more into technology development. Several different engine parameter sweeps were conducted, and the results are promising. However, it is not yet clear how to translate this concept into a practical engine.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
There is strong collaboration between the National Laboratories within the Co-Optima program in general, and it appears to be true here as well. The interaction with CRC with the fuels is good. It seems that there is other work on this project besides what was mentioned above. The presenter was not able to disclose the parties involved, but it also represents additional collaboration, which is good.

Reviewer 2:
The team has made excellent progress and is now partnering with ANL for some computational resources in CFD.

Reviewer 3:
Very good collaboration exists between several National Laboratories, Caterpillar, and Ford.

Reviewer 4:
There was mention of collaboration but not much detail was provided with regard to contributions made to the project. It is good that there is finally some simulation capability brought into the project to better help understand some of these fundamental processes. Compared to other Co-Optima projects, the collaboration and coordination in this project is much less pronounced.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The proposed future work to further increase the engine load and to increase the number of ducts is necessary and proper.

Reviewer 2:
It appears that the researchers have astutely determined the most important and potentially productive future work for this project. This came through in the discussion regarding raising the load with DFI and whether more than four ducts are possible.

Reviewer 3:
The proposed plan is outstanding, and this reviewer did not see any glaring holes.

Reviewer 4:
Proposed future work listed is to further understand the potential and tie up loose ends, and all the items are right on target. Going forward, the modeling work should catch up with the experimental work.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
This project supports DOE’s goals to maintain high efficiency and reduce toxic air emissions.

Reviewer 2:
The explanation of the relevance on Slide 3 is self-explanatory.

Reviewer 3:
The project is addressing the DOE goals for reducing petroleum use while simultaneously having cleaner combustion.

Reviewer 4:
This project is squarely aimed at overcoming barriers to a wider adoption of conventional diesel combustion in the MD and HD markets, as well portions of the LD market.

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

Reviewer 1:
The resources appear to be sufficient to maintain a good level of progress.

Reviewer 2:
There was no indication given that the program is resource limited.

Reviewer 3:
The resources are sufficient to continue the project.

Reviewer 4:
More modeling resources should be allocated to this project.

Presentation Number: ft078
Presentation Title: Heavy-Duty Mixed-Controlled Compression Ignition: Impacts of Fuel Properties on Combustion, Injection Characteristics, and Emissions Controls
Principal Investigator: Martin Wissink (Oak Ridge National Laboratory)

Presenter

Martin Wissink, Oak Ridge National Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

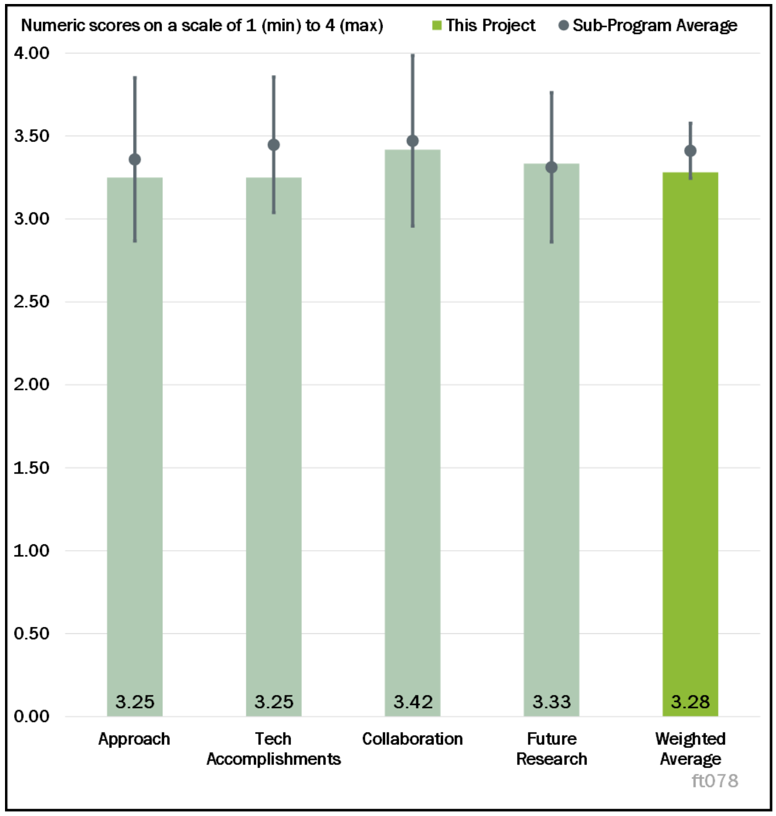

Figure 5-12 - Presentation Number: ft078 Presentation Title: Heavy-Duty Mixed-Controlled Compression Ignition: Impacts of Fuel Properties on Combustion, Injection Characteristics, and Emissions Controls Principal Investigator: Martin Wissink (Oak Ridge National Laboratory)

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

Reviewer 1:

The X-ray spray experiments and modeling are excellent examples of how to develop a fundamental understanding of the relationship between fuel properties and emissions. Add to that, the engine-out work that is being done, and this is an outstanding approach to understanding the differences between renewable diesel and diesel fuel with respect to emissions.

Reviewer 2:

Fuel spray and aftertreatment systems are both critical to emission control. Each of them can be a dedicated research project that is worth being funded by DOE. The reviewer did not quite understand why they were combined without providing enough information about how these two tasks are connected. Also, what is the focus of the project? It seems focused on in-cylinder fuel formation and combustion, but most of that work needs to be validated with the aftertreatment system. The reviewer understood that the future engine should be co-developed with the aftertreatment system. So, what could happen if the aftertreatment uses a different catalyst material? The reviewer thought the scope of this project should be better designed. Aftertreatment systems must be one of the key parameters being considered.

Reviewer 3:

The project examines the impacts of fuel properties on MCCI emissions. Biomass blendstocks, which were previously identified, are being examined for their impact on emissions.

Reviewer 4:
As identified in this project, increasing the accuracy of spray models, understanding the impact of fuel composition on emissions formation, and improving combustion during cold-start and low-load operation are all key technical challenges that need to be addressed for the development of more efficient engines with lower emissions. While understanding flow separation inside the injector nozzles is important, developing a better understanding of spray development and fuel/air mixing is critical for improving combustion and reducing emissions. Thus, it is imperative that the efforts of Task G.2.18 are not limited to cavitation. When exploring biofuel blends, it cannot be emphasized enough that the fuels being explored for HD MCCI are compatible with conventional CI engines. If this is not to be the case, then there is virtually no chance of the biofuels being investigated ever being adopted in the market.

Reviewer 5:
While it is very hard to give an in-depth analysis due to the sheer number of projects contained in this presentation, it appears that the projects are well designed and address the relevant technical barriers. (Also - how does the scoring work? Are all projects in the presentation given the same numeric score? What if there is one that is much better or worse than the others? How is this accounted for?) Disappointingly, engine hardware limitations prevent the study of many cold-start strategies.

Reviewer 6:
The multi-faceted approach, combining engine experiments, injection experiments, and modeling, is an appropriate methodology for developing a holistic understanding of the key physics as fuel properties change in MCCI engines. Unfortunately, many tasks are starting and ending at different times, challenging the narrative that this is a cohesive approach.

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 project made good progress on studying the fuel impact on cold start emissions and light-off, in-cylinder combustion, oxidation catalyst performance, and heating. Some delays due to COVID-19 are understandable.

Reviewer 2:
Many of the technical accomplishments have been hardware related as new systems were brought online for the investigation. Technical accomplishments regarding the diesel oxidation catalyst (DOC) light-off and injector cavitation appear to be on pace.

Reviewer 3:
Each of the tasks included in this project is a significant undertaking, and clearly a lot of work has been done over the past year. However, as per the report, a lot of the FY 2019 effort went into setting up and/or commissioning new test facilities and conducting baseline tests. PIs are encouraged to continue their efforts. Next year’s report with results and observations from the planned testing is expected to be more insightful. The data presented for MD/HD MM light-off/light-down temperatures is particularly interesting. It is encouraging to see the potential to lower both light-off and light-down temperatures. However, it is not clear if the observed trends are due to the change in cetane number (CN) (higher) or the variation in fuel composition (renewable diesel), or a combination of both. The PI is encouraged to develop a better understanding of the underlying mechanism (chemistry or physics, or combination) that leads to lower light-off and light-down temperatures. Finally, all PIs are encouraged to include quantifiable performance indicators in future reports in accordance with DOE guidance to reviewers for evaluating projects.

Reviewer 4:
There are some very impressive accomplishments in this work. The fuel spray work (both X-ray and modeling) is always impressive and yields great results. The reviewer referenced the light-off data when explaining why

the HD OEMs are looking into renewable diesel for the Environmental Protection Agency's (EPA) Cleaner Truck Initiative (CTI).

Reviewer 5:
Technical accomplishments are strong and mostly on track, even in the face of the pandemic.

Reviewer 6:
Many of the tasks reviewed here incorporated new experimental hardware, resulting in a relatively light set of results presented here.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
All sub-projects are engaging relevant stakeholders from the industry, academia, and suppliers.

Reviewer 2:
The collaboration between the National Laboratories is impressive.

Reviewer 3:
Strong collaboration was noted by this reviewer.

Reviewer 4:
The collaboration between project partners appears adequate.

Reviewer 5:
While each subtask made good progress, they seem to be relatively independent. The reviewer suggested highlighting collaborations with industry in "Technical Accomplishments."

Reviewer 6:
The collaboration and coordination varies by task. Tasks E.1.4.1 and G.2.18 appear to have good collaboration and coordination with one another, but this portion of the work has ended. Tasks F.2.4.1, E.2.2.9, and E.2.1/2.8 do not appear to have meaningful collaboration or coordination with one another.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The reviewer indicated the proposed research is outstanding. The reviewer suggested, however, that more work be done comparing biodiesel and renewable diesel in both in-cylinder emissions reduction and in the aftertreatment space. This is becoming a larger issue as California and the EPA move toward lower NO_x standards.

Reviewer 2:
The future research plan appears reasonable. The community eagerly awaits the fuel property impacts on emissions.

Reviewer 3:
The proposed future work is reasonable.

Reviewer 4:
The report does a good job of outlining the planned research activities for the next year. The activities identified are in alignment with the stated project objectives. Insufficient information is included in the report to assess the overall plans from the perspective of decision points and recovery options. However, this appears

to be a characteristic of Co-Optima project reports where several large projects are combined under one umbrella project for the purpose of reporting.

Reviewer 5:
The proposed work of Tasks E.2.2.9 and E.2.1.8 both will add value and understanding to MCCI effects on catalyst performance.

Reviewer 6:
The proposed future research should expand to consider various aftertreatment systems and catalyst materials. If only one will be tested, then the reason should be provided.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
The research activities outlined in this report are essential for evaluating the potential of MD/HD MCCI emissions compliance and thus support the overall DOE goal to develop more efficient and cleaner engines.

Reviewer 2:
This project allows for a better understanding of how fuel properties affect engine-out and tailpipe emissions. This will benefit both the fuel and transportation industries when designing future vehicles.

Reviewer 3:
These projects are strongly relevant to DOE goals and barriers.

Reviewer 4:
The projects reviewed here continue to have relevance to DOE's transportation research programs, providing insight on phenomena impacting emissions control performance in diesel engines—a major challenge for this technology, the success or failure of which will have significant impacts on energy efficiency in MD and HD transportation.

Reviewer 5:
The project is aligned in support of overall DOE objectives for clean and efficient transportation.

Reviewer 6:
The project is in line with DOE objectives to provide secure and clean mobility.

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

Reviewer 1:
The resources appear adequate for the proposed research.

Reviewer 2:
The resources appear adequate for the project objectives.

Reviewer 3:
The funding is sufficient for the proposed work.

Reviewer 4:
It appears that the resources for this project are sufficient.

Reviewer 5:
Resources seem sufficient.

Reviewer 6:
The funding levels are sufficient to support the efforts demanded by the tasks and their proposed future work.

Presentation Number: ft087
Presentation Title: Multimode, Co-Optimized, Light-Duty Vehicle Engine
Principal Investigator: Phil Zoldak (Hyundai-Kia North America)

Presenter

Phil Zoldak, Hyundai-Kia North America

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

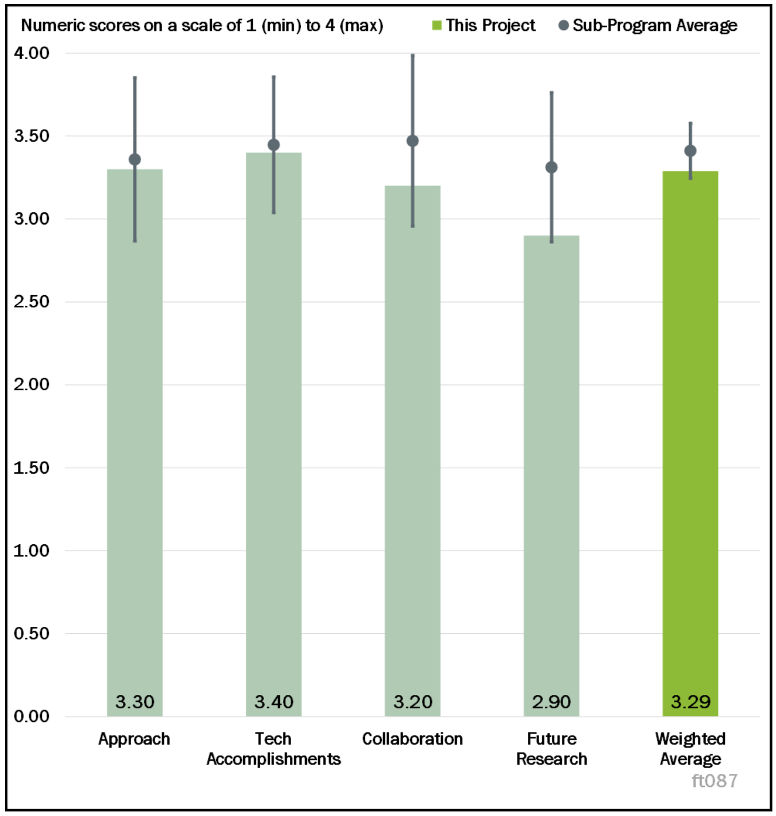

Figure 5-13 - Presentation Number: ft087 Presentation Title: Multimode, Co-Optimized, Light-Duty Vehicle Engine Principal Investigator: Phil Zoldak (Hyundai-Kia North America)

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

Reviewer 1:
This is a nicely crafted project to transfer technologies from national laboratory projects and the previous Delphi/Hyundai project into a more optimized GCI system by including the fuel properties into the design problem. The approach looks to be addressing all of the key areas of need to bring the system to life.

Reviewer 2:
In general, the approach in this project is excellent. The work is comprehensive, including engine experimental and simulation work. The approach also includes plans to increase the engine load and power output. One suggestion is to become more familiar with previous gasoline LTC work to better understand the dependence of gasoline autoignition upon several engine operational parameters.

Reviewer 3:
The work's goals are explicit. The breakdown of the tasks is reflective of the complexity of the underlying challenges. Carrying the information from other work—fuels surrogate selection, development directions, and demonstrations—is well planned. The focus on a practical demonstrator provides the framework of what must be accomplished to achieve the goals.

Reviewer 4:
The proposed project is planning to address relevant needs described as a part of the 2025 VTO technical goals to improve overall efficiency by increasing LD vehicle fuel economy using advanced SI plus GCI combustion hardware systems in conjunction with novel, co-optimized fuel technologies. The project team is not proposing any examinations of the beneficial impact of lubricating fluid or aftertreatment devices.

Reviewer 5:
The project is to develop a co-optimized fuel and MM SI/GCI engine combustion system that can achieve 15% vehicle fuel economy improvements. The project covers all engine-related development, such as hardware enabling MM combustion, three-dimensional (3-D) CFD, and fuel effect on GCI combustion. However, why is the aftertreatment not part of the scope? Most advanced combustion modes are not commercialized because they have other issues not related to combustion itself. Given the increasingly stringent emission regulations, the story is not complete if a combustion system is not co-optimized with the aftertreatment system.

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:
There appears to have been a lot of progress this year. The engine performance maps look very impressive, giving promise for satisfying the vehicle fuel economy improvements.

Reviewer 2:
The technical accomplishments are quite impressive. The 1-D and 3-D modeling feeds into the SCE and then into the MCE. The use of variable valve actuation and duration should be a big lever in achieving the goals of this project.

Reviewer 3:
This reviewer observed substantial progress for the first year even with 5 months of delay. The initial design modifications and progress toward a combustion system improvement, including alternative fuel candidates, were significant steps.

Reviewer 4:
The project made good progress and is overall on track.

Reviewer 5:
The reported progress was only discussing preliminary results evaluating hardware selection. The planned selection of novel fuels has been delayed and moved to be conducted during Year 2. Models to examine fuel combustion chemical mechanisms were developed for only four fuels and had not been discussed as a part of the presentation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The use of the collaborators shows in the progress that was made. Combustion simulation and fuels details—along with the design effort, turbo selection, and pull-ahead controls work—is well coordinated and seemingly well executed.

Reviewer 2:
The work from the partners looks very nice; it does not look like some of their work has yet reached engine testing, so it will be good to see more of that in the coming year. The work from the partners does look significant in terms of satisfying the final project goals, so the reviewer suspected the collaborations are working pretty well.

Reviewer 3:
The team of researchers is aligned as the subject project contributions include representatives of an OEM (Hyundai), a turbocharger supplier (Garrett-Motion), a petroleum fuel company (Philips 66), a National Laboratory (ANL), and academia (Michigan Technological University). It would be advantageous to add experts from NREL to expand knowledge and key contributions related to alternative fuels technologies and combustion models.

Reviewer 4:
This appears to be a good team consisting of an OEM, a university, and a fuel company. The coordination and collaboration appear to also be good among team members. This project could likely benefit from some collaboration with a National Laboratory that has experience in GCI, or possibly an injector company that is experienced in GCI.

Reviewer 5:
There is limited collaboration with National Laboratories and other OEMs, which is understandable because this project is cost shared by Hyundai.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The work plan as presented is well crafted to move the project toward a satisfactory completion. The reviewer would like to have seen more details into the aftertreatment development plans as that has been a big challenge for previous GCI projects. The low-load operation improvement plans look good, and the reviewer hoped that the project team will bring in the fuel co-optimization work too.

Reviewer 2:
The stated future work involving the exploration of intake air heating, spark assist, and possible mode switching is reasonable. However, it might be useful to explore boost sweeps as well, since that will directly influence the ignition properties for most gasoline fuels.

Reviewer 3:
The future research plan does not include examining the potential beneficial impact of novel, low-viscosity lubricant technologies nor assessing the impact of advanced emissions control systems. No specific plans are proposed to examine potential occurrence of the pre-ignition (also called mega knock or LSPI) phenomena taking place at low loads and low speed and strongly dependent on the quality of combusted fuels as well as specific composition of the lubricating oils.

Reviewer 4:
Future research was not mentioned; future steps for the program were.

Reviewer 5:
Very limited information is provided. The reviewer hoped aftertreatment can be part of the project and hopefully vehicle demonstration, instead of vehicle simulation.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
If the final vehicle can meet standards for the super ultra-low emissions vehicle with 0.030 grams/mile combined non-methane organic gases and NO_x (SULEV30) emissions and achieve a 15% reduction in fuel consumption, that offers a big gain in LD fuel consumption within the U.S. market.

Reviewer 2:
This project supports the DOE overall objectives to improve engine efficiency and reduce criteria emissions.

Reviewer 3:
This project is an application of developments that will lead to the VTO 2025 goals. The specificity of this project directly led by and primarily benefitting a single OEM in the long run seems somewhat limited. The evaluation of processes and approaches leveraged from other programs should increase so that the larger

community can benefit from the experience. The project plan and approach are sound and logical. The project contributors are well suited for their identified tasks. It will be great to see the progress made next year.

Reviewer 4:
The project is aligned in support of overall DOE objectives for clean and efficient transportation.

Reviewer 5:
The project is planning to address the DOE objective of up to 15% fuel economy improvements in LD vehicles, but the project has relatively restricted focus by planned examination limited to hardware and fuels, and not including emissions control devices and lubricating fluids.

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

Reviewer 1:
The proposed budget should be able to deliver planned project goals in a timely fashion.

Reviewer 2:
Budget and spend rates look about right for the project scope.

Reviewer 3:
The resources appear to be sufficient to achieve the target goals in the expected timeline.

Reviewer 4:
The project plan and approach are sound and logical. The project contributors are well suited for their identified tasks. It will be great to see the progress made next year.

Reviewer 5:
The resources appear adequate for proposed research.

Presentation Number: ft088
Presentation Title: Fuel Property Experimental Kinetics
Principal Investigator: Gina Fioroni (National Renewable Energy Laboratory)

Presenter

Gina Fioroni, National Renewable Energy Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 80% of reviewers indicated that the resources were sufficient, 20% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

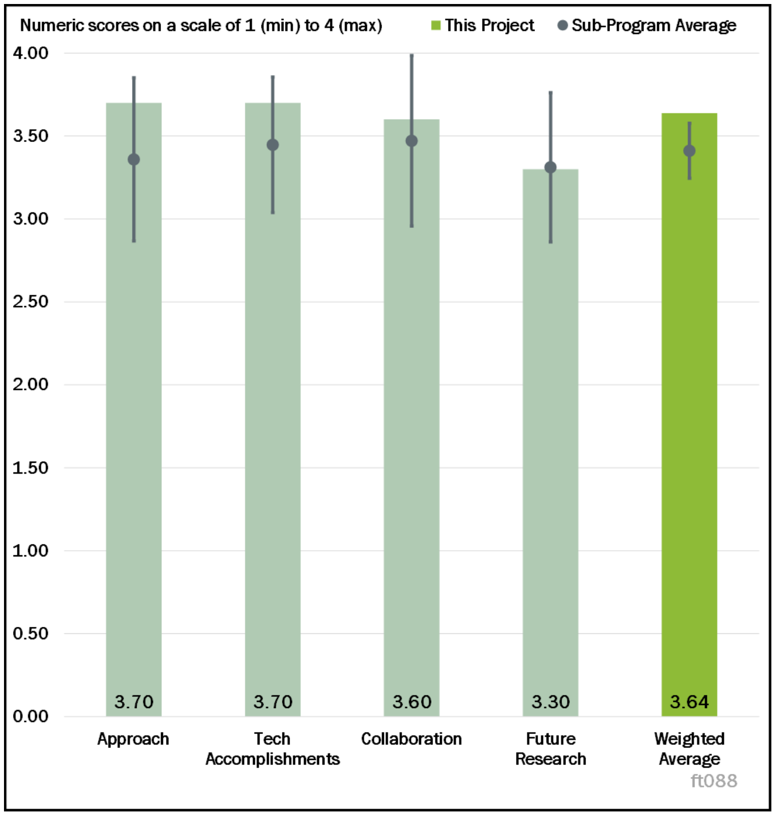

Figure 5-14 - Presentation Number: ft088 Presentation Title: Fuel Property Experimental Kinetics Principal Investigator: Gina Fioroni (National Renewable Energy Laboratory)

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

Reviewer 1:

The approach to better understanding the kinetics of autoignition, particularly the influence of mixing (phi-sensitivity) on autoignition, is critically important. Autoignition is the key to enabling any type of LTC and the key to understanding how to leverage fuel properties for advanced engines. This project uses a variety of tools, both experimental and simulation, to study these autoignition and fuel kinetics properties.

Reviewer 2:

This is excellent work. The research is identifying the fundamental kinetic mechanisms that lead to OS and ultimately could provide synergistic blending relative to the fuels' autoignition characteristics. It has the potential to ultimately facilitate fuel blending with lower carbon footprint blending agents that will allow advanced engine combustion configurations while maintaining compatibility with legacy fleets. It is still in its fundamental phase, but it is exciting.

Reviewer 3:

The team has a nice, systematic approach to characterize the kinetics.

Reviewer 4:

The approach brings to bear the chemical kinetics expertise of the various National Laboratories to identify blendstocks to gasoline to attain certain desirable fuel properties. World-class experimental measurements of the kinetic behavior are measured in the flow reactor, advanced fuel ignition delay analyzer (AFIDA), and the RCM.

Reviewer 5:
A good range and variety of tools are being applied to understand fundamental fuel behavior. It would be helpful to see more clarity and specificity on technical barriers being addressed. Currently, the program is targeted toward resolving a very high-level lack of fundamental chemistry knowledge. Building this out to clarify specific targets and gaps, which are critical to other development programs, would be a useful further step.

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:
Progress toward accomplishing the goals has been excellent. It is impressive to see how much has been learned about the dependence of phi-sensitivity upon different HC component structures and the ability to predict the performance of a fuel component based upon this information. The fuel phi-sensitivity index that has been developed should be a very useful tool going forward.

Reviewer 2:
The identification of the details of the fuel structure and its impact on the autoignition chemistry is outstanding new knowledge.

Reviewer 3:
It is great news that the higher pressure reactor design is done and can possibly be used soon.

Reviewer 4:
Excellent progress has been made in experimental fuel kinetics, with the autoignition characteristics of several blends tested and correlated. Several kinetic mechanisms have been improved. Measurements of phi-sensitivity have been made using the AFIDA apparatus.

Reviewer 5:
The work on flow reactors and understanding the fundamentals of chemical reaction shifts is very important and valuable work. Fundamental chemistry effects are a crucial part of the fuel-engine interactions, and this project is delivering insightful results toward understanding these factors. This effort should be an expanded focus of the Co-Optima program. There is solid progress on the RCM studies at ANL, though these appear to have been hampered by a laboratory move that delayed results. However, clarifying further, and improving the tie to, the overall project objective would be a useful exercise to ensure understanding of the project's connection to the larger effort.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
Excellent collaboration exists between NREL, ANL, PNNL, and several universities.

Reviewer 2:
There is excellent collaboration with the partner National Laboratories.

Reviewer 3:
This project shows a high degree of coordination and collaboration among the partners. The AFIDA and RCM work complement each other well.

Reviewer 4:
As with the other Co-Optima projects this reviewer critiqued, the collaboration is very strong and productive.

Reviewer 5:
Recognizing that the project itself is inherently cooperative, requiring collaboration with a range of different laboratories, the connections between the National Laboratories involved in this specific effort is not obvious. Moving forward, the connection between different subproject goals, focus, and activities should be enhanced and highlighted.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The researchers appear to have identified the fundamental aspects of the problem that needs further investigation and have planned out a reasonable approach to obtaining that information.

Reviewer 2:
Proposed future work looks to continue and build upon the work thus far. There needs to be additional clarity on potential breakpoints and go/no-go decisions to mitigate risk of program failure. Note that kinetic mechanism development is focused on prototypical ACI fuels, and therefore project timing is dependent on other programs highlighting properties for a prototypical ACI fuel and down-selecting potential candidates. Given this, a decision point on this effort would be appropriate.

Reviewer 3:
More chemical kinetic investigations of stoichiometric gasoline mixtures with EGR should be carried out as applicable to the LD industry.

Reviewer 4:
The proposed future work looks to be appropriate and an extension of previous success to accomplish the overall goals. The move toward more diesel-like fuels is probably needed, although it should also be viewed with an eye toward how it fits into the overall goal of improving efficiency and reducing GHG footprint as well. Most proposed e-fuel solutions tend to center around simpler HCs rather than long-chain ones. Long-chain HCs certainly tend to mimic diesel fuel more accurately than shorter ones, in general. But, they also tend to come at a higher cost of yield and expense (both energy in processing and dollars). It would be good to keep these multi-variable effects in mind.

Reviewer 5:
The reviewer was a bit concerned about the fit of the work in the overall Co-Optima program since it is very fundamental work and the experimental studies on mixed-mode ACI will likely be conducted without much input from this work. How much impact has the project team considered on engine testing and fuel choices to date? What about the future?

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
This project is very relevant to DOE's goals and objectives. Understanding the fuel kinetics and phi-sensitivity of these fuel components is mission critical to fundamentally improving engine combustion for improved efficiency and GHG reduction.

Reviewer 2:
This work could play a critical role in improving a fuel's performance for enhanced engine efficiency and at the same time be on the glide path for reducing the carbon footprint of the fuel.

Reviewer 3:
The work does support the DOE goals of increased engine efficiency by laying the fundamentals for new fuels.

Reviewer 4:
This work is aimed at understanding fuel property behavior and fuel blends to enable high engine efficiency.

Reviewer 5:
The project's focus is on fundamental understanding of fuel properties, which is of clear value to the research community. How this understanding directly connects with the higher level Co-Optima research goals needs to be highlighted. What are the ultimate deliverables, and how do they fit within the larger Co-Optima narrative and contribute to overall Co-Optima program outcomes?

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

Reviewer 1:
It seems that the funding is sufficient.

Reviewer 2:
Project resources seem sufficient for the scope and scale of the effort.

Reviewer 3:
Resources are sufficient and not excessive.

Reviewer 4:
Resources are sufficient to accomplish the stated goals.

Reviewer 5:
This type of fundamental science work to understanding autoignition and fuel properties would benefit from some additional resources to move progress along more quickly. Improved experimental equipment and facilities and improved simulation capability would be of benefit to this work.

Presentation Number: ft089
Presentation Title: Heavy-Duty Advanced Compression Ignition
Principal Investigator: John Dec (Sandia National Laboratories)

Presenter

John Dec, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers indicated that the resources were sufficient, 0% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.

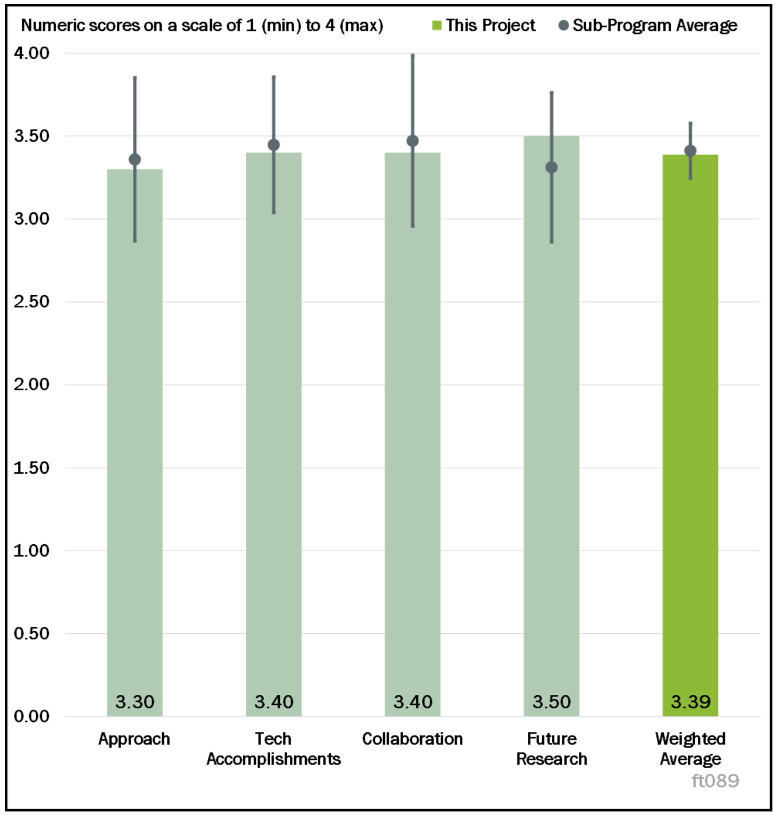

Figure 5-15 - Presentation Number: ft089 Presentation Title: Heavy-Duty Advanced Compression Ignition Principal Investigator: John Dec (Sandia National Laboratories)

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

Reviewer 1:

The current approach of including three engine projects and making conclusive findings with integrated results is excellent! Well-integrated CFD for all three platforms can make the analysis stronger in this project. The existing approach will address most of the needs, but to judge “improving combustion-phasing control,” transient and cycle-by-cycle engine data should be studied.

Reviewer 2:

The reviewer appreciated the growth of this project to include multiple combustion approaches. All of the ACI approaches have significant challenges remaining to be addressed before they are feasible for production implementation in HD engines; pursuing multiple pathways at the same time should allow for cross-knowledge and a faster path to technology development. The reviewer was also glad to see that modeling support tasks have been brought in as well; good modeling tools are critical to development of the ACI systems.

Reviewer 3:

The approach taken to document autoignition metrics was excellent. The impingement study lacked the same effort in metrics and variation. The wide variation in the tasks makes the cohesion of conclusions unclear. How do these efforts complement each other?

Reviewer 4:

The overall goal of this effort is to understand fuel properties that can improve engine performance and emissions. Three different engine projects were presented for this review. Individually, each effort is well designed, planned, and executed toward the goal of understanding fuel property impacts on advanced combustion strategies. A comment from this reviewer is that the various combustion strategies are more similar than different, and it is misleading to use different acronyms for them (i.e., they are different shades of gray, and rather than give them all different names it would be more beneficial to describe them and give them names that are indicative of where on the spectrum of “gray” that they fall). There seems to be a penchant for new acronyms and names; taking a step back and standardizing nomenclature would be beneficial, at least in the opinion of this reviewer.

Reviewer 5:
The idea of exploring the potential for changes in fuel composition and characteristics to improve MD and HD engines, which are primarily diesel powered, is good. It seemed to the reviewer that there is tremendous overlap between parts of this project and project ACE157 with the same PI. It would be helpful to articulate the synergies and distinctions. Is it hoped to develop a new fuel that will not need to be augmented like low-temperature gasoline combustion (LTGC)-additive-mixing fuel injection (AMFI)?

It seemed to the reviewer that for any changes in fuel characteristics to be acceptable for this market, they will have to be capable of maintaining high efficiency at maximum load, which is an important operating condition for these engines, especially in the HD sector. To that end, this reviewer thought engine projects 1 and 2 will be extremely challenging when using gasoline-like fuels, an expression that was used during the presentation. Achieving high load with LTGC and GCI will be extremely difficult without something like AMFI. Engine project 3, which the reviewer interpreted to be more of an MM operation, makes more sense in terms of a single fuel.

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 some slight delays were encountered due to the COVID-19 pandemic, the efforts have made very good progress and their delays are understandable given the pandemic.

Reviewer 2:
Despite the unavoidable effects by COVID-19, the project has made very good progress and is on track. The project results show strong accomplishments on Objectives 1 and 2 from the work done at SNL, which is very interesting.

Reviewer 3:
There was some good technical progress on all the tasks, including the new ones. With so many tasks to cover, it is difficult to tell exactly how much progress has been made toward the goal of this chunk of Co-Optima.

Reviewer 4:
Significant progress was made in several areas. The individual contributors provided very detailed explanations of their results, both expected and unexpected. Identifying the limitations of using OI as a metric was challenged and explanations given. The evaluations of fuel blends led to useful conclusions. Some tasks are too new to draw conclusions or gain insight.

Reviewer 5:
Two of the projects are just starting so it is too early to expect significant results. The results for the LTGC are interesting but seem to be for relatively light loads, phi = 0.36. The custom blend (CB) #1 fuel looks very interesting.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:
The teams all have good collaborations among the Co-Optima areas. The reviewer encouraged the three engine teams to communicate about their findings to see where there may be cross-knowledge and how their findings might support mode switching and other factors that could be important for commercial technology transfer.

Reviewer 2:
Collaboration looks very good as with all Co-Optima projects. The reviewer was curious about the extent to which the industry partners, Cummins and Caterpillar, are engaged in discussions on the technical work plan, in addition to offering equipment support.

Reviewer 3:
The project is well coordinated among the four groups at three National Laboratories. The reviewer understood that a good portion of the activities are supposed to occur in the future. Strong integration of CFD results with engine experimental studies for all the studied experimental platforms is very important for in-cycle combustion and emission analysis to provide conclusive outcomes from this project.

Reviewer 4:
The efforts were spread between many laboratories, and each performed their tasks well. The overlapping focus from contributors can sometimes slow progress, but this work seems to escape that.

Reviewer 5:
While the individual efforts are coordinated with Co-Optima and engage with universities and OEMs as appropriate, the most significant concern of this reviewer is that the three efforts reviewed in this presentation appear to be wholly separate from one another with virtually no coordination. The overall Co-Optima goal is to co-optimize engine and fuels, but there is no attempt to coordinate the results and efforts of these three projects with one another, and thus it is not at all evident how these efforts actually lead to Co-Optima achieving its goals. A coherent plan for ultimately determining “best” (or even “better”) combinations of fuel, hardware, and combustion strategy is warranted. This could, for example, be approached as determining what fuel properties allow for the most flexibility in hardware, or that allow for the broadest range of engine operation with a given strategy. Alternatively, it could be approached as determining what combustion strategy or strategies are most tolerant to variations in fuel properties. Perhaps data to do so have been collected, and this meta-analysis simply needs to be done.

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. Note: if the project has ended, please state project ended.

Reviewer 1:
The future work plans look good and should continue to push the tasks toward their targets.

Reviewer 2:
Individually, the planned next steps for all of these efforts are logical and appropriate.

Reviewer 3:
Given the current project objectives, the work planned is logically laid out.

Reviewer 4:
The planned activities are logical next steps. It is important that engine combustion and control analysis will also include cycle-by-cycle engine transient data.

Reviewer 5:
The future work is focused on the specific tasks, and this reviewer would like to have seen how this array of tasks comes back to a cohesive collection to allow directions and decisions to be made in co-optimization efforts. The tasks seem too specific for such a large variation of tasks.

Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:
These tasks support the need to improve MD/HD fuel economy and are areas of interest to the HD community.

Reviewer 2:
The fundamental tasks and investigations that comprise this single project will aid various efforts in the fuel and IC engine areas. The characterization of new fuel-ignition metrics and spray formation and evolution is in step with taking more steps in ACI and the emissions and fuel economy benefits that are shown in this project. The cascading of techniques and discoveries made in this project need to be vetted as this reviewer is concerned that the evaluations are specific to the individual efforts being undertaken.

Reviewer 3:
The idea of exploring the potential for changes in fuel composition/characteristics to improve MD and HD engines, which are primarily diesel powered, is good. It is relevant to DOE objectives.

Reviewer 4:
Yes, this project directly supports the DOE Strategic Objective to "Deliver the scientific discoveries and major scientific tools that transform our understanding of nature and strengthen the connection between advances in fundamental science and technology innovation." The outcomes of the project provide stepping stones toward fuel-efficient, clean IC engines.

Reviewer 5:
To the extent that these efforts are aiming to improve engines and fuels, these efforts are aligned with DOE's objectives. However, as noted above, more effort is needed to ensure that these efforts align with Co-Optima's goals.

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

Reviewer 1:
Budgets look fine for the work scopes.

Reviewer 2:
The amount of work that is described in these efforts is remarkable. The task breakdown, the analysis execution, and the presentation of results using so many different contributors are well done.

Reviewer 3:
The resources are sufficient for achieving project success in a timely fashion.

Reviewer 4:
It appears that the support is sufficient.

Reviewer 5:
The team has access to required resources to conduct this project.

Acronyms and Abbreviations

AFC	Alternative Fuel Corridor
0-D	Zero-dimensional
100LL	100 low lead
3-D	Three-dimensional
ACEC	Advanced Combustion and Emissions Control
ACI	Advanced compression ignition
AEC	Advanced Engine Combustion
AFIDA	Advanced fuel ignition delay analyzer
AI	Artificial intelligence
AKI	Anti-knock index
AMFI	Additive-mixing fuel injection
AMR	Annual Merit Review
ANL	Argonne National Laboratory
BETO	Bioenergy Technologies Office
BOB	Blendstocks for oxygenate blending
Ca	Calcium
CA50	Crank angle at 50% mass fraction burned
CB	Custom blend
CeO_2	Cerium oxide (ceria)
CFD	Computational fluid dynamics
CFR	Cooperative fuel research
CI	Compression ignition
CN	Cetane number
CO	Carbon monoxide
CO_2	Carbon dioxide
CRC	Coordinating Research Council
CTI	Cleaner Truck Initiative
DFI	Ducted fuel injection

DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
E15	Gasoline blended with 10.5%-15% ethanol
ECN	Engine Combustion Network
EGR	Exhaust gas recirculation
EPA	U.S. Environmental Protection Agency
FY	Fiscal year
GCI	Gasoline compression ignition
GDCI	Gasoline direct injection compression ignition
GDI	Gasoline direct injection
GHG	Greenhouse gas
GM	General Motors
HC	Hydrocarbon
HCCI	Homogeneous charge compression ignition
HD	Heavy-duty
HOV	Heat of vaporization
HPF	High-performance fuels
HRM	Homogeneous relaxation model
iHOV	Instantaneous heat of vaporization
K	Empirical factor (or constant)
L	Liter
LBNL	Lawrence Berkeley National Laboratory
LD	Light-duty
LEV	Low-emission vehicle
LLNL	Lawrence Livermore National Laboratory
LSPI	Low-speed pre-ignition
LTC	Low-temperature combustion
LTGC	Low-temperature gasoline combustion

LW	Livengood-Wu
MCCI	Mixing-controlled compression ignition
MCE	Multi-cylinder engine
MD	Medium-duty
ML	Machine learning
MM	Multi-mode
MON	Motor octane number
MOU	Memorandum of understanding
NMR	Nuclear magnetic resonance
NO	Nitric oxide
NO_x	Oxides of nitrogen
NREL	National Renewable Energy Laboratory
NTC	Negative-temperature coefficient
OEM	Original equipment manufacturer
OI	Octane index
OS	Octane sensitivity
PACE	Partnership for Advanced Combustion Engines
PAH	Polycyclic aromatic hydrocarbon
Pd	Palladium
PFS	Partial fuel stratification
PGM	Platinum group metals
PI	Principal investigator
PIONA	Paraffins, iso-paraffins, olefins, naphthenes, and aromatics
PM	Particulate matter
PMI	Particulate matter index
PN	Particle number
PNNL	Pacific Northwest National Laboratory
PPCI	Partially pre-mixed compression ignition

Pt	Platinum
P-T	Pressure-temperature
Q&A	Question and answer
R&D	Research and development
RANS	Reynolds-averaged Navier-Stokes
RCM	Rapid compression machine
Rh	Rhodium
RON	Research octane number
SACI	Spark-assisted compression ignition
SCE	Single-cylinder engine
SCR	Selective catalytic reduction
SI	Spark ignition
SNL	Sandia National Laboratories
SOI	Start of injection
SON	Supercharged octane number
SPI	Stochastic pre-ignition
SULEV	Super ultra-low emission vehicle
$SULEV_{30}$	Super ultra-low emissions vehicle with 0.030 grams/mile combined non-methane organic gases and NO_x
T50	Temperature at which 50% of the distillate fuel is recovered in a distillation experiment
T90	Temperature at which 90% of the distillate fuel is recovered in a distillation experiment
TDC	Top dead center
TWC	Three-way catalyst
U.S.	United States
$ULNO_x$	Ultra-low NO_x
USCAR	United States Council for Automotive Research
VTO	Vehicle Technologies Office
WTW	Well-to-wheels

Y	Yield-sooting index
Zero-RK	Zero-order Reaction Kinetics