3. Decarbonization of Off-Road, Rail, Marine, and Aviation Technologies

The Vehicle Technologies Office (VTO) supports research, development, demonstration, and deployment (RDD&D) of new, efficient, and clean mobility options that are affordable for all Americans. The office's investments leverage the unique capabilities and world-class expertise of the national laboratory system to develop new innovations in vehicle technologies, including: advanced battery technologies; advanced materials for lighter-weight vehicle structures and better powertrains; energy-efficient mobility technologies and systems (including automated and connected vehicles as well innovations in connected infrastructure for significant systems-level energy efficiency improvement); innovative powertrains to reduce greenhouse gas (GHG) and criteria emissions from hard to decarbonize off-road, maritime, rail, and aviation sectors; and technology integration that helps demonstrate and deploy new technology at the community level. In coordination with the other offices across the Office of Energy Efficiency and Renewable Energy and the U.S. Department of Energy (DOE), VTO advances technologies that assure affordable, reliable mobility solutions for people and goods across all economic and social groups; enable and support competitiveness for industry and the economy/workforce; and address local air quality and use of water, land, and domestic resources.

The Decarbonization of Off-Road, Rail, Marine, and Aviation (DORMA) Technologies subprogram supports RDD&D to develop and deploy new propulsion and efficient vehicle technologies in off-road, rail, marine, and aviation applications that reduce GHG emissions and achieve a net-zero economy by 2050, all while creating good paying jobs with the free and fair chance to join a union and bargain collectively.

The goal of this portfolio is to conduct coordinated research with industry, universities, and the national laboratories through Cooperative Research and Development Agreements (CRADAs).This subprogram conducts industry-led RDD&D for off-road medium and heavy-duty (HD) vehicles, including engines used for marine, rail, and aviation, focused on electrified and hybrid systems as well as powertrains that can utilize renewable fuels, such as advanced biofuels, H2, renewable diesel and e-fuels. The subprogram will coordinate with and utilize expertise from other Offices and VTO programs as needed.

The subprogram supports cutting-edge research at the national laboratories, in close collaboration with industry, while working closely with other agencies including the Environmental Protection Agency and Department of Transportation's Federal Railroad Administration and Maritime Administration, to achieve goals for decarbonization of these subsectors. It will use a multi-laboratory initiative, including high performance computing and hardware in-the-loop resources, for research to optimize vehicle efficiency which also will be applicable to hard to electrify on-road HD vehicles.

The subprogram also supports industry needs to develop predictive, high-fidelity sub-models and simulation tools that are scalable and can leverage future exascale computing capabilities. The activity will fund research of renewable fuel properties utilizing chemical kinetics modeling of different molecules to determine their impact on combustion efficiency and emissions. It will also develop numerical routines and sub-models of complex chemical reactions that can reduce the computational time and increase the accuracy required for high-fidelity engine models, making them viable for use by industry.

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 3-1 – Project Feedback

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaboration	Future Research	Weighted Average
DORMA001	Overcoming key barriers to H2ICEs—mixing pre-ignition and ultra-lean operation.	Ales Srna (Sandia National Laboratories)	3-7	3.25	3.50	3.38	3.13	3.38
DORMA002	Alcohol combustion in CI engines—understanding mixing ignition and pollutant emissions	Dario Lopez-Pintor (Sandia National Laboratories)	3-13	3.17	3.25	3.25	3.00	3.20
DORMA003	Soot Predictions from DNS of a lab-scale combustor with sustainable aviation fuels	Bruno Souza Soriano (Sandia National Laboratories)	3-21	3.50	3.50	3.50	3.13	3.45
DORMA004	Mixing-controlled compression-ignition combustion with low-lifecycle-CO_2 fuels	Chuck Mueller (Sandia National Laboratories)	3-28	3.63	3.50	3.75	3.63	3.58
DORMA005	Alcohol spray and H_2 jet experiments and modeling	Lyle Pickett (Sandia National Laboratories)	3-33	3.60	3.50	3.50	3.40	3.51
DORMA006	Low Lifecycle Carbon Fuel (LLCF) combustion and emission models	Scott Wagnon (Lawrence Livermore National Laboratory)	3-39	3.63	3.50	3.75	3.63	3.58

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaboration	Future Research	Weighted Average
DORMA008	Slashing Platinum Group Metal (PGM) in Catalytic Converters An Atoms-to-Autos Approach	Kevin Gu (General Motors)	3-43	3.50	3.50	3.58	N/A	3.51
DORMA010	Off-Road Decarbonized Fuel Transient Performance	Muni Biruduganti (Argonne National Laboratory)	3-49	3.33	3.17	2.83	3.17	3.17
DORMA012	Enabling Hydrogen Combustion for Large-Bore Locomotive Engines through Advanced CFD Modeling	Muhsin Ameen (Argonne National Laboratory)	3-53	3.13	3.13	3.25	3.25	3.16
DORMA014	Implementing low lifecycle carbon fuels on locomotive engines – CRADA with Wabtec	Dean Edwards (Oak Ridge National Laboratory)	3-58	3.30	3.20	3.40	3.20	3.25
DORMA015	Predictive CFD Tools for Low-Carbon Fueled Off-road Internal Combustion Engines	Riccardo Scarcelli (Argonne National Laboratory)	3-63	3.00	3.33	3.00	2.83	3.15
DORMA016	Renewable methanol-fueled engines for marine and off-road applications	Jim Szybist (Oak Ridge National Laboratory)	3-66	3.50	3.50	3.67	3.33	3.50
DORMA018	SAF Combustion and Contrail Formation Research	Julien Manin (Sandia National Laboratories)	3-69	3.25	3.00	3.25	3.00	3.09
DORMA019	Multi-phase flow studies of SAFs for industry-relevant conditions and geometries	Brandon Sforzo (Argonne National Laboratory)	3-73	3.83	3.67	3.67	3.83	3.73

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaboration	Future Research	Weighted Average
DORMA020	Sustainable Aviation Fuel (SAF) Contrail Modeling	Matt McNenly (Lawrence Livermore National Laboratory)	3-79	2.83	2.83	3.17	2.83	2.88
DORMA021	Simultaneous Greenhouse Gas and Criteria Pollutants Emissions Reduction for Off-Road Powertrains	James McCarthy (Eaton)	3-83	3.70	3.70	3.50	3.60	3.66
DORMA022	Development of a Flex-Fuel Mixing Controlled Combustion System for Gasoline/Ethanol Blends Enabled by Prechamber Ignition	Adam Dempsey (Marquette University)	3-88	3.75	3.75	3.25	3.50	3.66
DORMA025	Fully Electric Powered Hydraulic Assisted Compact Track Loader	Perry Li (University of Minnesota)	3-92	3.33	3.67	3.67	3.33	3.54
DORMA026	Articulated Dump Truck (ADT) Electrification—Greenhouse Gas Reductions and Commercialization of New Technology	Brij Singh (John Deere)	3-95	3.67	3.33	3.17	3.50	3.42
DORMA027	Control of aldehyde emissions from alcohol-fueled non-road engines	Sreshtha Majumdar (Oak Ridge National Laboratory)	3-99	3.30	3.30	3.40	3.20	3.30
DORMA028	Comprehensive Integrated Simulation Methodology for Enabling Near-Zero Emission Heavy-Duty Vehicles	Andrea Strzelec (University of Wisconsin-Madison)	3-105	3.13	3.13	3.63	3.25	3.20

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaboration	Future Research	Weighted Average
DORMA029	Fast Simulation of Real Driving Emissions from Heavy-duty Diesel Vehicle Integrated with Advanced Aftertreatment System	Hailin Li (West Virginia University)	3-109	3.33	3.17	3.17	3.33	3.23
DORMA030	Opposed-Piston 2-Stroke Hybrid Commercial Vehicle System	Ming Huo (Achates Power)	3-112	2.80	3.20	3.30	2.80	3.06
DORMA032	High Efficiency Ultra Low Emissions Heavy-Duty 10L Natural Gas Engine Project	Tim Lutz (Cummins)	3-118	3.63	3.63	2.38	3.50	3.45
DORMA033	High Pressure Fast Response Direct Injection System for Liquified Gas Fuels Use in Light-Duty Engines	William de Ojeda (WM International Engineering)	3-122	3.17	3.67	3.17	3.50	3.46
DORMA037	Sustainable Aviation Fuel Characterization	Gina Fioroni (National Renewable Energy Laboratory)	3-125	3.40	3.50	3.50	3.10	3.43
DORMA038	Towards Accurate Combustion and Emissions Modeling of Sustainable Aviation Fuels	Debolina Dasgupta (Argonne National Laboratory)	3-131	3.83	3.50	3.33	3.50	3.56
DORMA040	Optimized Low Carbon Fuel Range Extender (HyREX)	Jon A. Dickson (Cummins)	3-136	3.38	3.38	3.25	3.25	3.34
DORMA041	Low greenhouse gas NO_x control	Dhruba Deka (Pacific Northwest National Laboratory)	3-140	3.50	3.20	3.30	3.50	3.33

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaboration	Future Research	Weighted Average
DORMA042	Unforeseen challenges with renewable fuels	Konstantin Khivantsev (Pacific Northwest National Laboratory)	3-146	3.00	3.00	3.33	3.00	3.04
DORMA043	Low-load cycle emission control	Yong Wang (Pacific Northwest National Laboratory)	3-151	3.70	3.50	3.80	3.50	3.59
DORMA045	Biodiesel poisoning of close-coupled SCR catalysts for off-road engines	Todd Toops (Oak Ridge National Laboratory)	3-156	3.63	3.38	3.50	3.25	3.44
DORMA046	Ammonia for 4-stroke Marine Dual Fuel and Gas Engines (Retrofits and New)	Scott Curran (Oak Ridge National Laboratory)	3-161	3.50	3.75	3.00	3.00	3.50
DORMA047	High-Efficiency Mixing Controlled Compression Ignition Combustion of Propane Dimethyl Ether Blends	Sage Kokjohn (University of Wisconsin)	3-165	2.83	3.00	3.00	2.67	2.92
DORMA051	Fuel effects on aviation engine emissions – a modeling tool for SAF screening	Dario Lopez-Pintor (Sandia National Laboratories)	3-169	3.50	3.50	3.38	3.13	3.44
DORMA052	Simulation of Jet Engine Performance using SAF Blends	Shashank Yellapantula (National Renewable Energy Laboratory)	3-174	3.50	3.50	3.83	3.50	3.54
Overall Average				3.39	3.38	3.36	3.26	3.37

Presentation Number: DORMA001
Presentation Title: Overcoming key barriers to H2ICEs—mixing pre-ignition and ultra-lean operation
Principal Investigator: Ales Srna, Sandia National Laboratories

Presenter

Ales Srna, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

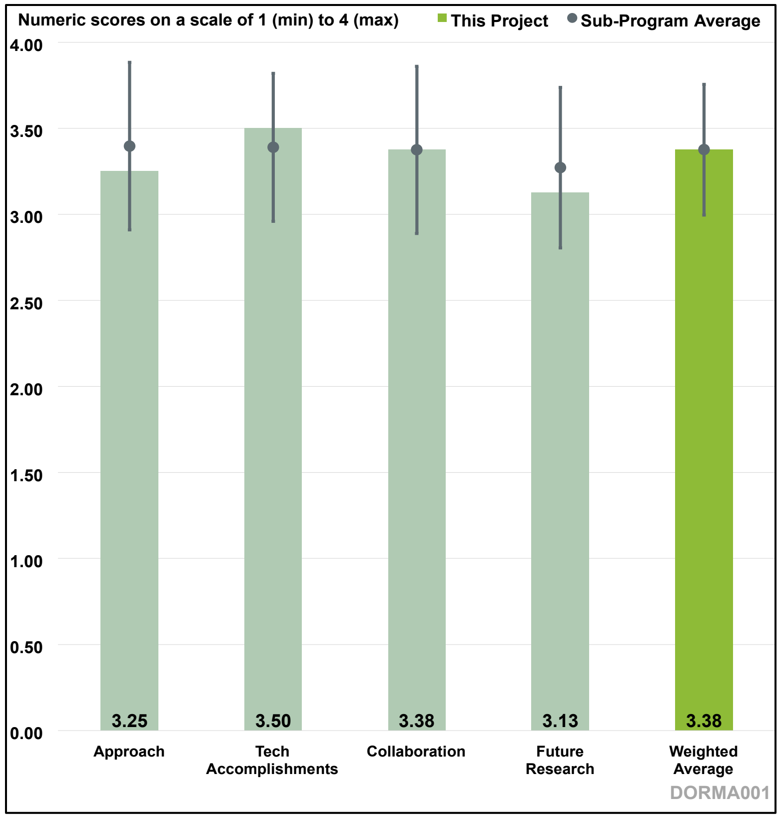

Figure 3-1. Presentation Number: DORMA001 Presentation Title: Overcoming key barriers to H2ICEs—mixing pre-ignition and ultra-lean operation Principal Investigator: Ales Srna, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer observed that the project focuses on hydrogen (H_2) internal combustion using both a pilot ignition source and pre-chamber spark ignition, noting that both approaches are likely in the future. The reviewer suggested considering both retrofit and new engine design approaches. The reviewer asked whether homogeneous charge compression ignition is possible with H_2 fuel in internal combustion engines (ICEs) and whether high compression ratio allows for late injection compression ignition of H_2 direct injection (DI) fuel. The reviewer remarked that the future design space is varied and unclear and acknowledged that efforts to organize the possible operation space would be useful to the engine community.

Reviewer 2

This reviewer stated that the project's tasks are designed to overcome barriers that have impeded the wide-spread use of H_2-fueled ICEs. According to this reviewer, the ultimate goal of the project is for H_2-fueled ICEs to command a significant market in the transportation sector, thereby reducing the harmful emissions from conventional liquid-fueled combustion engines and achieving zero GHG emissions. The reviewer observed that a CRADA with Caterpillar and other entities from industry and academia provides a framework for investigating combustion in a single-cylinder engine. The project also includes computational fluid dynamics (CFD) to simulate in-cylinder H_2 injection and flow dynamic processes.

The reviewer considered the single-cylinder engine configuration appropriate for the project's intended purposes. The reviewer urged the principal investigator (PI), however, to make clear which results and processes in this configuration will carry over to the more complex multi-cylinder configuration of commercial engines, acknowledging that the PIs posed a related question on Slide 28 asking whether optical engine results are fully representative of production/metal engine performance.

This reviewer deemed the use of zero-dimensional (0D) or one-dimensional (1D) models to understand complex combustion processes a reasonable approach, noting that low-order transport configurations can provide significant insight and data to validate detailed numerical models of combustion. The reviewer explained that there are aspects of combustion that are not necessarily impacted by differences in transport (e.g., the size of soot precursor particles is independent of the flaming configuration). The reviewer suggested that future presentations should identify which information from 0D or 1D models is relevant to the more complex in-cylinder environment of an engine, where turbulence, swirl, three-dimensional (3D) transport, etc., exists, since it was not clear in this presentation. The reviewer also questioned the broader applicability of models that require significant tuning to capture H_2 heat flux, referring to Slide 16 and noting that the presentation did not discuss how tuning would be carried out or the broader applicability of the models to the results.

The reviewer pointed out that the project addresses many basic in-cylinder processes associated with fuel injection, mixing, swirl, ignition, flame/wall interactions, engine operation under different conditions of injection pressure, mixture distribution, injector configurations, effects of lubrication oil droplets, etc. The reviewer found it challenging at times to understand the rationale for selecting conditions to investigate and how the results obtained would inform a predictive CFD capability. The reviewer observed that the project is focused on engine testing, where operational conditions are set, and the results are discussed. While results from individual components were clearly presented, the reviewer was unable to discern from the presentation, in the limited time available, how the components fit together to provide a clear path to the ultimate long-term objective of the project. For example, the term 'phenomenology' on Slide 17 was not specifically defined and was therefore difficult to link to something measurable. Similarly, photos of a multi-port injector were shown, but it was not clear what quantitative information or data were obtained from the injector (e.g., penetration rate, width of the jets) or how this data would be used in modeling). The reviewer recommended that future presentations include a flow chart or other graphic showing how the individual parts fit together and contribute to the whole.

The approach to close the knowledge gap impeding H_2 ICE development by conducting experiments using optical and laser-imaging diagnostics in a heavy-duty engine with computer modeling was unclear to this reviewer, who commented that computer modeling usually involves measurements followed by predictions. The reviewer observed that the presentation did not specify what is being measured by laser imaging, how the measurements are used in simulations, or what inputs were used for the computer modeling and numerical framework.

The reviewer remarked that the role of oil droplets was not clearly presented, pointing out that Slide 4 shows droplets of lubricating oil on the surface of a piston while Slide 16 shows photos of oil droplets from a single-hole injector, raising questions about the origin of the oil droplets shown on Slide 16. The reviewer expressed a need for clarification of the oil droplet concern.

Lastly, this reviewer mentioned a need for more clarity regarding the choice of operating conditions employed in the investigation of in-cylinder mixture formation, e.g., what guided the choice of swirl ratios of 0.5 to 3.5.

Reviewer 3

This reviewer concluded that the project is well designed and will contribute to addressing some of the challenges with H_2 ICEs. The timeline was deemed by the reviewer to be reasonable for the scope of the project. The reviewer pointed out that the combustion studies' operating conditions are limited and recommended expanding the studies to include high-pressure injection (200 – 300 bar), which has the advantage of high brake efficiency and power density, as well as port fuel injection, which may reduce particulate emissions compared to direct injection.

Reviewer 4

The reviewer stated that the project presents a comprehensive summary of the technical barriers to H_2 ICEs and asserted that the long list of challenges and the itemized list of knowledge gaps highlight the need for extensive research. The reviewer questioned whether an H_2 ICE product can be quickly launched in the market to gain customer acceptance, as the project perspective on Slide 4 suggests, without compromising performance or emissions.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

This reviewer praised the team's mixture preparation experiments and modeling and highlighted the importance of the project's collaboration with Lyle Pickett to understand the possibility for in-homogeneity. The reviewer also affirmed the usefulness of the early versus late injection results and the hydrocarbon-induced pre-ignition studies for future engine designers.

Reviewer 2

The reviewer acknowledged that extensive engine testing was carried out during this reporting period but noted that it was not always clear how the many individual components of the testing program fit together. The reviewer stated that the snapshots of results revealed significant technical accomplishments that were achieved in this reporting period, observed that there are many parts to this project, and commended the PIs for summarizing key results. The person concluded that most of the barriers to implementation of H_2 ICE technology are being addressed with the possible exception of H_2 supply and storage infrastructure, which is outside the scope of this project but may be appropriately addressed within the DOE Bioenergy Technologies Office or the DOE Hydrogen Program.

Reviewer 3

This reviewer praised the project's combustion results, which provide valuable insights on pre-chamber fueling, the impact of swirl and H_2 interaction on in-cylinder mixture distribution, and the effect of H_2 on auto-ignition of hydrocarbons.

Reviewer 4

The reviewer appreciated the clear outline of the milestones completed in 2023 and those in progress in 2024. The reviewer commended the project's experimental work, documentation of the engine swirl effects, insightful data, and visualizations of H_2 ICE pre-chamber ignition and in-cylinder processes. The reviewer found the characterization of differences relative to natural gas combustion helpful.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer pointed out that Slide 6 mentions a number of collaborations. The connection with Lyle Pickett was described by the reviewer as excellent. This reviewer indicated that it would be helpful if involved partners were identified within the results slides.

Reviewer 2

The reviewer observed that the team is quite large, encompassing about nine components, with Caterpillar being the lead. With so many team members, it was not always clear to the reviewer how the components fit together. For example, it was not clear how Argonne National Laboratory's (ANL's) in-cylinder CFD of H_2 ICEs, which includes pre-ignition studies, fits together with the University of Duisberg-Essen's CFD on in-cylinder H_2 mixture formation. The reviewer questioned whether ANL is using CONVERGE and the academic partners a different numerical framework, noting that the presentation did not identify which codes were used. The reviewer pointed out that CFD will require inputs such as property data and kinetic mechanisms for combustion simulations, as well as assessments of uncertainty in the simulations, yet no discussion of the accuracy of the simulations was incorporated. The reviewer questioned how the international universities in the project were selected for the CFD modeling effort, expressing particular interest in knowing the unique competencies that motivated the choices. Since the presentation provided little information on the CFD modeling, the reviewer found it difficult to assess the modeling component of the project (e.g., inputs required, numerical methods used, adaptive gridding [if incorporated], computational time, validation). The reviewer presumed that Caterpillar has assessed these matters during the biannual meetings among the team members.

Reviewer 3

The reviewer commented that collaboration and coordination with other institutions is well documented and encouraged the team to keep it up.

Reviewer 4

The reviewer stated that the work is part of a CRADA with Caterpillar and that the project includes collaboration with Sandia National Laboratories. The person observed that the project also receives input from a wide range of industrial original equipment manufacturers (OEMs), government, and universities.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

This reviewer can affirm that pre-ignition was likely driven by residual gas. Noting that residual-gas-driven pre-ignition was mentioned in the presentation as a future topic, the reviewer affirmed the importance of investigating this mechanism and encouraged the team to spend time on it. The reviewer remarked that both the future mixture preparation and pre-chamber work will be useful.

Reviewer 2

The reviewer observed that future plans were presented in general terms. The future plans include addressing in-cylinder mixture formation, pre-ignition, and wall heat loss, among other aspects. The reviewer noted that science-based correlations for pre-ignition mechanisms were mentioned, but it was not clear what precisely would be correlated and what experiments would be required.

The reviewer was interested in the modification of the optical engine to permit interchangeable swirl combustion geometries, although. The motivation for this modification (i.e., the gaps that needed to be filled, such as the swirl level) was not presented.

This reviewer recommended that a pictorial representation of the project be incorporated in the presentation to show how the components fit together, including national lab, industry, and academic partner contributions. Some detail on the CFD efforts would also be useful, such as a property database, the kinetic mechanism for combustion simulations, validation, etc.

The reviewer remarked that comments on the hydrogen infrastructure for production, supply, storage, delivery, etc., would be useful to include in order to provide context to the overall goal of deploying H_2 ICEs in the market by the 2027 timeframe noted in the presentation. The reviewer acknowledged that the DOE Hydrogen Program may already be solving hydrogen infrastructure issues but asserted that studies such as this one would be enhanced by the deflection of concerns about storage, supply, safety, etc.

This reviewer pointed out that in the introduction (Slide 3), the PIs have headings entitled “Relevance” and “Long-Term Objective.” The reviewer suggested that it would be helpful to have a box with the heading “Approach.”

Reviewer 3

The reviewer applauded the proposed future research, adding that it will contribute to overcoming in-cylinder mixture formation and pre-ignition challenges as well as ignition system challenges and wall heat loss. The reviewer recommended addressing additional challenges affecting the commercialization of this technology, such as the impact of water produced on the ICE components, in the proposed future research.

Reviewer 4

This reviewer reported that the project plans to continue to investigate the mixture formation and pre-ignition in the combustion cylinder as well as to expand the scope to investigate ignition systems and wall heat losses. The reviewer asserted that providing the next period’s milestones would improve the presentation.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This reviewer expressed an expectation that H_2 ICEs will be important in the medium- and heavy-duty high-power, high-duty-cycle domain and affirmed the usefulness of this project’s work for future H_2 ICE research and development (R&D).

Reviewer 2

The reviewer concluded that the project’s H_2 ICE R&D is highly relevant to the VTO subprogram objectives in that H_2 ICEs have potential to help decarbonize emissions when integrated into the market. The reviewer observed that the team combines many elements in its development of H_2 ICEs, all of which are incorporated to address performance and emissions.

Reviewer 3

This reviewer stated that the project supports the overall VTO subprogram objectives for decarbonization of difficult-to-electrify sectors with high-power-density applications by helping to close the knowledge gaps pertaining to H_2 ICE in-cylinder processes and control strategies.

Reviewer 4

The reviewer affirmed that the work is relevant, noting that H_2 ICEs are being actively developed by OEMs for decarbonization of difficult-to-electrify industrial sectors.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This reviewer remarked that the project's resources appear to be sufficient.

Reviewer 2

The reviewer said that the resources seem adequate for this large project but cautioned that more details (e.g., overhead rates, scientist and technician salaries, equipment costs, etc.) beyond the bottom-line costs for the project provided in the presentation are needed for the reviewer to adequately evaluate the project's resources. The person added that an ultimate judgement would have to come from a cost/benefit analysis based on DOE's investment relative to the commercialization potential of the technology under investigation.

Reviewer 3

This reviewer observed that the project is on track and milestones are being met with the current funding level.

Reviewer 4

The reviewer concluded that the resources and experimental facilities for this project are adequate.

Presentation Number: DORMA002
Presentation Title: Alcohol combustion in CI engines—understanding mixing ignition and pollutant emissions
Principal Investigator: Dario Lopez-Pintor, Sandia National Laboratories

Presenter

Dario Lopez-Pintor, Sandia National Laboratories

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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

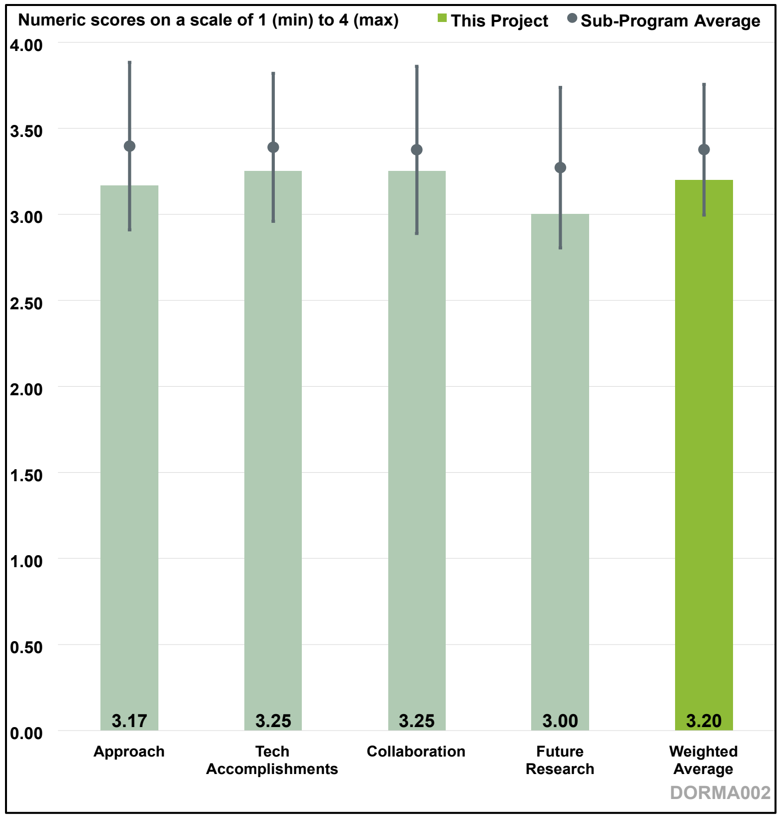

Figure 3-2. Presentation Number: DORMA002 Presentation Title: Alcohol combustion in CI engines—understanding mixing ignition and pollutant emissions Principal Investigator: Dario Lopez-Pintor, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer stated that the project is on track and technical barriers are adequately addressed. According to the reviewer, a logical approach to synchronize work across mixing, ignition, and combustion tasks was laid out early in the presentation and then discussed in the technical accomplishments section. The reviewer noted that the technical accomplishments exhibit a clear progression to a dual-fuel solution with an active pre-chamber and observed that results from literature were used to guide active pre-chamber work.

Reviewer 2

The reviewer gave this project a rating of “fair” for its approach to performing the work of addressing technical barriers related to the use of lower carbon intensity alcohol fuels, namely ethanol and methanol. The reviewer pointed out that the project’s approach of studying the ignition and combustion of high-octane, low-cetane alcohol fuels (methanol and ethanol) in a direct compression-ignition engine configuration is not novel and does not contribute to alleviating barriers to methanol or ethanol utilization. Direct compression-ignition of highly ignition-resistant alcohol fuels has been studied in various research programs and has been implemented commercially in a small number of vehicles and vessels. The reviewer observed that despite being commercially deployed for over a decade, direct compression-ignition has not seen significant growth. The reviewer asserted that methanol and ethanol are fundamentally well-suited to spark-ignition combustion processes because of their extremely high octane numbers, but they are poorly suited to direct compression-ignition combustion because of very low cetane numbers. The reviewer further noted that alcohol ignition chemistry has been shown repeatedly in the literature to be particularly unresponsive to both commercial and experimental ignition improvers, and this project only re-confirms those results. The reviewer recommended that the project shift to commercially and technically relevant approaches to utilization of lower-carbon-intensity alcohol fuels. These approaches include both pilot-ignition processes for large-bore, low-speed marine engines and spark-ignition processes for higher-speed, smaller-bore boat and off-road engines.

Reviewer 3

This reviewer acknowledged that the project addresses some key aspects of mixing-controlled compression ignition (MCCI) combustion of the alcohol fuels, such as spray penetration, lift-off length, ignition delay, and 3D CFD simulation. However, the reviewer pointed out that some of the project's research areas are not well aligned with MCCI combustion. The relevance and motivation behind port fuel injection (PFI) spray characterization and PFI-led passive pre-chamber combustion characterization in the optical engine were unclear to the reviewer. Although the reviewer found the concept of active-pre-chamber-assisted MCCI combustion interesting, the reviewer questioned whether it is a pragmatic solution considering the cost, complexity, and controllability challenges. The person asserted that doping a large quantity of 2-ethlyhexyl nitrate is also impractical. This reviewer concluded that the project is not sharply focused on developing practical solutions that address the key technical barriers for MCCI combustion, including robust and efficient low-load combustion, cold startability and emissions, and full-range combustion strategy considering emissions and efficiency.

Reviewer 4

The reviewer stated that the project addresses important issues to enable methanol and ethanol, two potential renewable fuels, for off-road applications. The reviewer affirmed the importance of all focus areas of the project, including mixing, ignition, and combustion, and suggested including emissions as an equally important area for investigation, noting that it has been well-established that the pollutant emissions from methanol and ethanol fuels significantly differ from those of conventional diesel. The reviewer conjectured that different emission control catalysts and engine control strategies will likely be needed for the systems to meet the low tailpipe emission standards. The reviewer explained that emission control technology has advanced to the stage that it is now a part of engine/fuel system rather than an aftertreatment system; thus, including emissions measurements in the early stages of the project and studying how the engine-out emissions are affected by various parameters is beneficial for the development of the entire system.

Reviewer 5

This reviewer conveyed that ethanol and methanol were identified as the most promising fuel candidates to replace diesel in an effort to decarbonize the off-road vehicle fleet. According to the reviewer, this project attempts to characterize the mixture formation of ethanol/methanol, understand ignition, and develop fundamental understanding of combustion strategies for engines using these fuels to achieve a similar performance to that of diesel compression ignition engines. The project structure is focused on three main tasks: mixture formation, ignition fundamentals, and engine performance and emissions. The reviewer affirmed that the project's approach to gaining a fundamental understanding and characterization of alcohol fuels in direct injection engines is sensible and recommended evaluating how emissions for ethanol and methanol combustion compare to those for diesel combustion to confirm the continued relevance of this project to meet VTO goals.

Reviewer 6

The reviewer remarked that the three focus areas within the project's approach are well explained and make sense. The reviewer questioned whether in-cylinder chemical species measurements, which may have been mentioned as proposed future research, are possible within the ignition focus area, asserting that such measurements along with thermal mapping seem appropriate and would further detail the changes imposed in oxygen concentration.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

This reviewer commented that the project's technical accomplishments clearly follow the project schedule, with challenges identified and progress made at each step. The reviewer asserted that wall wetting from observed deep penetration of liquid methanol can be mitigated with fuel/intake heating. The reviewer noted that ether blends were found to be infeasible for MCCI because of the high amounts required. The reviewer noted identification of alcohols scavenging radicals and suppressing ether ignition. This can be addressed by burning ether before injection of alcohol. The reviewer added that active pre-chamber is needed to avoid the misfire that is observed with passive pre-chamber.

Reviewer 2

Acknowledging that the project has made technical accomplishments and progress, the reviewer rated the project's progress "satisfactory" because of weaknesses in the accomplishments that were highlighted. This project has used a variety of experimental and modeling techniques to study in-cylinder behavior (including injection processes) of methanol. However, the technical accomplishments presented focus on physical and chemical phenomena related to the direct compression-ignition of methanol and ethanol. The reviewer conveyed that these learnings, such as the significant challenges associated with igniting these high-octane fuels, already existed in literature. Specifically, prior literature has already documented the 1,000 Kelvin ambient environment threshold for achieving autoignition with methanol and ethanol and the large amounts of ignition improvers that must be added to methanol or ethanol to significantly impact thresholds for ignition. The reviewer commended the project for studying PFI of methanol and ethanol for use in a pilot or dual-fuel or pre-chamber combustion system, noting that these technical findings addressed barriers to utilization of these fuels. Further work on utilization of methanol and ethanol with high-energy ignition systems was recommended by this reviewer.

Reviewer 3

The reviewer conveyed that the project is on track against the plan. The reviewer's main concerns are the relevance of some of the tasks to MCCI combustion and the extent to which the project contributes to the advancement and adoption of the MCCI combustion technology for alcohol fuels.

Reviewer 4

The reviewer commented that technical progress in most of the project's focus areas was well demonstrated in the presentation. Noting that emission measurements for nitrogen oxides (NO_x) were presented for the fuels with additives, the reviewer observed that emissions of aldehydes, which have very low thresholds, were not reported in the presentation. The person cautioned that aldehyde emissions can be critical and may strongly influence the mixing/ignition/combustion strategies. It was not clear to the reviewer how the baseline engine-out NO_x emissions for the diesel case were determined. The reviewer recommended using the best available diesel fuel technology as the baseline.

Reviewer 5

Pointing out that the U.S. DRIVE Net-Zero Technical Team and the 21st Century Truck Partnership Internal Combustion Engine Technical Sector Team roadmaps have identified ethanol and methanol as fuels with near-net-zero-carbon potential, this reviewer affirmed that the project is on track to help characterize these non-petroleum fuels and provide an understanding of fuel property effects on NO_x and particle emissions. The reviewer remarked that these alcohol fuels are not suitable for MCCI in modern diesel engines due to low ignitability, lower energy densities, compressibility, lubricity, and material compatibility challenges. The person reported that the project has developed a database with OH radical, infrared, and liquid imaging of in-cylinder processes of pre-chamber-ignition methanol combustion for CFD development and validation. The project has also established the minimum level of ether mixing needed for reliable ignition across a range of operating conditions that span typical off-road duty cycles. The project is currently characterizing various mixing regimes and has revealed various challenges with methanol port injection and high latent heat of vaporization. Finally, the reviewer conveyed that the project has been able to achieve stable combustion at a wide range of operating conditions through pre-chamber fuel mixing and addition of large amounts of ethers (40%—50% diethyl ether and diethylene glycol diethyl ether).

Reviewer 6

The reviewer remarked that the measurements and observations are progressing in line with the project plan. The reviewer questioned whether there is a crank angle window to inject a pilot that allows the kernels to form, and how much timing flexibility (efficiency) that leaves. The reviewer also questioned whether the project data indicate which changes are needed in the engine combustion chamber (or injector/nozzle) to enable methanol and/or ethanol to be used in a practical application. The reviewer expressed interest in an explanation of the directions for any aftertreatment and a projection of how the results differ from current fuels with such catalyst formulations, asking whether the results point to a likely need for greater precious metal content or different catalyst approaches versus current applications.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer pointed out that although bowl design is very important to controlling NO_x and soot with MCCI, the only mention of bowl design in the presentation was a statement that a production bowl was utilized. Collaboration with current industry partners to investigate improved geometry for DI of alcohols. The reviewer suggested that a CFD design of experiment could be used to evaluate sensitivities of ethanol and methanol to a number of bowl design parameters. The reviewer also suggested that industry partners validate the CFD with data from Sandia National Laboratories.

Reviewer 2

This reviewer was impressed by the collaboration and coordination across the project team and external partnerships, noting the importance of this collaboration and coordination in maximizing the value of experimental capabilities that exist within the project.

Reviewer 3

The reviewer remarked that the mix of partners for this project is good but observed that the activities are scattered across a wide range of different technical topics. It was not clear to the reviewer how these different tasks complement each other to advance MCCI combustion for alcohol fuels.

Reviewer 4

This reviewer recommended that partners in emissions research and emissions control catalyst development be added to the team to ensure that emissions control is an integrated part of this project.

Reviewer 5

This reviewer described the project's collaboration and coordination as outstanding, with a mix of industrial partners, multiple national laboratories, and several universities. The reviewer also noted that the project is conducted in close cooperation with U.S. industry through the Advanced Engine Combustion Working Group.

Reviewer 6

The reviewer suggested showing the contributions of each collaborator on the results slide to provide reviewers with a better understanding of where and how collaboration contributes to the findings and conclusions, pointing to Slide 22 as an example.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer conveyed that three future research tasks were proposed. The reviewer remarked that the first task, characterizing heat transfer and wall temperature in a methanol-fueled MCCI engine, will be useful for industry partners to evaluate this fuel as drop-in with current hardware but noted that the utility of this point was not explicitly covered in the presentation. The reviewer asserted that piston and injector specifications will impact heat transfer and recommended identifying sensitivities related to these specifications. The second and third tasks, exploring methanol premixed combustion with a pilot and developing and validating kinetic models, respectively, were described by the reviewer as a natural progression from the technical accomplishments to date.

Reviewer 2

The reviewer remarked that this project's proposed future research is only somewhat aligned with alleviating barriers to utilization of lower-carbon-intensity methanol and ethanol fuels in off-road and marine applications. The person asserted that future work should focus on industry-relevant combustion systems that rely on high-energy ignition of premixed methanol or ethanol. This can include a broad range of physical systems, such as pilot ignition, pre-chamber ignition, or direct spark ignition, all of which present different barrier/opportunity tradeoffs and are being pursued by industry.

Reviewer 3

This reviewer commented that the proposed future work captures some key areas of MCCI combustion for alcohol fuels. Piston and cylinder head surface temperature and heat transfer measurements, for example, are of practical significance, and dual-fuel combustion can be a feasible path. The reviewer encouraged the project's efforts that deepen the understanding and generate relevant engine test data toward developing high-fidelity, predictive combustion models. The person affirmed the importance of future research on ignition chemistry but noted that flame propagation measurements may not be strongly relevant, considering the nature of compression ignition. The reviewer recommended that the project team think strategically about the framework of the MCCI combustion approach on which the project will focus to address the key technical barriers (i.e., cold start, low-load performance, full-range combustion strategy). This will help make the proposed future research more organized and cohesive.

Reviewer 4

Because emissions measurements are planned only during the final period of the project, the reviewer concluded that the project plans to employ an after-treatment emissions control solution. With the stringent emissions regulations for aldehydes, it is unlikely a simple after-treatment device can solve the problem or can be a cost-effective solution, according to the reviewer.

Reviewer 5

This reviewer related that the project, as presented, is 50% complete, with significant milestones yet to complete in Fiscal Year (FY) 2024. If the current year milestones are all met on time, proposed future research includes developing an understanding of piston and cylinder head heat transfer for a methanol-fueled MCCI engine, establishing a database detailing the evolution of ignition and combustion for premixed alcohol ignited by pilot injections of a highly reactive dual-fuel (diesel and dimethyl ether [DME]), and additional CFD modelling and chemical kinetics to capture ignition and flame propagation of methanol. The reviewer affirmed that these tasks are a logical continuance to further the understanding of mixed alcohol MCCI combustion. The reviewer recommended undertaking an investigation and analysis of NO_x, GHG, and particulate matter (PM) emissions under experimental conditions to verify modeling predictions, as the current mixing modeling does not capture the experimental results. The reviewer asserted that alcohol combustion in compression ignition engines should produce lower criteria emissions than diesel but expressed interest in seeing experimental results showing the extent of the emission reductions.

Reviewer 6

This reviewer concluded that the project's proposed future work is reasonable. The person remarked that improving the environmental impact of difficult-to-electrify applications while allowing these applications to perform as expected requires continued evaluation of replacement or modified fuels that can easily be managed by the supply chain within the current U.S. production stream.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer stated that the project supports VTO subprogram objectives to minimize formation of emissions and develop a better understanding of how fuel properties affect advanced combustion systems.

Reviewer 2

This reviewer stated that the project's current implementation and approach are not relevant to the VTO objective of increasing utilization of next-generation, lower-carbon-intensity fuels (methanol and ethanol). However, by changing the approach to focus on practical combustion systems, the project could reduce barriers to utilization of these fuels, thereby delivering relevance to the VTO objectives.

Reviewer 3

Asserting that MCCI combustion should be the primary path for alcohol fuels in off-road applications, the reviewer concluded that the high-level technical relevance of the project is sound. However, the reviewer expressed concern that some of the tasks are not strongly tied to MCCI combustion and that there is insufficient focus on some of the known challenges for compression ignition of fuels with lower autoignition reactivity, considering the large body of works in this area.

Reviewer 4

This reviewer deemed the project highly relevant to advanced engine and fuel technologies, noting that methanol and ethanol are two renewable fuels that can potentially accelerate the decarbonization of the transportation sector, particularly the hard-to-electrify off-road engine.

Reviewer 5

The reviewer remarked that this project supports the decarbonization of the off-road transportation sector, a major objective of the VTO DORMA program, through fundamental research to understand alcohol combustion in compression ignition engines. The characterization research conducted through the project is a first step toward enabling the use of net-zero-carbon fuels for off-road transportation. The reviewer conveyed that the U.S. National Blueprint for Transportation Decarbonization, which states that 79% of the total fuel consumed today by off-road vehicles is diesel, identifies the use of sustainable liquid fuels and the reduction of ethanol carbon intensity as vehicle improvement strategies for the off-road transportation sector.

Reviewer 6

This reviewer concluded that the project's identification of candidate fuels for advanced engine technologies is well aligned with the VTO DORMA program's objective of enabling difficult-to-electrify applications to continue to perform and improve their environmental impact. The reviewer observed that this project seeks to improve the applicability of available fuels.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This reviewer stated that the project is well organized, spreading responsibilities across a variety of facilities, including Sandia National Laboratories' Combustion Research Facility (CRF), Argonne National Laboratory, and multiple universities. The reviewer asserted that the project's resources are sufficient to meet the milestones.

Reviewer 2

The reviewer described the project's FY 2023 budget of $1,050,000 as excessive and the FY 2024 budget of $450,000 as sufficient.

Reviewer 3

This reviewer remarked that the project's resources are adequate for its milestones and timelines.

Reviewer 4

The reviewer observed that the team had adequate resources and was making good progress in the project.

Reviewer 5

This reviewer concluded that the project's funding is sufficient to meet its fundamental research objectives in FY 2024 and that the project is well organized and on track to meet its stated milestones. The person noted that while the presentation showed FY 2023 funding of $1,050,000 and FY 2024 funding of $450,000, it was not clear how much funding was utilized during which fiscal year and over the various tasks of the project.

Reviewer 6

The reviewer remarked that the project seems well managed. The objectives are being met using the skillsets of the project's contributors. Analysis details are thorough and support the plans and directives. The reviewer observed that the project's timeline, contributors, and facilities were adequate to support progress.

Presentation Number: DORMA003
Presentation Title: Soot Predictions from DNS of a lab-scale combustor with sustainable aviation fuels
Principal Investigator: Bruno Souza Soriano, Sandia National Laboratories

Presenter

Bruno Souza Soriano, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

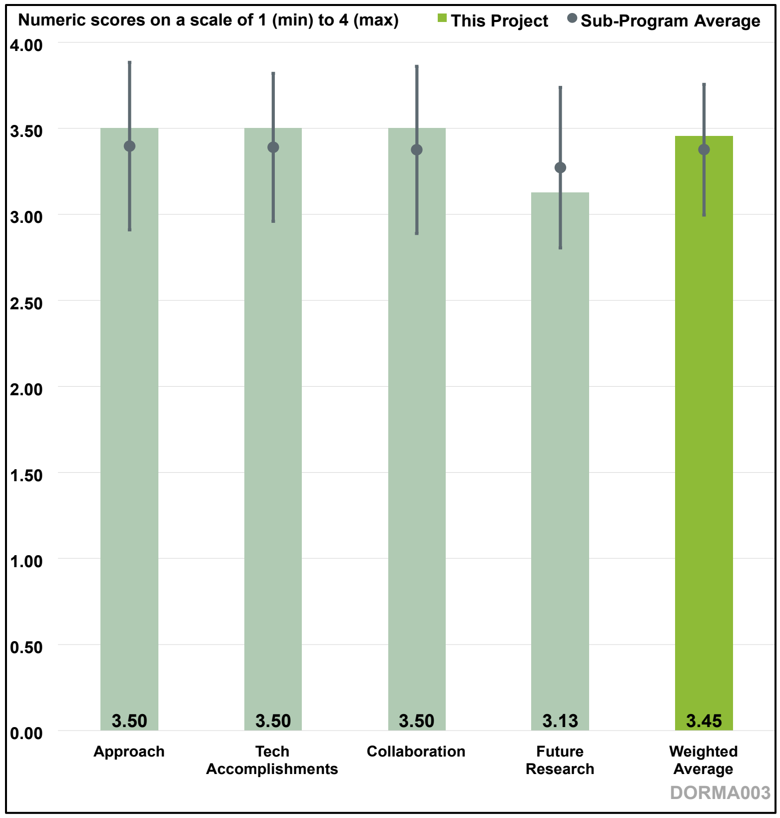

Figure 3-3. Presentation Number: DORMA003 Presentation Title: Soot Predictions from DNS of a lab-scale combustor with sustainable aviation fuels Principal Investigator: Bruno Souza Soriano, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

This reviewer remarked that the project is addressing potential shortcomings in turbulent combustion modeling and soot modeling for Jet-A and sustainable aviation fuel (SAF) in flow conditions suitable for capturing the key processes occurring in gas-turbine combustors. The person noted that direct numerical simulations (DNS) completed and planned have the potential to provide high-quality data for improving combustion and soot modeling applicable to large eddy simulations (LES) and that progress to date indicates a high probability of meeting the overall goals of the project.

Reviewer 2

The reviewer conveyed that this project is working toward overcoming barriers to SAF adoption by addressing the lack of understanding of soot production processes for SAF combustion. This reviewer affirmed that the project will advance understanding of soot emissions by creating DNS simulations of relevant turbulent flames that implement multiphase fluid dynamics, polycyclic aromatic hydrocarbon chemistry, and soot chemistry models. According to the reviewer, the investigators aim to produce simulations of turbulent soot-producing flames with fidelity exceeding the current state of the art. The investigators will use LES to establish DNS boundary conditions for a swirl-stabilized flame. DNS-simulated soot measurements will be compared with experimental observations. The reviewer described the project tasks as well-chosen and logical and the timeline as reasonable.

Reviewer 3

This reviewer reported that the project is addressing the multi-faceted technical challenge of accurately predicting soot produced by gas turbine combustion of SAF-relevant fuels, which requires accurate modeling of the combustion, soot inception and growth, soot oxidation processes, and other processes. The project will leverage DNS to capture the multi-modal multi-phase spray swirl combustion that occurs in the gas turbine engine, evaluating the DNS techniques and soot modeling approaches with laminar configurations before applying them to more challenging combustor setups. The reviewer affirmed this approach and mentioned the project team's collaboration with several other groups to facilitate achievement of project objectives. Noting that the project's two-year duration is short for a project of this scope, the reviewer nonetheless observed that the project team is not only on track to achieve the research goals, but is also mining data from the DNS to extract key information about the combustion process (e.g., effect of backscatter, flame propagation modes) and has developed a neural network based technique to advance flamelet strategies. The reviewer applauded the team's elucidation of key underlying physics in these areas, adding that the project's findings will significantly add to the research community's knowledge base on SAF performance in gas turbine engines.

Reviewer 4

This reviewer stated that the approach of this project is to use experimental results from various combustion configurations to understand processes associated with soot formation and to validate numerical models for soot produced from jet fuels (Jet-A and C1) in the configurations selected. The configurations include a laminar flame configuration ('canonical configuration,' though that term was not defined in the presentation), a counterflow flame, and a burner with spray injection at the bottom. The reviewer described the configurations (excepting the Cambridge burner) as "rather fundamental in their operation." The reviewer explained that a range of simulation tools and models are applied to these configurations to provide data for evaluating models of soot formation and kinetic mechanisms for oxidation.

The reviewer pointed out that the configurations selected by the project (e.g., a laminar counterflow burner with no turbulence present) are often used in fundamental studies to elucidate certain aspects of combustion physics in isolation. Premixed flames, counterflow burners, etc., are appropriate for this purpose and can shed light on fundamental processes associated with soot formation, gaseous GHG emissions, and turbulence models. The reviewer highlighted that results from fundamental burner designs need to then be linked to inform operation and design of more efficient engines. It is not clear which specific fundamental results (e.g., oxidation chemistry, soot model, turbulence models) can be carried over to a practical engine, or how the results obtained from this project would reduce emissions that affect GHG or contrail formation. As an example, the reviewer asked whether the finding that 'premixed flames have a larger contribution to the heat release rate' is also relevant to the environment of a jet engine.

The reviewer observed that the Cambridge burner configuration incorporated spray injection at the bottom, to which adaptive mesh refinement reactive flow solvers, including spray, soot, and radiation models, were applied. However, the reviewer noted that the models were not described, so it was not possible to know how detailed the spray modeling was. The reviewer expressed interest in determining optimal conditions for rapid evaporation of the injected spray to initiate combustion, which was not discussed during the presentation.

According to this reviewer, soot and turbulent flow models were mentioned during the presentation, but it was not evident to what extent the models validated with the basic burner designs are applicable to a real jet engine. The reviewer would have appreciated a discussion of the models' applicability to real engines.

The reviewer also reported that the presentation was missing a discussion of the reason naphthalene was chosen as a representative soot precursor in the model. The reviewer asked why C_2H_2 or some other molecule was not chosen.

The reviewer noted that the presentation repeatedly referred to modeling and experiments for Jet-A and pointed out that Jet-A itself is too complex for modeling. A surrogate must be developed for it. No surrogate was noted in the presentation that the reviewer could recall, so the reviewer was unable to evaluate its efficacy or applicability and the circumstances for validating it.

The reviewer recalled that the configuration used in the project for soot modeling was a counterflow flame. The connection of this configuration to a practical combustor or engine was unclear to the reviewer. In this configuration, liquid is completely eliminated by vaporization, and the flow is one-dimensional, which is dissimilar from a jet engine, where multiphase effects could be present and the flow is not one-dimensional. The reviewer asked whether the project team expects that a robust soot model will result from simulations of soot using validation data from this burner. Acknowledging that a connection likely exists between the model configuration and a practical engine, the reviewer remarked that the link was not clear in the presentation.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

This reviewer stated that the DNS simulations of the Cambridge swirl burner with Jet-A and C-1 have found that backscatter of turbulence energy from small to large turbulence scales is occurring for certain conditions and may be important for lean blow-out (LBO) predictions. LBO is an important combustor operability characteristic for assessing SAF impacts. The project has developed and validated deep neural network (DNN) subgrid models for three dissipation rates appropriate to manifold (or flamelet) approaches to modeling turbulent combustion and demonstrated a significant improvement in accuracy in predicting these dissipation rates for the Cambridge burner burning C-1, which was not used for training the DNN subgrid models. The reviewer remarked that the current Jet-A and C-1 fuel soot chemistry and soot evolution modeling in two-dimensional DNS simulations of counterflow flames is showing good comparisons with low-pressure experiments (or DNS with the more detailed Lawrence Livermore National Laboratory chemistry). The reviewer was encouraged by these results, describing the project's work as an excellent step in preparing for the more complex DNS simulations with soot and radiation for the Cambridge swirl burner.

Reviewer 2

This reviewer found that the study has been productive so far, remarking that the multiphase DNS simulating a University of Cambridge swirl-stabilized burner is working. The reviewer acknowledged the investigators for identifying complex extinction and reignition behaviors and determining the relative heat release rate for premixed and non-premixed zones of the flame. The project has demonstrated that extinction and reignition events are related to turbulent backscatter, which is only captured with DNS and cannot be captured with LES. The team has identified fuel effects on LBO behaviors. Simulations using a reduced jet fuel mechanism for a laminar counterflow flame were used to demonstrate that this mechanism could accurately predict the location of soot precursors. The results of the simulation were compared with a counterflow experiment; the location of soot production was very accurately identified, though the soot volume fraction was somewhat overpredicted. The investigators explored fuel effects and strain rate effects on soot production. The reviewer praised the team for its accomplishments to date.

Reviewer 3

The reviewer acknowledged the thoroughness of the PIs' analysis of past DNS results from the swirl combustor setup. The reviewer remarked that premixed edge flames have been shown to dominate the combustion process through modal analysis, adding that the results further show the effect of deflagration fronts working with ignition fronts to sustain the turbulent flame. The reviewer is interested in seeing an evaluation of the particular effects of these modes at conditions very close to LBO. This is already partly addressed in the project through correlating LBO to edge flame displacement speed, which itself correlates to derived cetane number. The reviewer is also interested in the turbulence back-scatter and its stabilizing effect on LBO, which suggests possibilities of tuning turbulence to suppress LBO and illustrates the need for LES models to incorporate back-scatter. The reviewer affirmed that the constrained DNN approach shows good agreement with DNS and offers an improved approach to multi-modal flame modeling.

Reviewer 4

The reviewer commended the team for getting a lot of results from their efforts over the past year. The reviewer was impressed by the DNS of the complex environment of the lab-scale aero-combustion, the turbulence modeling, and the soot modeling. The reviewer was interested in the LBO correlation with flame displacement speed and the finding that LES turbulence models do not capture back-scatter extinction regions and found the effort of 'training dataset selection' potential useful.

The reviewer presumed that a Jet-A surrogate was used in the soot modeling effort but noted that it was not specified. Likewise, the kinetic mechanism was not described, and the modeling of soot volume fraction (SVF) was not very clear. The reviewer pointed out that the role of thermal and transport properties in the simulations was not discussed but could have an effect on discrepancies.

The reviewer refuted the assertion that the conditions of the counterflow flame configuration were similar to those of swirl flames, pointing out that the counterflow configuration ostensibly produces a well-defined transport while transport within a spray flame is more chaotic, with both turbulence and swirl being present. Since the counterflow flames completely eliminated the liquid phase by vaporizing it, there were no fuel evaporation effects in the counterflow environment, whereas fuel evaporation effects would be present for a swirl-stabilized spray flame. The reviewer suggested that some discussion of how counterflow burner results can be connected to, or inform, operation of a jet engine would be appropriate.

This reviewer described the soot experiments in the counterflow configuration as impressive but questioned the assertion that the SVF results show satisfactory agreement, noting that some of the comparisons seem to show significant differences. For example, while broad trends of SVF are captured by the numerical modeling, comparing measured and simulated SVFs for ethylene with models from Lawrence Livermore National Laboratory and the PeleLMeX code illuminates some discrepancies; in some cases, differences of an order of magnitude exist between measured and simulated SVF, and in other cases, differences are 30% or more, as shown in Slides 19 and 20. The reasons for the differences and a strategy to close the gap were not discussed. The reviewer suggested that there are many potential reasons for these differences, including failure to validate a kinetic mechanism that incorporates soot precursor chemistry in a way that would promote its generality (i.e., using data from only one combustion configuration vs. several), inaccuracies of thermal and transport properties (e.g., diffusion coefficients, gas thermal conductivity), rate constants in the kinetic mechanism not being known to a high degree of accuracy, choice of reactions in the mechanism, and an insufficient number of soot precursor reactions being incorporated.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer applauded the project's excellent use of existing experiments and collaborations with both Lawrence Livermore National Laboratory and the University of Illinois at Urbana-Champaign on chemistry models for Jet-A and SAF that include soot precursors. The reviewer suggested that additional collaborations may be needed in the future to validate the models at higher pressures using sooting flame experiments with Jet-A and/or SAF at pressures higher than a few atmospheres.

Reviewer 2

This reviewer conveyed that Sandia National Laboratories leads the project and coordinates with two other national laboratories and three universities on DNS implementation, soot modeling, experimental data, and chemical mechanism development.

Reviewer 3

This reviewer commended the project's collaborations, remarking that the collaborations were strategically chosen to provide support with soot modeling, mechanism reduction, and experimental validation of computational approaches. Acknowledging the likelihood that the current collaborators significantly contributed to the progress of this work, the reviewer did not see a need for more collaborators.

Reviewer 4

The reviewer remarked that the project team is excellent. It incorporates two national laboratories and three academic partners, with one being international. The team has considerable expertise with experiments and modeling. The data produced seem accurate and the numerical modeling rigorous.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer stated that the project plans to complete the Cambridge burner simulations with correct geometry, both without soot and including soot and radiation. This reviewer expressed confidence that the planned work would be completed, considering the simulations already completed. The reviewer noted, however, that the timeline for future work on higher pressure simulations or improved soot modeling was not clear from the presentation.

Reviewer 2

The reviewer affirmed that the next steps in this project are well-planned and expressed an expectation that the project's goals will be achieved, considering the promising results to date. Building off previous soot model validation and multiphase DNS success, the next steps are to implement soot and radiation models within DNS and to refine the boundary conditions. At a later time, the project will explore pressure effects on soot behavior, though experimental measurements at elevated pressure are not available for validation.

Reviewer 3

The reviewer related that the PIs have defined several pathways for future research. First, the team will complete DNS of the Cambridge combustor with the reduced mechanisms and developed soot model. Proposed future efforts would extend simulations to higher pressure conditions, implement a new soot model, and leverage ongoing work on molecular dynamics simulations to advance capabilities to predict soot in greater detail through particle size distribution, chemical composition, and morphology. The reviewer acknowledged that these are challenging tasks but affirmed the value of the proposed work in aiding understanding of soot effects over a wide range of scales.

Reviewer 4

While this reviewer stated that the plan for future research, especially the plan to compare and improve models, made sense, the person cautioned that the presentation did not include specifics of how this comparison and improvement would be carried out or discussion of the associated consequences. The reviewer recommended that the team validate the inputs to the simulation tools (e.g., soot models, kinetic mechanism with improved rate constants, property database appropriate for the temperature and pressure conditions of interest) prior to beginning experiments/simulations at elevated pressures. The reviewer pointed out that if the 1 atm differences cannot be resolved, going to higher pressure will introduce more complications, and more adjustments will be needed to close gaps between experiments and numerical simulations.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer stated that the project is working on improved subgrid turbulent combustion models that may improve simulations of combustor operability (such as LBO and ignition), which is important to assessing fuel impacts. The project is also working to improve soot modeling, which will contribute to improved predictions of aircraft engine emissions of soot and can be an input to contrail formation models.

Reviewer 2

This reviewer concluded that the project is relevant to the VTO objectives. The project is using high-fidelity simulations to understand soot emissions from SAF. The reviewer remarked that a predictive soot model would enable faster and more cost-effective screening of SAF candidates, leading to cost savings for the aviation industry and environmental benefits through emissions reduction.

Reviewer 3

This reviewer asserted that the project supports and is relevant to the DORMA program. The reviewer remarked that SAF has the potential not only to aid decarbonization through a net-zero-carbon approach, but also to reduce soot emissions, because of the fuel’s inherent chemical composition and/or physical properties. Thus, SAF should be leveraged to reduce emissions.

The reviewer commented that the DNS efforts of this project and subsequent predictive modeling capabilities have potential to alleviate the 50% blending requirement with Jet-A, leading to use of 100% SAF with lower sooting tendencies. The findings of the detailed analysis of DNS data improve understanding of the combustion and LBO processes and facilitate ideas for implementing techniques to enhance engine safety by addressing issues such as LBO. Furthermore, the DNS work is leading to pathways that can be followed by LES for improved turbulent combustion modeling. Noting that LES is the approach of choice for evaluation of practical combustion systems, the reviewer commended the PIs for extremely useful and relevant work.

Reviewer 4

This reviewer affirmed that the project is relevant to combustion of SAFs in aviation systems, stating that the project, if successful, will influence the achievement of net-zero-carbon aviation. The project's goal is ultimately to achieve a predictive and efficient numerical solver to evaluate the combustion of alternative fuels. The reviewer noted that the PIs expect to improve turbulent and soot formation models in combustion systems through this study. Included are soot models under what are referred to as realistic configurations.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer deemed the project team, codes, and high-end computing capabilities of this project to be sufficient, noting that the work builds on expertise and capabilities developed over many years, thereby improving and extending these capabilities.

Reviewer 2

This reviewer concluded that the resources of the project are sufficient and the budget is reasonable, adding that the investigators have the computational infrastructure and technical expertise to perform the simulations outlined in the presentation.

Reviewer 3

While the computational resources seemed sufficient to the reviewer for the project to make progress toward its goals, the financial resources ($125,000) seemed limited and the timeframe seemed short for a project of this scope and technical difficulty.

Reviewer 4

This reviewer concluded that the resources are adequate for the proposed and accomplished work.

Presentation Number: DORMA004
Presentation Title: Mixing-controlled compression-ignition combustion with low-lifecycle-CO2 fuels
Principal Investigator: Chuck Mueller, Sandia National Laboratories

Presenter

Chuck Mueller, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

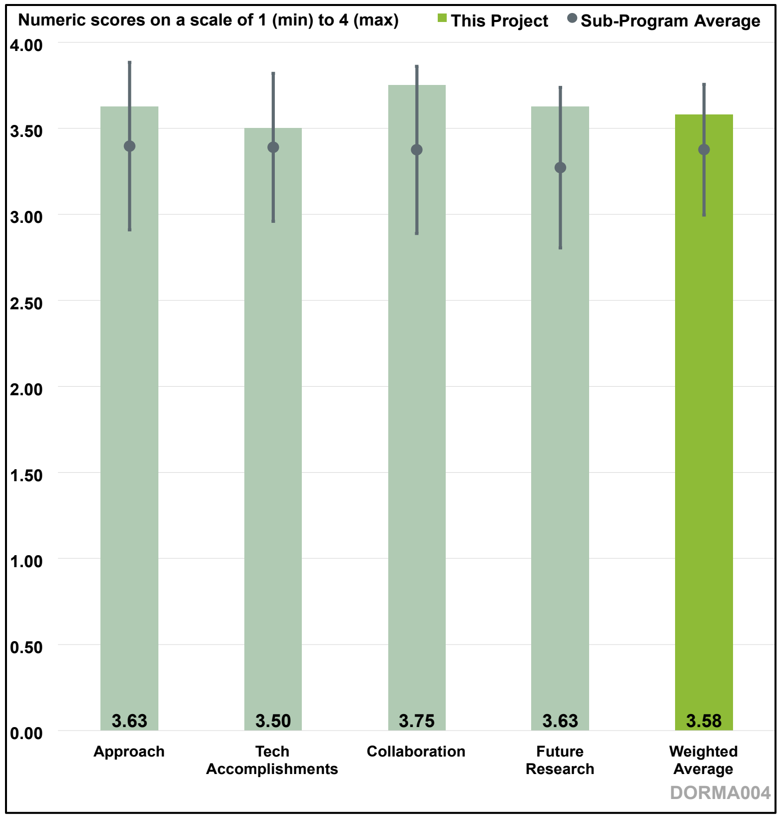

Figure 3-4. Presentation Number: DORMA004 Presentation Title: Mixing-controlled compression-ignition combustion with low-lifecycle-CO2 fuels Principal Investigator: Chuck Mueller, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer commended the testing with the Deere six-cylinder engine, noting that using a production engine for this evaluation is likely a key step in achieving broader application of the technology. The companion modeling with various partners was also deemed beneficial by the reviewer. The reviewer remarked that work to visualize low-carbon fuels at Sandia National Laboratories would be beneficial to the engine community.

Reviewer 2

This reviewer praised the project for determining the conditions to control gaseous and particulate emissions from diesel combustion processes, noting the project's excellence. The PI has assembled a team with a wide range of expertise, including OEMs, partners from academia and national laboratories, and no less than 20 industry partners. The approach combines testing of ducted fuel injection (DFI) in a multi-cylinder metal engine and experiments in the Sandia National Laboratories optical engine. The fuels being investigated include biodiesel (i.e., methyl ester mixtures), a renewable diesel, and dimethyl ether, among others. The milestones include targets for engine testing, spray systems, life cycle analysis, commissioning of a DME fuel injection system, and ultimately an assessment of the benefits of DFI as a technology for reducing particulate and gaseous emissions.

Reviewer 3

The reviewer described this project as well designed, noting that the timeline is reasonably planned and the sound approach builds on prior work with ducted fuel injection for reduced diesel particulate matter. Pointing out that engine durability is a key concern for off-highway customers, the reviewer recommended establishing or quantifying the DFI durability with respect to diesel combustion before exploring the extension of DFI in low-lifecycle-carbon-dioxide (CO_2) fuels.

Reviewer 4

This reviewer commended the project for its steps toward moving DFI into multi-cylinder engines, which is very important in bringing this technology from the laboratory to the field. The reviewer also commended the project for performing sensitivity studies on the misalignment of the ducts with injector sprays rather than just on injector holes. Lastly, the reviewer commended the project for exploring the LLCF space to leverage the low-emissions capability of DFI with LLCF. The reviewer remarked that the results are promising, although it is still unclear whether the multiscale engine work will be successful.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer commented that the production engine DFI alignment work and sensitivity analysis and the low-carbon fuels interaction study, which includes oxygenated fuels, are useful and interesting. The simulations on misalignment are also helpful from the production engine perspective. The reviewer highlighted the importance of understanding fuel sensitivity to DFI.

Reviewer 2

The reviewer noted that the project reported an extensive array of technical accomplishments, which are discussed below.

The reviewer found the DFI retrofit especially interesting, presuming it would not require a complete engine design to implement but rather could be installed on an existing engine platform. The reviewer recalled that the PI noted issues with cavitation in alignment. It was not clear where cavitation would occur and what supersaturations could be sustained for the fuel systems investigated to create conditions favorable for cavitation to occur. The reviewer asserted that more research is needed to better understand conditions where cavitation could occur.

In the study of rotational misalignments, soot reduction was considered possible with misaligned injectors. The connection between soot and injector alignment was not clear to the reviewer. Although CFD results were shown, the connection with soot was not discussed.

The reviewer found the development of the multi-cylinder engine installed at Excel Engineering impressive. The complexity of the engine hardware seems quite extensive to the reviewer. The reviewer observed that the initial DFI engine results seem conflicting. The table in Slide 12 shows changes in soot to be enormous, depending on the operational torque mode. It is unclear whether soot with an upward arrow (ΔSoot) means less soot production or more soot production. If it means more soot production, then some of the numbers indicate huge increases in soot depending on the operational mode. The reviewer was unsure of the correct way to interpret the table.

The simulation of DFI combustion was unclear to the reviewer because details were lacking. While some results were shown, the details of the simulations were not discussed.

The reviewer observed that DME is a popular fuel being considered for commercialization and asked about realistic expectations for DME commercialization and the prospects for a 'DME economy.'

Reviewer 3

The reviewer said the preliminary results on the application of MCCI combustion with low-lifecycle-CO_2 fuels are promising and offer valuable insights on the importance of fuel oxygenation to engine-out NO_x and particulate emissions.

Reviewer 4

This reviewer commended the project for its promising technical progress to date, expressing hope that the most recent emissions results will demonstrate the project's capacity to shift the soot–NO_x tradeoff even farther. The reviewer acknowledged that the actual market penetration of LLCF in each respective DORMA market and the amount of low carbon leverage these markets can provide remain uncertain.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer praised the experiments and testing with the Deere engine and the modeling at King Abdullah University of Science and Technology, describing them as outstanding. The reviewer observed that other institutions are also exploring DFI technology and highlighted the importance of having numerous R&D institutions exploring the technology in preparation for future DFI adoption.

Reviewer 2

This reviewer observed that there is significant collaboration and coordination among the partners. This is an enormous project with more than 20 CRADA partners. Each team has its own set of deliverables. Some of the descriptions of the deliverables seemed perfunctory to the reviewer. For example, Georgia Tech is responsible for DFI experiments and theory, along with other collaborators.. But there was no substantive discussion so it was not possible for this reviewer to evaluate.

Reviewer 3

This reviewer remarked that the collaboration and coordination within the project team, which includes partners from industry, academia, and national laboratories, is well documented in the presentation.

Reviewer 4

The reviewer commented that the PI has assembled an excellent team of collaborators and participants for this project. Engine OEMs, universities and national laboratories are all part of the team working on this technology. It was clear to the reviewer that the PI has been successfully gathering collaborators for quite some time.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer mentioned that a comment was made about reduced DFI efforts at Sandia National Laboratories. This reviewer expressed hope that others will continue efforts to understand and optimize the technology, as the reviewer believes the concept has merit, especially in high load applications. The reviewer remarked that the interaction of DFI with newer low- and zero-carbon fuels will be very useful.

Reviewer 2

The reviewer stated that future work will continue multi-cylinder and single-cylinder engine testing of renewable diesel, DME, biodiesel, and blends. The reviewer asked what feedstock is used to produce the renewable diesel. The reviewer noted that the plan includes investigation of volatility effects of oxygenated fuels. The reviewer recommended that the PI develop a flow chart highlighting the role of each entity in achieving the overall objectives, if such a flow chart does not already exist, to enable audiences of presentations such as this to better understand how the various components are being organized to achieve the overarching objective of the project. The presentation should then elaborate on a few specific elements selected by the project team.

Reviewer 3

The reviewer described the proposed future research as comprehensive. The CRADA focuses on multi-cylinder metal engine and single-cylinder optical engine testing of DFI with low-lifecycle-CO_2 fuels, while the core focuses on testing of low-lifecycle-CO_2 fuels with conventional diesel combustion.

Reviewer 4

This reviewer observed that the project is fast approaching a critical phase, where multi-cylinder engine results will need to be put forth, with tolerance and manufacturing information, to move the engine from the lab to the real world. While the reviewer viewed the proposed future work as the correct work, they acknowledged uncertainty as to whether this technology can be successfully commercialized. The reviewer expressed concern that if the project stalls, there may not be many opportunities to optimize any of the variables, such as number of injector holes, injector hole diameter, and stand-off distance to the duct.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer believes this technology could have a significant impact, especially in compression ignition engine applications that run high-load duty cycles, where soot formation is most problematic. The reviewer commended the project for its outstanding focus on lower soot and modifying the classic NO_x–soot tradeoff curve. The reviewer acknowledged that the additional complexity and cost are a concern but said the impressive performance improvements are likely to encourage others to utilize the technology.

Reviewer 2

This reviewer commented that the project is exceptionally relevant to the VTO program with its emphasis on emissions from operation of combustion engines in ground transportation systems.

Reviewer 3

This reviewer explained that the project supports the overall VTO subprogram objective of providing low-cost, secure, and clean energy technologies to move people and goods by helping to close the knowledge gaps pertaining to the development of combustion strategies that simultaneously lower engine-out NO_x, soot, and lifecycle CO_2 emissions.

Reviewer 4

The reviewer expressed the opinion that this project's work is important to the future of DORMA technologies, both from a fuels point of view and an emissions reduction point of view. The reviewer pointed out that DFI and LLCF support the DOE mission to decarbonize and comply with future air quality emissions regulations in hard-to-electrify markets.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The resources appeared to be sufficient to this reviewer.

Reviewer 2

This reviewer noted that there are a lot of partners for this project and that the budget seems realistic for the work that is being done.

Reviewer 3

The reviewer stated that the investigators are on track to meet the milestones outlined in the project plan with the current funding levels.

Reviewer 4

This reviewer observed that the resources appear to be sufficient to continue and maintain progress on this project.

Presentation Number: DORMA005
Presentation Title: Alcohol spray and H2 jet experiments and modeling
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 felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 80% of reviewers felt that the resources were sufficient, 20% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

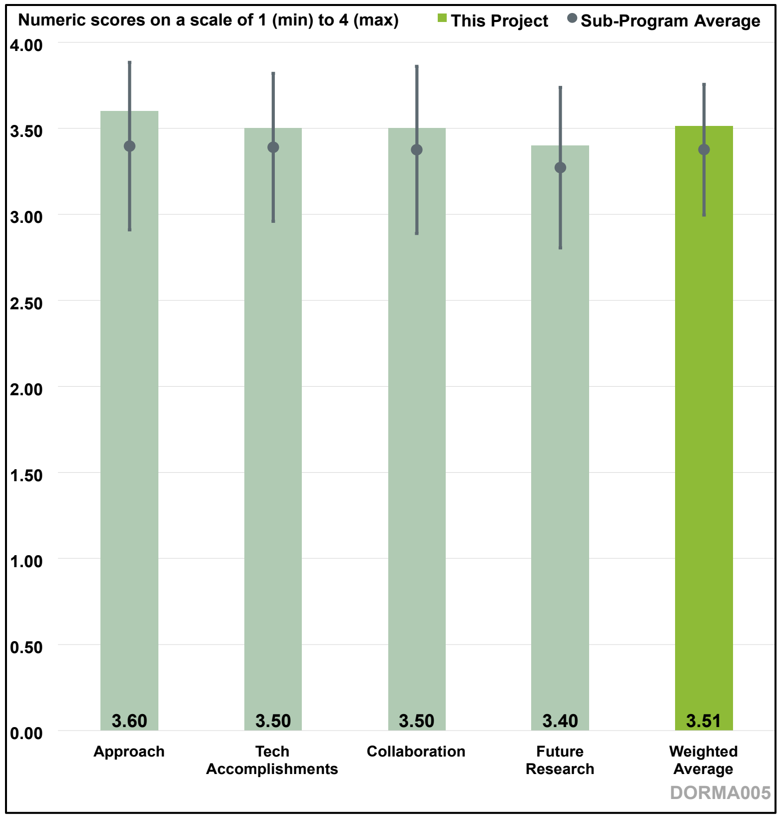

Figure 3-5. Presentation Number: DORMA005 Presentation Title: Alcohol spray and H2 jet experiments and modeling Principal Investigator: Lyle Pickett, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

This reviewer commented that the project is well designed. The reviewer noted that more time may be needed to address H_2 injection barriers. The reviewer conveyed that the project handles methanol vaporization challenges with intake/fuel heating and multiple injections. The proposed future work presented included improved methanol modeling to fill an identified need. The reviewer cautioned that mixture fraction and temperature modeling of supersonic H_2 flow modeling may take more time than scheduled given the diagnostic and modeling challenges presented, which include supersonic flow, temperature distribution of the under-expanded jet, and hardware acquisition/fabrication.

Reviewer 2

The reviewer stated that this project is applying state-of-the-art experimental spray diagnostic techniques to the new challenges of understanding spray physics for non-conventional fuels (hydrogen and methanol). It is also effectively leveraging CFD “virtual experiments” to supplement the experimental diagnostics that are being carried out, in order to determine where gaps in the predictive capabilities of CFD exist. The reviewer concluded that the work being carried out under the project directly contributes to addressing technical barriers related to the direct utilization of lower-carbon-intensity hydrogen or methanol in combustion engines. The only weakness the reviewer identified in this project is the use of light-duty gasoline injector hardware for the methanol work. The reviewer acknowledged that this may have been a necessary compromise to begin the project work and take a “first look” at methanol spray physics but stressed that it will be essential to rapidly transition the work to more representative injector hardware, as major differences in the spray configuration can impact which physical processes are dominant in the development of the spray and which physics are most important for CFD software to capture to allow for predictive modeling.

Reviewer 3

The reviewer affirmed that the technical approaches used by the project to address key areas in characterizing spray behavior of low-carbon fuels are sound. The reviewer emphasized the importance of the H_2 jet characterization and modeling for designing appropriate fuel–air mixture formation in H_2 engines. Regarding methanol spray, the reviewer stated that further clarification is needed on the decision to investigate gasoline direct injection (GDI) spray instead of diesel-like high-pressure direct injection spray. If the team intends to study dual-fuel MCCI using GDI to introduce methanol to the engine cylinder, this needs to be clearly communicated.

Reviewer 4

This reviewer praised the approach that is being taken to address the technical barriers and acknowledged the steps being taken to address the key problems arising from the fluid properties.

Reviewer 5

This reviewer commented that the project uses outstanding experimental capabilities to generate and provide crucial information on spray behavior, ignition, and other combustion phenomena. The reviewer observed that the application of these capabilities to the understanding of fuel mixing, ignition, and combustion of low-carbon-intensity methanol and hydrogen for off-road vehicle systems is timely and needed. The reviewer asserted that improving the efficiency of combustion and generating the understanding that permits robust engine design (e.g., preventing or minimizing preignition of H_2) will eliminate barriers to technology implementation. The reviewer noted that methanol’s high latent heat of vaporization is both a barrier and a benefit, as it cools the chamber but may extend spray penetration, leading to wall impingement.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer stated that the methanol spray experiments and corresponding CFD work have been completed, but challenges remain with respect to matching experimental data. The reviewer pointed out that the use of multiple small injections may limit scalability to high-load conditions. The reviewer also stated that H_2 jet experiments and corresponding CFD work have been completed, and the project plans to address new barriers with supersonic flow and a cold jet temperature.

Reviewer 2

This reviewer remarked that the project has made effective progress against the project plan. The team has identified the role of flash boiling on methanol spray collapse and the challenge of predicting this behavior using commercial CFD codes. The reviewer noted that this important result directly guides DOE and industry work toward resolving gaps in the predictive capabilities needed to design internal combustion engines capable of utilizing lower-carbon-intensity methanol fuel. The reviewer also observed that the project has made important discoveries regarding hydrogen sprays and the role that hydrogen cooling and sonic phenomena have on spray performance.

Reviewer 3

The reviewer commended the project for excellent progress toward generating high-quality experimental data and for providing insightful findings on the fundamental physics involved during the fuel injection process for methanol and H_2.

Reviewer 4

This reviewer remarked that the examples and measurements presented provide the intended insight. Noting that the project is doing fundamental work to provide insight, the reviewer asked if the team has thought about cell size, cell count, or geometric sensitivity. The reviewer asked if the variation in nozzle orifice geometry altered the approach to meshing and if the effect of supersonic flows (mentioned as a computation challenge) altered the approach to mesh generation.

Reviewer 5

The reviewer commented that this work on methanol and hydrogen combustion has extended the understanding of flow, mixing, ignition, and combustion phenomena in important ways. The reviewer asserted that combining CFD with high-fidelity experiments is providing new and deeper insights than most other research has been able to provide. For example, these experiments have shown a very complicated response of methanol liquid spray mixing to mild fuel heating. Moreover, these experiments have shown the underlying liquid interactions when using a split injection, which explain the origin of benefits for methanol spray from multiple injection strategies. In the case of hydrogen gas jet, the combination of hydrogen injection and gas dynamics phenomena (shock waves, reflecting waves, Mach disk structures) during H^2 injection. The reviewer noted that this work enables the design of advanced engines by providing the information to develop better fuel injection simulation.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

This reviewer commended the excellent collaboration within CRF facilities for simultaneous experimental and modeling work and noted that additional collaboration exists with Argonne National Laboratory, Convergent Science, and the Engine Combustion Network. The reviewer mentioned some collaboration with Caterpillar in relation to DORMA002, which is also conducted at the CRF.

Reviewer 2

The reviewer praised the project for being an example of effective collaboration and coordination across DOE and industry efforts. The use of a variety of collaborative structures, including a CRADA, the Sandia-organized Engine Combustion Network, individual external collaborations with Argonne National Laboratory and Convergent Science, and internal coordination with adjacent DOE projects within Sandia National Laboratories, demonstrates to this reviewer that the project team is actively pursuing opportunities to disseminate its findings and transfer learnings as efficiently as possible.

Reviewer 3

This reviewer stated that the project is well connected to partners and that the project's spray characterization data is foundational to partners' activities. The reviewer expressed a desire to see more engagements from industrial partners to steer the scope of the project and provide critical inputs on hardware selection and operating boundary conditions.

Reviewer 4

The reviewer remarked that the exchange of findings between the collaboration partners appeared to be effective and useful. The reviewer appreciated seeing the contributors, by topic, in the slides. The reviewer suggested that input from injection system manufacturers, if not already included, would help guide the range of variation.

Reviewer 5

This reviewer observed that the project is characterized by broad engagement and that it connects with the engine and combustion community through the Engine Combustion Network, a platform for sharing experimental and numerical data. The person also noted that there is CRADA support from Caterpillar on both methanol and hydrogen in addition to the DOE project.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

This reviewer concluded that the proposed future work addresses most barriers described in the preceding slides. The person cautioned that relying on intake manifold heating creates cold-start and low-load operational and packaging challenges while increasing cost. The reviewer recommended exploring and testing methods for pre-heating the fuel prior to injection as a substitute to intake heating.

Reviewer 2

The reviewer asserted that the project's proposed future research is well aligned with the DOE mission to alleviate barriers to lower-carbon-intensity fuel utilization. Further, the proposed research is regarded as well aligned with the experimental capabilities of the lab and the expertise of the researchers. The reviewer commented that the diagnostic development for hydrogen sprays is an excellent use of the lab and DOE resources, as it yields high-fidelity data that will be critical to advancing predictive tools, yet it is an area in which industry is unlikely to invest because of the precompetitive nature of the effort.

Reviewer 3

This reviewer strongly encouraged the project team to gather adequate input from the industry on the most representative hardware and testing boundary conditions, suggesting that the HDEV4 may not be the most relevant selection for H_2. The reviewer also highlighted the importance of coordinating and aligning on the injector hardware between the constant volume combustion chamber spray characterization and the fuel–air mixture formation characterization planned for the optical engine at Sandia National Laboratories. The reviewer stated that it is imperative to clarify what type of fuel injection system and overall combustion strategy are intended for the methanol spray characterization.

Reviewer 4

This reviewer observed that mentioning the challenge of obtaining injectors without proprietary protection seems misplaced for such fundamental work. The reviewer recommended normalizing the variation in hole geometry such that an understanding of large variations in geometries is presented to determine model prediction impacts, leading to increased simulation confidence.

Reviewer 5

This reviewer affirmed that the plan for future experiments will lead to new knowledge of the essential physics and chemistry of the spray and combustion behavior of the fuels investigated and illuminate ways to overcome the technology barriers that limit the effective implementation of the fuels. The reviewer noted that the detailed future plans are targeted toward addressing key barriers that need to be understood for fuel injection system and engine design.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer stated that the project supports VTO subprogram objectives to develop a better understanding of how fuel properties affect advanced combustion systems.

Reviewer 2

This reviewer remarked that the project is relevant to DOE goals to remove barriers to the introduction of lower-carbon-intensity fuels for off-road and marine transportation. The project directly contributes to removing barriers to implementation of hydrogen and methanol by providing high-fidelity data and understanding of key spray physics for these novel fuels.

Reviewer 3

The reviewer expressed the opinion that the project is well aligned with the VTO subprogram objectives but highlighted the need to strengthen the project's relevance to practical applications. For instance, it was not clear to the reviewer how GDI spray characterization for methanol contributes toward the application of MCCI combustion strategy for off-road applications. The reviewer also pointed out the need to align the selection of an H_2 injector and operating boundary conditions with the practice in the industry.

Reviewer 4

This reviewer observed that the project investigates less-known details of spray mechanics for candidate low- or zero-CO_2 fuels. The person said that the complications of implementing the two fuels studied within the project, compared to incumbent fuels (diesels), warrant revisions to simulation models. The reviewer affirmed that the project's objectives support advanced engines and fuels.

Reviewer 5

The reviewer remarked that this project is highly relevant to DOE goals and objectives and that it addresses research needs to support the utilization of low-carbon fuels in future engines.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This reviewer stated that direct collaboration with an engine and/or injector OEM could greatly enhance the project. An OEM collaborator could assist with acquiring hardware (a noted challenge), fuel heating, and scaling injections for high load conditions (a noted barrier).

Reviewer 2

The reviewer expressed concern that the project's resources are slightly insufficient to accomplish the broad range of work needed to support both hydrogen and methanol utilization.

Reviewer 3

This reviewer asserted that the project's resources are sufficient to support the tasks and the timeline.

Reviewer 4

The reviewer observed that the project is timely and is on track to meet its objectives. However, the reviewer felt that there should be more emphasis on the model implications of the findings and assessments of the predictions included.

Reviewer 5

This reviewer remarked that the project's funding appears to be sufficient and is spread over a long enough period to achieve highly impactful outcomes, noting that continuity of support has enabled an extremely important capability at Sandia National Laboratories.

Presentation Number: DORMA006
Presentation Title: Low Lifecycle Carbon Fuel (LLCF) combustion and emission models
Principal Investigator: Scott Wagnon, Lawrence Livermore National Laboratory

Presenter

Scott Wagnon, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

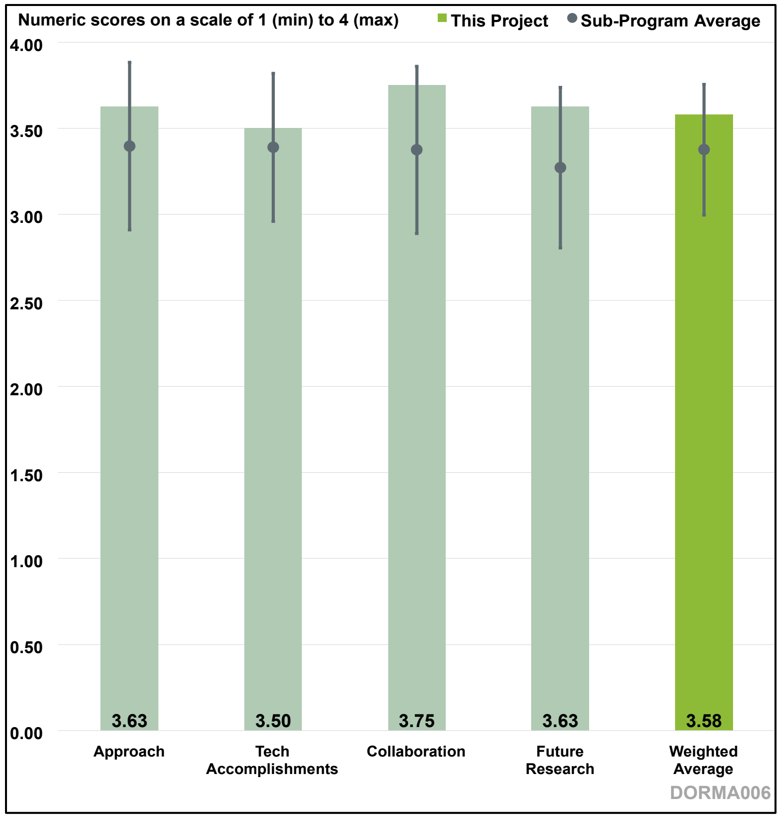

Figure 3-6. Presentation Number: DORMA006 Presentation Title: Low Lifecycle Carbon Fuel (LLCF) combustion and emission models Principal Investigator: Scott Wagnon, Lawrence Livermore National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer commended the project for excellent developments. The reviewer questioned whether there are fundamental ways to speed up or automate part or all of the process. The reviewer asked if a fuel molecule could be input from first principles, leading to production of an initial detailed chemical kinetic model.

Reviewer 2

This reviewer concluded that the project is well designed, technical barriers of the work scope are being reasonably addressed, and the timeline is reasonably planned, with the project currently 42% completed.

Reviewer 3

This reviewer emphasized the importance of developing and improving the kinetics models to the decarbonization efforts in DORMA. The person added that developing surrogates that accurately predict fuel behavior, and validating that behavior, are very important. The reviewer praised the project for addressing each of these barriers in a very positive and successful way.

Reviewer 4

The reviewer remarked that the work supports an improved understanding of a variety of future fuels and provides essential information to enable the design of future combustion systems for transportation. The person pointed out that predictive modeling remains a grand challenge for DOE and that the kinetic modeling tools need to be developed to allow robust modeling.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

This reviewer stated that the Jet A and SAF chemical kinetic developments will be useful for the R&D community and that the validation work in the rapid compression machine and University of Connecticut burners is essential. The reviewer was glad to see the Zero-order Reaction Kinetics (Zero-RK) solver software and Global Pathway Selection Zero-RK reducing software published for open use.

Reviewer 2

The reviewer acknowledged that the project is doing challenging work and affirmed that reasonable technical progress has been made toward accomplishing the goals of the project plan. The person expressed concern, however, that many of the milestones have not yet been met. It was not clear to the reviewer how well the research community understands the kinetic mechanisms for these lighter fuels based on the results presented in the report.

Reviewer 3

This reviewer was impressed by the progress the project has made to date, particularly in the modeling and validation portion of the project, and by the nine-component surrogate that almost identically matches the target fuel. The reviewer recommended considering the use of artificial intelligence/machine learning to explore fuels even more thoroughly and rely less on expansive (and expensive) experimental validation.

Reviewer 4

The reviewer praised the project for its productive work on models of jet fuels to support SAF development. The models include combustion properties such as sooting tendency. The reviewer mentioned that the project’s improvements to software for combustion chemistry modeling (Zero-RK) have reduced the run time for simulations that incorporate detailed chemistry, and the software has been publicly shared via GitHub. The project has also made improvements to global pathway selection software and shared it publicly.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer pointed out that most of the collaboration presented is with Argonne National Laboratory and the University of Connecticut. The reviewer encouraged the project to continually reach out to other researchers to validate the models in different combustion contexts.

Reviewer 2

This reviewer praised the project’s collaboration and coordination with other institutions and industry partners.

Reviewer 3

This reviewer found the project team impressive, noting the national laboratory and university representation. The reviewer observed that the team has coalesced well and is collaborating excellently on experiments and simulation. The reviewer commended the project for skillfully leveraging the limited resources of global participants.

Reviewer 4

The reviewer stated that this team has broad collaborations worldwide and has a history of active engagement with industry, academia, and other national laboratories. The team remains highly collaborative, as it has been in the past.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

This reviewer concluded that the cyclo-alkane chemical kinetic and SAF model developments will be useful.

Reviewer 2

The reviewer described the proposed future research as exhaustive and clearly defined but expressed skepticism about the likelihood that the project will achieve its targets. Nevertheless, this reviewer recommends the inclusion of artificial neural networks (machine learning models) for future research of reduced models to use in simulation.

Reviewer 3

This reviewer observed that the future work for this project appears to be aiming at reducing the barriers even further and building upon recent successes. The reviewer commended the project for improvements to the simulation tools and for making these improvements available to the community at large, describing these developments as excellent.

Reviewer 4

This reviewer asserted that the expansion of the kinetics studies to consider more fuels and fuel blends and further improvements of these kinetics are of great value to the community and will help overcome barriers and enable robust design calculations. The past and present contributions from this team were described by the reviewer as outstanding. The reviewer expects the outputs of this work to remain highly impactful. The reviewer remarked that key elements of the work are not only enabling high-fidelity considerations of combustion chemistry but accelerating the speed of simulations to enable practical design simulations with adequate consideration of chemistry.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer remarked that the renewable fuels mechanisms are very important and suggested that the R&D communities would benefit from confirmation that good models also exist for other popular low-/zero-carbon fuels.

Reviewer 2

This reviewer said the project will help to close the knowledge gaps of low-lifecycle-carbon fuels and that it supports the overall VTO subprogram objectives for decarbonization of difficult-to-electrify sectors.

Reviewer 3

The reviewer stated that this project is very relevant to DOE's DORMA program objectives, noting that it supports both experimental and simulation efforts to enable decarbonization.

Reviewer 4

The reviewer conveyed that this project yields combustion chemistry models that enable alternative and advanced fuel utilization. The SAF and low-carbon-fuels work are considered by the reviewer to be essential. The reviewer pointed out that the kinetic mechanisms and detailed understanding of combustion chemistry produced by this project are needed for model-based design.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This reviewer stated that the project's resources appear to be sufficient.

Reviewer 2

The reviewer was not sure the project's current funding levels will be sufficient to address the remaining challenges and barriers outlined in the report, given that so many milestones have not yet been completed.

Reviewer 3

This reviewer remarked that the resources appear to be sufficient to achieve the goals of this project.

Reviewer 4

The reviewer mentioned that the good levels of long-term funding enabled the project to develop highly useful outcomes for combustion kinetics.

Presentation Number: DORMA008
Presentation Title: Slashing Platinum Group Metal (PGM) in Catalytic Converters An Atoms-to-Autos Approach
Principal Investigator: Kevin Gu, General Motors

Presenter

Kevin Gu, General Motors

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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

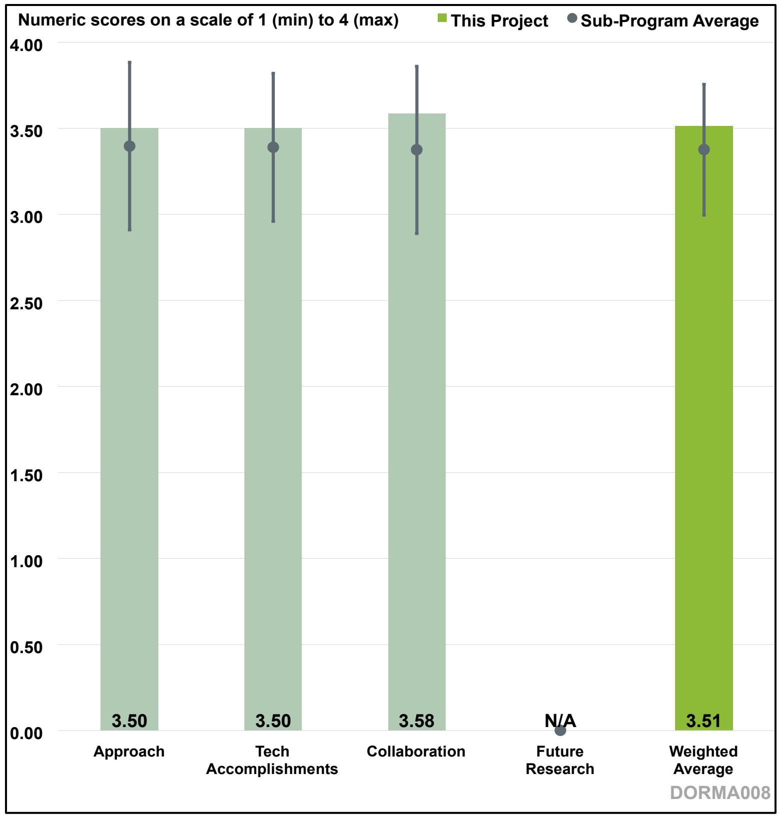

Figure 3-7. Presentation Number: DORMA008 Presentation Title: Slashing Platinum Group Metal (PGM) in Catalytic Converters An Atoms-to-Autos Approach Principal Investigator: Kevin Gu, General Motors

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer observed that the team has the expertise, technical support, and industry partners needed to complete the research project. The reviewer noted that the research project follows a well-established technical approach used in the past, which starts with core samples in a chemical lab and includes vehicle products. The timeline is considered well planned. The reviewer expects that the project will be completed as planned based on the evident planning, available resources, and expertise and effort of the team.

Reviewer 2

The reviewer conveyed that the team developed a group of ceric oxide-modified aluminum oxide (Al_2O_3) supports and demonstrated that those supports enhanced the three-way catalyst (TWC) performance of palladium (Pd) and rhodium as compared with the Al_2O_3-supported catalysts. The team evaluated the catalysts after aging the samples under well-established industrial catalyst aging protocols and on an engine dynamometer to ensure that the results were practically relevant. The reviewer noted that while these accomplishments are remarkable, the presentation lacked sufficient information to compare the newly developed catalysts to the state-of-the-art commercial TWCs that are designed for similar applications. The reviewer asserted that TWC technology has advanced to the stage that sophisticated selections of support materials and placement of PGM are commonly implemented in commercial catalysts. A major objective of those industrial approaches, according to this reviewer, is to reduce PGM usage. The reviewer recommended, therefore, that the goal of PGM reduction for this project be based on the best available technology in the market rather than a set of simple base cases.

Reviewer 3

This reviewer stated that the research plan was laid out well to achieve its goals and the partners were well chosen for their contributions.

Reviewer 4

This reviewer described the Atoms to Autos approach as a clever, multi-pronged approach to achieving a 50% reduction in PGM loadings while maintaining emissions performance meeting the super-ultra-low-emission vehicle 30 standard. The reviewer noted that reducing the size of the PGM particles allows for a nearly atomic dispersion that has strong resistance to migration and aging.

Reviewer 5

It was clear to this reviewer that the project addresses technical barriers related to reducing PGM loadings. The reviewer conveyed that the project also achieved prolonged lifetime and improved durability with the support modification. The strategy to achieve the goals was considered reasonable by the reviewer; the use of alumina–metal oxide supported catalyst particles allows comparison to a baseline catalyst (metal–alumina supported catalyst). The reviewer stated that the presented results show significant advantages with avoidance of large particles and ability to create a more robust catalyst while decreasing PGM content.

Reviewer 6

The reviewer said that a new lean/rich aging protocol was established and light-off temperatures were characterized before and after aging.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

Noting that a limited amount of data was presented, this reviewer observed that progress has been made in this project and that the progress is well supported by the two patents granted, one patent pending, and one paper published.

Reviewer 2

This reviewer stated that the team developed a group of supports with surface modification to enhance the TWC activity of the PGM component. The team scaled up the sample preparation process and prepared a reasonable quantity of samples to prepare sets of full-sized catalysts for engine dynamometer testing. The team then aged the catalysts under industry-recognized protocols and finally demonstrated that the newly developed catalysts could reduce the PGM usage. The reviewer noted that although the results did not demonstrate achievement of the original PGM reduction target of 50%, the targets were very nearly achieved, and the project demonstrated the feasibility of a 25% PGM reduction. The reviewer remarked that the important finding from this project is that PGM reduction is feasible on TWC, even after nearly 50 years of intensive academic/industrial research and development effort.

Reviewer 3

The reviewer commended the project for achieving many great technical accomplishments, including meeting the required NO_x and hydrocarbon standards, in spite of various constraints on the project, including loading. The person noted that the project does not appear to have met the carbon monoxide (CO) standards within these same constraints. The improvements in maintaining smaller particle size and particle size distributions with the preparation and aging processes used appear to the reviewer to be technical accomplishments that have not yet been reported to the extent possible. The reviewer expressed hope that these accomplishments will be included in publications.

Reviewer 4

This reviewer praised the project for the excellent progress that has been made. The person conveyed that a design concept was prepared, optimized, and aged, and that the design demonstrated thrifting in excess of the target (60% versus 50%). Currently there is a prototype device being canned for engine and vehicle testing.

Reviewer 5

The reviewer remarked that the milestones in all three funding periods appear to have been met except for the one involving ongoing engine performance testing. Some milestones experienced delays of 3–4 months because of complexities arising from partnering agreements. The reviewer was glad to see that the formulation was able to be modified and prototype scaling/testing continued. The reviewer observed that the project appears to have met its metrics in mid-2023, and the last year has been spent conducting aging testing and final testing, which is ongoing. The reviewer stated that the data presented provides a clear picture of progress toward a catalyst that is more durable, contains less PGM, and is able to be scaled. Additionally, the reviewer asserted that the use of metal–oxide support keeps particle size down when compared to baseline catalyst, and the lower particle size likely plays a significant role in helping to maintain activity of the catalyst. Beyond the milestones, the reviewer found the project’s two granted patents, one pending patent, and one publication worth noting. The publication is in a high-profile catalysis journal and provides a modified chemisorption method that could have impact for the broader catalysis community.

Reviewer 6

This reviewer’s evaluation was only done for the third budget period, since the review is constrained to just the past year. The project demonstrated 50% reduction in PGM and filed three patent applications, with two granted so far.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer conveyed that the team collaborates with one national laboratory, one OEM, one catalyst supplier, and two universities. The contribution from Pacific Northwest National Laboratory was not clear to the reviewer. The reviewer asserted that the current team has all the expertise needed for the success of this project, so no additional collaborators are needed.

Reviewer 2

This reviewer stated that close collaborations among the academic institutions, catalyst manufacturer, and OEM are apparent. The team successfully translated novel ideas from lab scale to engine dynamometer demonstration. The reviewer recommended including a state-of-the-art commercial TWC from BASF in the evaluation to fully assess the practical potential of the technology developed in this project.

Reviewer 3

This reviewer remarked that the project's team of collaborators was very well suited to implementing its approach, relying in large part on work from the University of Central Florida for its approach to catalyst preparation.

Reviewer 4

The reviewer commended the project team for excellent research collaborations between an OEM (General Motors [GM]), a Tier 1 supplier (BASF), a national laboratory (Pacific Northwest National Laboratory), and multiple universities with clear roles.

Reviewer 5

The reviewer observed that the diverse project team brings unique expertise to the project and asserted that a project of this type requires expertise in single-atom catalyst development, catalyst scale-up, catalyst characterization, and understanding kinetics/mechanism of activation and deactivation. Both GM and the University of Central Florida team members have expertise in single-atom catalyst development; it was not clear to the reviewer why both groups were needed and how their contributions were unique and not duplicative. The reviewer was surprised that the project did not include some economic modelling, at the least to demonstrate the impact of the PGM reduction. The person speculated that the project may be at too premature of a stage for economic modelling at this time.

Reviewer 6

The reviewer commended the project for having a nicely formed team with clearly defined roles. The reviewer recommended showing the contributors on the technical accomplishment slides in the future.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer noted that no future work is proposed because the project is supposed to be completed soon.

Reviewer 2

This reviewer stated that the project is ending in June 2024.

Reviewer 3

This reviewer remarked that the project has ended from a practical view, except for one more potential publication with additional results.

Reviewer 4

The reviewer conveyed that the project is 90% complete, noting that ongoing work will be finished to end the project.

Reviewer 5

This reviewer said that the project is basically at the end of the funding period, with 90% of funds having already been expended. The reviewer did not identify any issues with the presented information but did have some questions. First, the reviewer asked if atomic layer deposition methods might offer better results or control of the catalyst composition. The reviewer asked if the reason atomic layer deposition methods were not considered is because they are not cost competitive relative to the solution coating methods followed by calcination that were used. Second, the reviewer asked why the alumna is needed at all if the CeO_x could serve as a support and if this choice is also driven by the economics.

Reviewer 6

The reviewer reported that the project ended in June 2024.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This reviewer concluded that the project is relevant to advanced engine and fuels technology. The person asserted that reducing the catalyst by 50% will reduce dependence on imported material and improve the competence of the U.S. vehicle industry.

Reviewer 2

The reviewer asserted that PGM is critical for internal combustion engines to meet environmental emission regulations. The person noted that reducing PGM usage has been a challenging task and that decades of research and development effort have been devoted to it because of the scarcity of PGMs. The reviewer observed that the results from this project demonstrate that there is still room for improvement in this area, and the reward can be significant.

Reviewer 3

This reviewer remarked that reducing the use of PGMs by 50% to meet emission standards would result in major cost savings for automotive OEMs on ICE-powered vehicles using new low-carbon fuels. Thus, the project is relevant.

Reviewer 4

The reviewer said the project is extremely relevant to DOE goals to reduce reliance on precious metals.

Reviewer 5

This reviewer concluded that the project goals and approach are well aligned with VTO interests in developing improved catalysts or formulations for engine systems. The reviewer noted that reducing PGM content is imperative and expressed the view that the connection between performance and understanding composition and dynamics at the atomic level is critical. The reviewer observed that the project team missed an opportunity (to a minor degree) to make the connections between the atomic level and performance a little more strongly throughout the presentation. While the reviewer felt that the overall vision demonstrated these connections well, they could have been reinforced more strongly throughout the presentation.

Reviewer 6

The reviewer pointed out that reduction of PGM usage in engine exhaust aftertreatment is an objective of the VTO program.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer stated that the team has excessive resources, including equipment, space, industry support, and expertise, for the success of this project.

Reviewer 2

This reviewer commended the team for making good progress with the research funding, observing that the industrial partners (GM and BASF) contributed significant effort to the project.

Reviewer 3

The reviewer said the institutions and their capabilities were sufficient for this project.

Reviewer 4

This reviewer concluded that the resources are sufficient because the project is nearly complete.

Reviewer 5

The reviewer observed that the project had all the resources it needed given the diverse skill sets of the partners and their expertise in all the areas needed to develop the catalyst, understand how it operates, and scale/test it.

Reviewer 6

This reviewer conveyed that the project was completed with the allocated budget, although with delays that were not a result of insufficient funds.

Presentation Number: DORMA010
Presentation Title: Off-Road Decarbonized Fuel Transient Performance
Principal Investigator: Muni Biruduganti, Argonne National Laboratory

Presenter

Muni Biruduganti, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

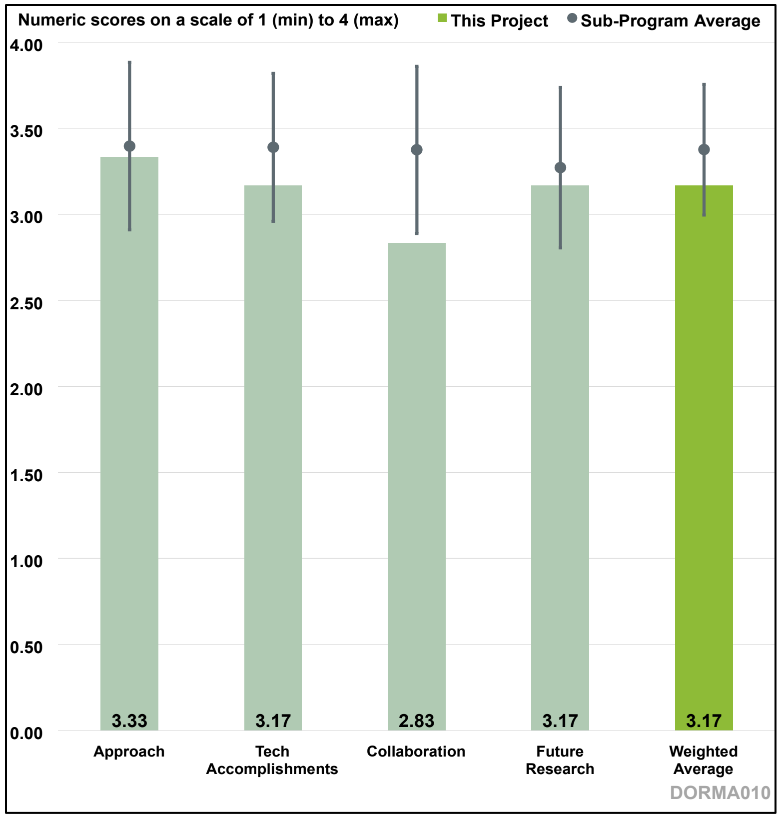

Figure 3-8. Presentation Number: DORMA010 Presentation Title: Off-Road Decarbonized Fuel Transient Performance Principal Investigator: Muni Biruduganti, Argonne National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer asserted that the use of a powerful tool (Autonomie) for this powertrain development study promises valuable outcomes. Combining engine combustion and development studies coupled to the powertrain simulation should lead to an effective powertrain design. Using the engine-in-loop approach has been shown many times in the past to be an effective way to design and anticipate propulsion challenges of different powertrain options. That application in this case—for off-road systems where the duty cycle and engine and powertrain needs to serve can vary widely across the off-road sector and vary extensively from on-road design—is a strength of this project.

Reviewer 2

The reviewer noted the project is evaluating H_2 ICE transient performance for non-road applications and using hardware-in-the-loop to simulate the application while operating the engine in the test cell. The reviewer added the real-time non-road equipment model uses Autonomie for the vehicle dynamics and transient set point to the engine controls (in the test cell).

Reviewer 3

The reviewer commented that switching engines from Navistar to Cummins seems to add technical risk to the project. Getting the engine to perform correctly in a test-cell dynamometer takes times and effort. Switching to another engine could impact product schedule and cost. The reviewer noted that there could be an impact on redoing simulation results for the transient differences between engines.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer acknowledged the ANL team currently has a Navistar 13-liter diesel engine in their test cell. The team has also upgraded the test cell to accommodate hydrogen for the Cummins B6.7H (a 6.7-liter H2 ICE engine), which is scheduled to be tested in a future year. The Cummins engine is not yet in production, so testing it will be delayed to FY 2026. An interim step will be to use the Cummins B6.7NG (a natural gas-fueled engine) in FY 2025 and to test its operation using blends of natural gas and hydrogen. ANL is also upgrading the on-site hydrogen fuel storage system from tube trailers to liquid hydrogen tanks.

Reviewer 2

The project is leveraging expertise at ANL with Autonomie and leveraging facilities from SuperTruck and existing partnerships, which has enabled good progress to this midway point in the project. The testbed appears to be mostly in place, and a new H_2 ICE will be acquired/installed to complete the project objectives. But the most challenging aspects, the advanced virtual vehicle simulation, have been developed using the existing 13-liter diesel engine. The project team has demonstrated the ability to simulate hybrid architecture. The engine will arrive in 2026, but the reviewer asked if that is guaranteed, as this will significantly impact the project timeline. The team has demonstrated the integration of engine–model signals, so that the engine is being commanded to operate as needed for the virtual vehicle to meet the duty-cycle demands, and this is further improving integration. Transient drive-cycle requirements are being emulated, albeit with some throttling of the rate of change of engine start. Nonetheless, the powertrain simulation capability looks like it is far along in the development process.

Reviewer 3

The reviewer asserted that a more detailed comparison of the five different off-road drive cycles with the engine dynamometer and engine simulation results from a transient perspective is needed. It was stated a low-inertia dynamometer was used and simulation results were compared with the dynamometer response. There seems to be some difference between the two. The reviewer would like to see the actual vehicle comparison as well. Later in the presentation, some emissions results were shown. The dynamometer response can have a significant impact on emissions results during transients.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer indicated the presentation shows good collaboration between different project team members and organizations.

Reviewer 2

The reviewer remarked that the team is primarily ANL with some support from Navistar and Cummins. Navistar is providing a 13-liter diesel engine as in-kind support. ANL is also negotiating with Cummins for an H_2 ICE that is expected to arrive in late 2025. This reviewer acknowledged that the national laboratories are allowed to run projects independently, but in general the reviewer's expectation is that ANL would have engaged other partners, be they the engine manufacturers or others, to support the program. For example, ANL should strongly consider getting a non-road machine manufacturer to help get vehicle duty cycles to feed into real-time Autonomie. Duty-cycle data were drawn from field data generated by the University of Helsinki on another Decarbonization of Off-Road, Rail, Marine, and Aviation (DORMA) project.

Reviewer 3

The reviewer observed that there are no universities involved in this project. The ANL–industry collaboration looks very effective from the work being accomplished, but there is a missed opportunity here for training new engineers through this project, either through summer interns, student design projects, or graduate thesis research. Since Autonomie is widely used in academia as well as by the laboratories and industry, there should be an effort to engage students in this activity. Interaction with Navistar and potentially with Cummins to enable H_2 ICE studies are both evidence of good industry engagement. But a missing element is direct involvement with an off-road equipment original equipment manufacturer (OEM). The team is making use of data from the University of Helsinki and University of Nebraska, but the presentation did not make clear whether those collaborations or resource leveraging are active collaborations under this project. In the question-and-answer period, it was clarified that these data are from other/previous DORMA projects. So, the reviewer concluded, there is no active university engagement under this project.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer commented that the H_2 ICE in a range of virtual powertrain designs, exploring the engine's performance with the challenges of H_2 combustion, is an excellent topic to explore. The team seems poised to accomplish some very good work, and the most challenging systems for the hybrid powertrain design are already in place. But there seems to be risk related to the acquisition of the H_2 ICE. As a risk-mitigation strategy, the team will install a natural gas version of the desired test engine—as a step toward getting the H_2 version of the test engine—to be ready for its arrival.

Reviewer 2

The reviewer asserted the overall future tasks are clear and make sense technically. Since the study is focused on transient response, more effort should be put into comparing back to different off-road standardized cycles.

Reviewer 3

The reviewer strongly recommended doing more work to generate realistic duty cycles from agricultural or industrial equipment, noting that this is exactly the sort of thing that an external partner could provide (in-kind) or help generate.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said this project is very relevant to support VTO objectives. Hydrogen engines are an important tool for meeting carbon-reduction goals.

Reviewer 2

The reviewer stated this project is both highly relevant to the general topic of improving efficiency and performance of off-road vehicle systems, but also to the deep decarbonization of such systems.

Reviewer 3

The reviewer affirmed the project is relevant to the VTO objectives, adding that the current relevance is limited while using the 13-liter diesel engine. It will be better once the project team has the H_2 ICE available.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said the project seems to have sufficient resources for the project.

Reviewer 2

The reviewer affirmed the funding seems adequate to achieve the project objectives.

Reviewer 3

The reviewer indicated the budget of $500,000 in FY 2024 is sufficient for testing if Navistar and Cummins really provide some additional in-kind engineering support to ensure that their donated engines will operate well in a test cell.

Presentation Number: DORMA012
Presentation Title: Enabling Hydrogen Combustion for Large-Bore Locomotive Engines through Advanced CFD Modeling
Principal Investigator: Muhsin Ameen, Argonne National Laboratory

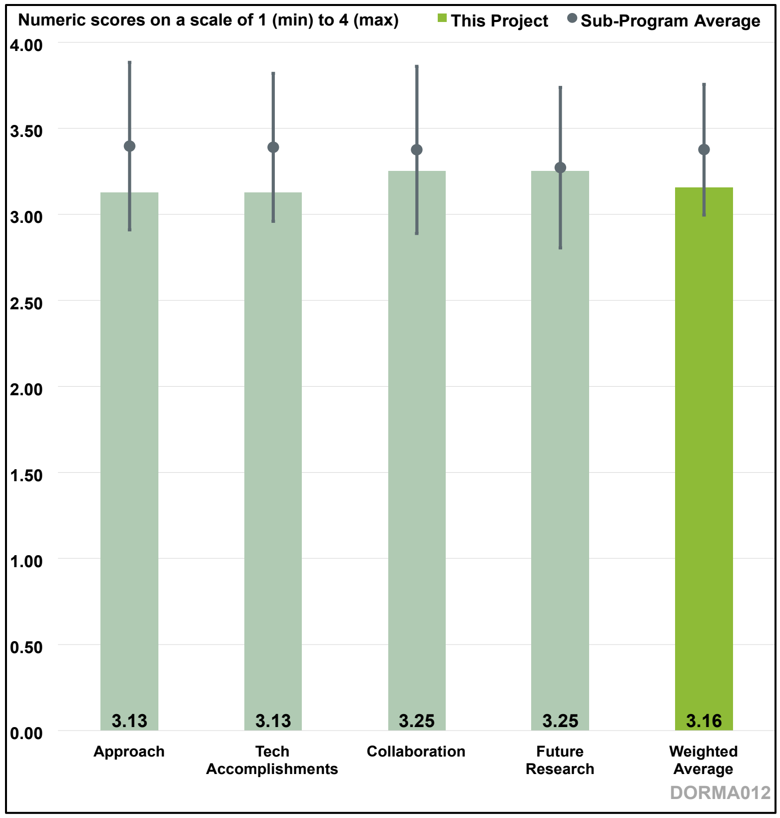

Figure 3-9. Presentation Number: DORMA012 Presentation Title: Enabling Hydrogen Combustion for Large-Bore Locomotive Engines through Advanced CFD Modeling Principal Investigator: Muhsin Ameen, Argonne National Laboratory

Presenter

Muhsin Ameen, Argonne National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer believed the noted barriers are being addressed very well. There are clear tasks to either solve, eliminate, evaluate, or validate barriers. Where there is a chance that barriers may not be completed, solved, or overcome, the desired level of outcome (such as “improve”) is noted. Additionally, the project appears to be well set up to navigate any unforeseen challenges and/or unplanned results. The project team is working through an unanticipated barrier to the baseline H_2/diesel PFI configuration work—the delays at Oak Ridge National Laboratory (ORNL). Alternative mitigation plans are being worked on.

Reviewer 2

The reviewer indicated the milestones set for the project address all key barriers for hydrogen combustion in large bore engines. The approach for validating the CFD simulation with experimental data is a commendable approach to developing a dependable simulation tool for further technology advancements. Some key questions that need to be addressed include: (1) What the air/fuel ratios are for the (diesel/H_2) mixture during the different substitution rates. The 300% increase in NO_x suggests a richer mixture with increased substitution rate. The reviewer thought NO_x reduction should be placed as an important milestone in the approach. (2) The use of main injection timing (MIT) as a tool to control combustion is fairly well known in conventional diesel combustion; while this exercise is a good approach for CFD validation, the findings of control of start of combustion, peak pressure, etc., are not novel for advancing the use of hydrogen/diesel dual-fuel. It would help to understand the end result of the MIT influence and how it is going to be used for NO_x mitigation, pre-ignition mitigation, knock mitigation, etc.

Reviewer 3

Overall, the reviewer stated it is a reasonable approach for a project focused on CFD to pair with the experimental work being conducted at ORNL. The progression of validation and then CFD experiments conducted ahead of experimental work is good, since it uses the CFD to inform the experimental work conducted later. The reviewer looks forward to seeing whether and how this can accelerate the experimental program. With the objective (shown on Slide 3) to use the simulations to "...enable up to 100% operation on hydrogen and low-carbon fuels...", the reviewer expressed concern about the availability of fuel models for the low-carbon fuels. Since 100% hydrogen substitution is not applicable, there will be a low-carbon diesel component to the combustion process. There are limited, and often out-of-date, models for renewable diesel and biodiesel. There is also no mention of validation of the models with low-carbon fuels.

Reviewer 4

The reviewer commented that the technical approach is shown to be able to predict combustion events and abnormal combustion, adding that the results have not been correlated with experiments.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewed noted that the nine technical accomplishments appear to be addressing the objectives of the project well, noting the development of robust simulation tools to accurately evaluate various low-carbon fuels for use in the rail industry and eventually contribute to the development of a suitable low-carbon-fueled engine. Technical accomplishments, such as the results of the hydrogen substitution rate testing, provide clear indications of the impact on ignition performance and emissions reduction and are adequately informing future testing needs and next steps.

Reviewer 2

The reviewed affirmed that the results of the study are highly relevant and would be a rich dataset to compare against experimental data. The simulation results have covered basic engine parameter investigation that could be used to validate and refine the model with CFD data. The reviewer noted two further points: (1) Technical Accomplishment 7/9 is highly relevant for hydrogen combustion. This accomplishment would benefit further by identifying in-cylinder conditions that would influence pre-ignition, such as hot spots, residual trapped gas, etc. The current findings related to advanced MIT resulting in better flame propagation are well documented in previous literature. The value of CFD simulation would be to identify specific areas of concern in a given combustion chamber geometry that would lead to pre-ignition conditions. (2) Technical Accomplishment 8/9 is also a very important dataset related to crevice volume. For hydrogen combustion, crevice volume is highly important and its effect on pre-ignition is uncertain. The results do not seem to discuss the effect of crevice volume on pre-ignition.

Reviewer 3

The reviewer noted some delays in validation due to delays on experimental testing. The reviewer expected to see a recycle loop on some work completed thus far once the ORNL engine is operational and data are available to validate, such as some of the initial simulations report findings that are consistent with the literature and positive control authority for the diesel injection through a range of injection timings, for example. This is good validation of basic model functionality, but it is not immediately clear whether or how these types of findings represent a step forward on the path to dual-fuel diesel–hydrogen combustion, since they are broadly expected trends. Further, as this work progresses, it will be useful to re-examine many years of DOE's and other's funded work on dual-fuel combustion to understand where the outcomes of this project merely duplicate the prior findings and what material is truly unique and novel.

Reviewer 4

The reviewer appreciated the systematic parameter study and regression analysis. For the results shown on Slide 7, the reviewer requested inclusion of engine operating conditions (e.g., rated?, speed and torque, indicated mean effective pressure [IMEP], intake manifold pressure, intake manifold temperature [IMT], volumetric efficiency, and fuel quantities). The reviewer also recommended the team include results for the swirl ratio equaling zero and show global lambda values at different substitution levels, since H_2 and diesel have different stoichiometric air/fuel ratios. The reviewer indicated it was unclear if the substitution ratio is by energy content. For results shown on Slide 9, the reviewer requested inclusion of global lambda values; for combustion efficiency, the reviewer requested a breakout of diesel combustion efficiency and H_2 combustion efficiency, if possible. It is equally important to show how the presence of H_2 impedes diesel auto-ignition and ignition delay.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer remarked that the project team's collaboration with industry as well as national lab and CFD software partners is showcased well.

Reviewer 2

The reviewer expressed that collaboration between the parties appears to be strong. This reviewer acknowledged potentially missing something but did not believe the delays at ORNL have anything to do with collaboration. To that end, the partners seem to be working on a potential alternative plan should delays persist.

Reviewer 3

The reviewer pointed out it was early in the project and thus difficult to see how effective the collaborations are between the different parties, though they make sense on paper. Partners at ORNL indicated good feedback and connectivity on operating maps thus far.

Reviewer 4

The reviewer noted there was nothing to add.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer indicated the proposed future research is well supported and obvious based on the technical accomplishments. Future tasks toward fine-tuning of causes of abnormal combustion, emissions modeling, and the impact of fuel mixing accuracy on wall heat transfer models should yield targeted results based on the baseline information obtained during the baseline study.

Reviewer 2

The reviewer stated the proposed experimental validation is the most critical part of this project. An in-depth validation of CFD results would be the key success criteria for this project.

Reviewer 3

The reviewer acknowledged there is a broad swath of future research topics laid out for this project It would be useful to highlight any opportunities to down select the work and focus on key, enabling topics to move the overall hydrogen engine for rail projects forward. The reviewer encouraged focusing on using CFD tools to answer significant questions that cannot be answered easily experimentally. For example, injection timing trends are very straightforward and quick to implement in an experimental project, but things like compression ratio, exhaust gas recirculation (EGR) levels and temperatures, air systems, and piston shapes are much lengthier processes to explore experimentally. By focusing the simulation work on these aspects, it can help accelerate the project more quickly than things that are readily done experimentally. In addition, using simulation to understand phenomena of the combustion process could be an area to find value using CFD.

Reviewer 4

The reviewer indicated that correlation with experiment is a key milestone to yield improvements in the predictability and quality of results in future research. For engine-out emissions prediction, the project team should include unburned H_2 prediction. To prepare for closed crankcase ventilation (CCV), the team should attempt to predict H_2 in blowby for PFI. It will be excellent if such research is able to elaborate blowby during both compression and expansion. The team should plan to highlight the differences between direct injected H_2 and PFI H_2 on blowby and how it impacts CCV.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer affirmed the project is relevant to the industry achieving 2050 net-zero emissions objectives and ensuring that any transition to low-carbon fuels or hydrogen will be feasible, economical, and efficient. Simulation models that can accurately evaluate various fuels will be key to advancing toward zero-emissions objectives and will inform the design of the next-generation locomotive engine.

Reviewer 2

The reviewer said this project is a very value-added fundamental study with nice progress shown.

Reviewer 3

The reviewer stated this project is highly relevant for the use of hydrogen in large bore engines with diesel pilot. Control of combustion in a diesel/H_2 mix is critical, and identifying conditions that result in abnormal combustion is the key unknown in hydrogen-fueled engines. Developing high-fidelity CFD simulations accelerates engine development time and reduces the cost of new technology development. However, projects like this that have an approach to validate the CFD models with focused engine experiments are highly relevant to gain confidence in further use of models for engine development.

Reviewer 4

The reviewer acknowledged the project is relevant to overall VTO subprogram objectives, focused on enabling hydrogen internal combustion engines for rail applications. The work is nicely connected to the experimental project lead by ORNL. That said, there is always a concern on the relevance of applied CFD programs completing straightforward development tasks and whether this type of work is appropriate for DOE laboratories. In this case, the reviewer concluded the connectivity to enable another project makes it reasonable for enabling the DOE objectives.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer asserted that the computing ability of ANL and experimental capability of ORNL are more than sufficient to accomplish the goals of this project.

Reviewer 2

The reviewer said the resources, as defined, appear to be sufficient. The ability to execute at ORNL could impact whether milestones are met in a timely fashion. This reviewer expressed confidence that milestones can be met based on the contingency planning that is occurring. Project proponents are staying close to the situation and have a plan to pivot if further delays at ORNL persist.

Reviewer 3

The reviewer indicated the resources are sufficient but would have liked to see a greater in-cash cost share versus in-kind given the scale and attributes of the project.

Reviewer 4

The reviewer looked forward to seeing timely availability of experimental data.

Presentation Number: DORMA014
Presentation Title: Implementing low lifecycle carbon fuels on locomotive engines – CRADA with Wabtec
Principal Investigator: Dean Edwards, Oak Ridge National Laboratory

Presenter

Dean Edwards, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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

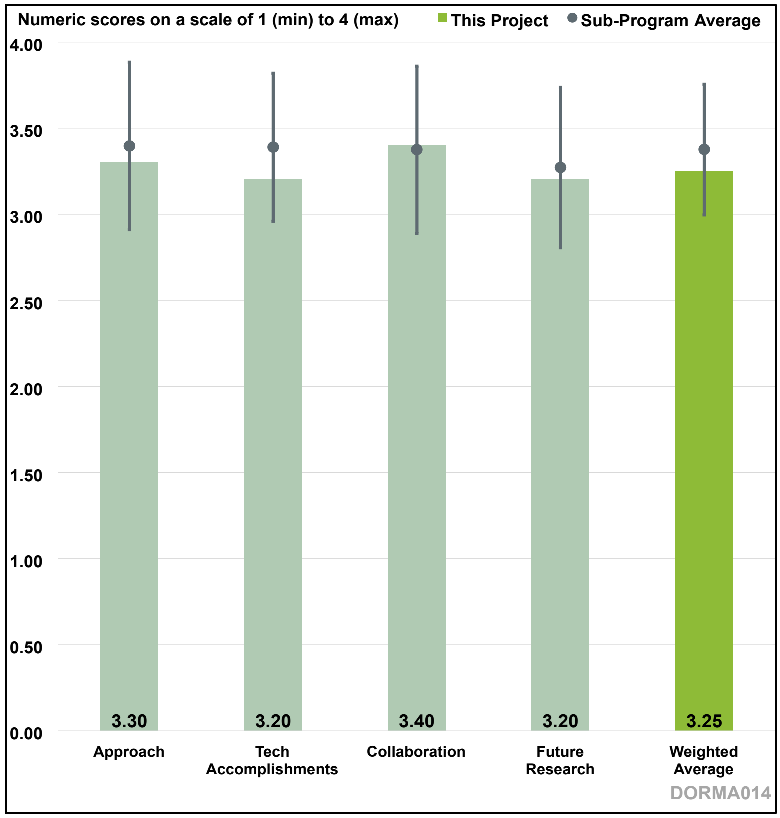

Figure 3-10. Presentation Number: DORMA014 Presentation Title: Implementing low lifecycle carbon fuels on locomotive engines – CRADA with Wabtec Principal Investigator: Dean Edwards, Oak Ridge National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer noted that, even though delays have hindered the timeline, there is leadership support and a plan to advance immediately when infrastructure upgrades are complete. Technical barriers have been identified and predicted outcomes are realistic. Efforts to maximize hydrogen substitution rate to reduce CO_2 and NO_x emissions have been identified, while acknowledging that dual-fuel ICEs are not a zero-emissions solution.

Reviewer 2

The reviewer provided two comments. (1) Engine testing infrastructure installation is a critical milestone that was undertaken and is the fundamental platform for any future work and validation of CFD models. (2) Hydrogen fueling infrastructure is the other task that is a critical barrier to developing engine testing facilities for alternative fuels.

Reviewer 3

The reviewer acknowledged having only general knowledge in this area, but added the project plan looks excellent assuming the rail engine is made into a dual-fuel system, where H_2 is one of the most reasonable fuels to add to the system, with a goal of decarbonizing the system as much as possible.

Reviewer 4

The reviewer acknowledged impressive progress has been accomplished. Thoroughness and care have been taken into consideration to ensure safe lab operation. The team underestimated the time and effort it took for the lab upgrade, fuel supply, permit approval, etc. That said, the investment and new capability will prove highly valuable for future research.

Reviewer 5

The reviewer pointed out that the project approach involves building new facilities, baseline engine testing, and then evaluation of different hydrogen fueling systems and their impacts on the ability to increase the hydrogen substitution ratio. The work addresses a key technical space of decarbonizing rail, where locomotives are in service for extended periods of time and hydrogen is of interest as a potential decarbonization pathway. The project has a logical progression, but the scope of work compared to the timeline is very aggressive. This raises the concern that there will be insufficient depth in each stage of the project, as there is significant time pressure to complete the work. The overall timeline was unreasonable, even at the early stages where significant new infrastructure development and installation was part of the project. The significant delays so far are not surprising.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer acknowledged that the range of demanding pieces for this project is high, especially the Wabtec engine installation and testing that may be near at hand. With two years to go, next year’s results will be critical in seeing how this dual-fuel approach works.

Reviewer 2

The reviewer noted the project design is complete; however, infrastructure upgrades have been delayed.

Reviewer 3

The reviewer indicated the project has a well-thought-out plan and is making solid progress with support from leadership. The reviewer suggested considering crankcase H_2 monitoring, purging, and pressure relief as additional safety measures, as well as monitoring engine oil during operation. Emissions measurement is not mentioned in the report. In addition to standard gas and PM measurement, this reviewer suggested considering H_2 emission measurement.

Reviewer 4

The reviewer stated that the completion of infrastructure tasks is an excellent accomplishment but noted the presentation did not show any preliminary data from test-cell commissioning.

Reviewer 5

The reviewer indicated that significant progress has been made into building facilities and installing infrastructure supporting this project. The new single-cylinder locomotive engine and support systems will give a solid platform for future development in the rail-engine space. That significant progress acknowledged, the reviewer added that the work has not surprisingly run behind schedule, slowing overall progress on the project. With little technical progress, it is challenging to assess.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer noted there are key partnerships that are needed to make this project work. Wabtec appears to have been very active, which is critical at this stage in the project.

Reviewer 2

The reviewer commented that the collaboration between ORNL and ANL provides an excellent platform for CFD model validation, and the coordination between Wabtec and ORNL has helped in developing a modern locomotive-engine research engine test facility.

Reviewer 3

The reviewer acknowledged this is a challenging facility upgrade project requiring extensive collaboration but is impressed with the progress despite the project being behind schedule.

Reviewer 4

The reviewer indicated the planned collaboration and coordination between the different parties looks appropriate, including close connection to a supporting engine OEM with significant cost-share and another national laboratory with substantial capabilities in CFD. The constellation of teams should make for an effective project. The reviewer acknowledged that it is early in the project to have a clear view on the efficacy of the teaming.

Reviewer 5

The reviewer noted it appears that collaboration efforts are solid; however, several issues related to inflation and supply chain have hindered completion of construction.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer indicated that future work is well-defined and should achieve the desired targets.

Reviewer 2

This reviewer asserted the single-cylinder approach to maximizing the substitution of hydrogen as well as testing the impact on NO_x aftertreatment seems workable. Having time trials with other fuels than diesel would be a great effort.

Reviewer 3

The reviewer stated that, as an outcome of this research, the team should recommend the feasibility and appropriateness of retrofitting older engines without EGR. This reviewer is optimistic that, for diesel locomotive engines equipped with EGR, common rail, and highly boosted turbo, the retrofit approach for H_2 substitute will be more practical.

Reviewer 4

The reviewer acknowledged that there is a significant amount of future work proposed. However, it appears that much of that work involves the evaluation of different hardware sets: injection systems, air systems, and compression ratio. This is concerning from both an operations and scientific perspective. Work that is a series of hardware changes can be difficult to execute in a national lab, and the industry-wide scientific understanding that this ultimately delivers is reduced. Further, the extensive work, short project duration, and already behind-schedule status, is concerning and suggests the final results from the project will have too much span and too little depth to be broadly useful. This reviewer would prefer to see a reduction in scope, with a focus on a smaller set of topics that generate real learnings to drive the industry—for example, a focus on a baseline diesel-based decarbonization scenario using renewable diesel or biodiesel and a high-substitution DI hydrogen configuration. Additionally, there is room for more depth and focus on emissions, not just hydrogen substitution for decarbonization.

Reviewer 5

This reviewer made two comments. (1) The emissions measurement capability of the test facility was unclear. (2) There is no mention of validation activity between CFD and engine data.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer indicated the relevance of this project is clear, since it clearly supports the DORMA goals to Decarbonize the Off-road, Rail, Marine, and Aviation sectors of transportation, which are difficult to electrify. This may be a uniquely interesting and difficult effort in this area.

Reviewer 2

The reviewer acknowledged that decarbonizing rail is challenging and requires test facilities that can cater to a range of fuels and engine designs. This CRADA provides researchers with an excellent tool to develop models as well as conduct highly relevant experiments.

Reviewer 3

The reviewer asserted this is an excellent project and very relevant.

Reviewer 4

The reviewer stated that short-term solutions for decarbonizing the rail sector and the ability to ensure existing ICEs can remain in use as dual-fuel assets are important.

Reviewer 5

The reviewed noted this project does support the VTO program objectives around identifying and evaluating technologies for decarbonization in the off-highway transportation sector. H_2 ICEs have been identified as a potential direction for decarbonization if lower-carbon hydrogen becomes available. Understanding the engine technology options for rail falls within this scope.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer stated that ORNL management is supporting this project well and Wabtec is a strongly supportive partner. As far as this reviewer can tell, the project has planned for sufficient resources.

Reviewer 2

The reviewer asserted that industry and national laboratories collaboration provides highly valuable technical, instrumentation, and computational resources.

Reviewer 3

The reviewer offered best wishes to the team to recover from the delay and is looking forward to the data generated from the lab.

Reviewer 4

The reviewer acknowledged it appears that the project is well-supported with resources; however, the ability of its proponents to execute the necessary infrastructure upgrades to allow the continuation of the project is critical to meeting deadlines and objectives.

Reviewer 5

The reviewer stated the resources are substantial and appropriate, noting the challenge with delivering milestones in a timely fashion is less a funding issue and more a result of the aggressive timing and scope.

Presentation Number: DORMA015
Presentation Title: Predictive CFD Tools for Low-Carbon Fueled Off-road Internal Combustion Engines
Principal Investigator: Riccardo Scarcelli, Argonne National Laboratory

Presenter

Riccardo Scarcelli, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 67% of reviewers felt that the resources were sufficient, 33% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

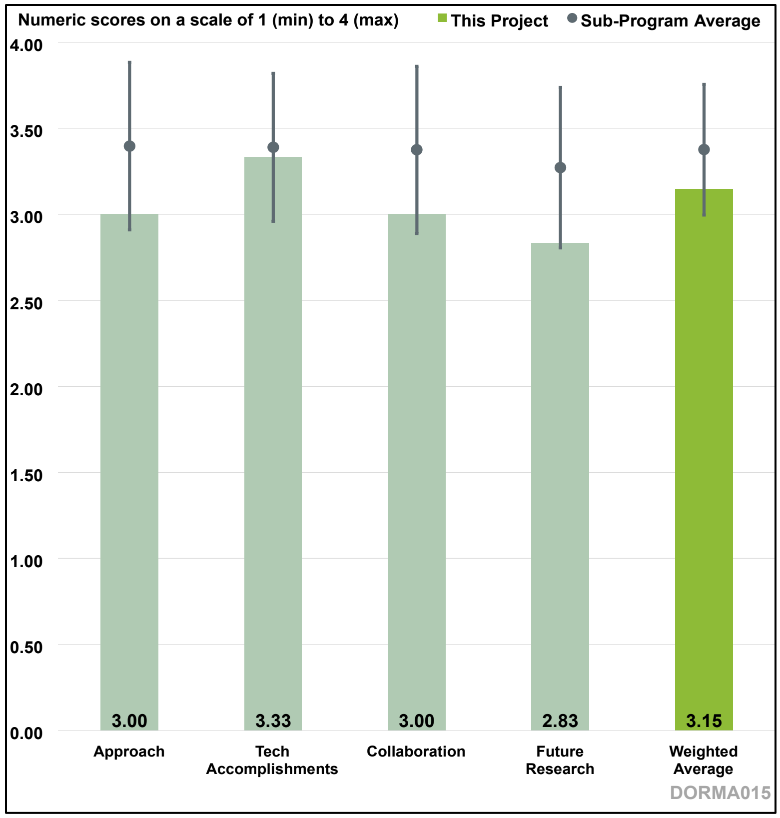

Figure 3-11. Presentation Number: DORMA015 Presentation Title: Predictive CFD Tools for Low-Carbon Fueled Off-road Internal Combustion Engines Principal Investigator: Riccardo Scarcelli, Argonne National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer stated the simulation provides valuable insights into the combustion process. Such capability will pay long-term dividends in accelerating development and issue resolution.

Reviewer 2

The reviewer asserted that the simplified intake port seems too simple, especially with PFI, and asked if there is any way to improve the model to have a more accurate geometry with both the intake valves and injector. This may have a significant impact on the cycle-to-cycle differences being seen in simulation. Additionally, the experimental data used for comparing cycle-to-cycle variation appears to be an average. This reviewer asked if there is a way to show best/worst experimental cycles for a comparison with the CFD data.

Reviewer 3

The reviewer commented this project couples a series of different topic areas focused on improvements to CFD modeling tools, with the overall effort aligned with improving these tools to aid development of engines using low-carbon fuels, particularly hydrogen and methanol. At first glance, the project is a collection of diverse topics, and the specific milestones for each one were not immediately clear from the materials, as they spanned such a range of topics. The live presentation made it clearer that these are different aspects that are important for effective models, and they are separated to address as such. Within this context, the project lays out a series of key aspects to address for improving the overall CFD toolset.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer indicated the project has made significant progress in meeting project tasks and no improvements are needed.

Reviewer 2

The reviewer asserted good overall progress thus far for a project that is in its relative infancy. Key milestones have been met, with the critical focus area identified. There are good comparisons between different fidelity models, including DNS/LES/Reynolds-averaged Navier-Stokes (RANS). The work on DNS has significantly improved over the last few years, which is exciting to see. It is, however, useful to understand the degree to which differences between DNS, with very high fidelity, and RANS, with low processor cost, are impactful for the overall utility of the results. The identification of mixing, and how mixing is being modeled, as the critical path forward is crucial for the future of the project and a good early step.

Reviewer 3

The reviewer stated that this report did not adequately describe boundary conditions such as bore, stroke, revolutions per minute, torque (%), intake manifold pressure and temperature, compression ratio, in-cylinder swirl ratio, etc. A summary table is recommended. The team suggested experimental data from Caterpillar (CAT) methane (CH_4)/H_2 testing have been used to validate the simulation but did not explain how the simulation data matched with experimental results before showing the cycle-to-cycle variation on Slide 7. The CCV discovery is quite insightful.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer indicated that the collaboration and coordination across project teams seems to be successful.

Reviewer 2

The reviewer noted adequate geometric parameters and simulation methods sharing are apparent among project partners.

Reviewer 3

The reviewer acknowledged the collaboration on this project is relatively narrow, including ANL as the lead with one OEM and a CFD code supplier. That said, the in-kind contribution from the OEM partner is appreciated. It will be important to see further signs of collaboration as the project moves forward.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer encouraged the team to predict H_2 combustion efficiency and H_2 emissions as future goals. This reviewer also posed a question to the project team, asking how to validate the conjugate heat transfer results from CFD.

Reviewer 2

The reviewer suggested perhaps adding an improved intake port model. Other than that, the future work is acceptable.

Reviewer 3

The reviewer observed the future work for the project continues to move ahead on a range of topics associated with improving CFD modeling tools. However, it was identified that the key aspect, especially for hydrogen combustion, was the mixing model. As the project evolves, this reviewer encouraged the team to consider reshaping the work to ensure this was fully addressed and would prefer to see a focus here rather than covering all topics.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said the work has a clear purpose and is of value to the industry given the focus on identifying and further developing improvements to modeling tools. It is relevant, given the pressure new fuels may place on existing understanding of model performance. Industry has a clear focus on low-carbon solutions, so improvements here can help the industry as a whole move forward.

Reviewer 2

The reviewer asserted this project definitely supports efforts for decarbonization and CO_2 emissions reduction.

Reviewer 3

The reviewer noted the project is well aligned with VTO objectives and the mission for national laboratories.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer indicated that the resources with ANL, CAT, and others are adequate for the project scope and timeline.

Reviewer 2

The reviewer offered the following suggestion: a smaller PFI spark-ignited engine has been studied to run H_2 with combustion data measurement, and this reviewer wondered if it would be valuable to validate the models to such existing data then re-apply them to a large bore and lower speed engine with prechamber.

Reviewer 3

The reviewer stated that the resources seem low relative to other modeling/simulation projects.

Presentation Number: DORMA016
Presentation Title: Renewable methanol-fueled engines for marine and off-road applications
Principal Investigator: Jim Szybist, Oak Ridge National Laboratory

Presenter

Jim Szybist, Oak Ridge National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

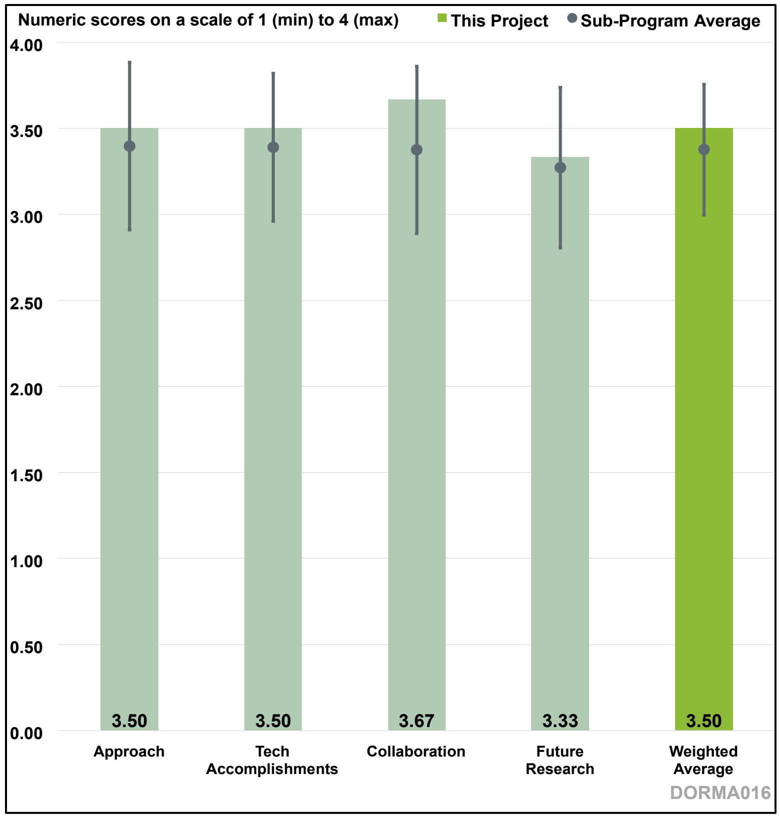

Figure 3-12. Presentation Number: DORMA016 Presentation Title: Renewable methanol-fueled engines for marine and off-road applications Principal Investigator: Jim Szybist, Oak Ridge National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer noted this is an extremely ambitious project, following three approach pathways simultaneously: (1) PFI methanol (MeOH) with a DI diesel pilot; (2) PFI of DME with DI MeOH, with catalytic MeOH dehydration to DME; and (3) MeOH prechamber spark ignition (SI) on three separate engine platforms.

Reviewer 2

The reviewer affirmed the project is on track.

Reviewer 3

The reviewer noted the project focused on three different combustion strategies, seeking to maximize performance. The strategies were PFI MeOH/DI diesel, PFI DME/DI MeOH, and active fueled prechamber. Engines are identified for each of these combustion modes, and a schedule is set for these. The information could have been strengthened with targets or expectations for them. The reviewer asked if there would be merit in focusing on one engine platform to consolidate the effort. The work included the development of a catalytic methanol dehydration for onboard DME production to support the second approach above. The reviewer added that the work could better clarify the state at which the effort is at.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer mentioned the project is in its early days. Engine platforms have been updated, and two have been installed and commissioned/baselined. The reviewer is looking forward to seeing the data that comes out of these test cells.

Reviewer 2

The reviewer noted solid progress has been made.

Reviewer 3

The reviewer indicated the project completed the installation and baseline of a CAT C18 engine at ORNL. Testing benchmarked discrete points using the CAT engine control unit (ECU) and ORNL open-access ECU. The project also installed and commissioned a single-cylinder version of the C18 engine at ORNL. The project fabricated a modified intake manifold for a prechamber cylinder head configuration. The aim of the prechamber was to prevent methanol pooling.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer affirmed strong partnership with CRADA partner Caterpillar and excellent working relationships with funding partners and additional collaborators. The reviewer also praised the impressive work with the senior design team at Colorado State University.

Reviewer 2

The reviewer noted that strong collaborations with an OEM and suppliers are apparent.

Reviewer 3

The reviewer observed that the project is configured as a CRADA with Caterpillar as the primary collaborator. The project features partners, Gane Energy, BASF, Colorado State University, and the Methanol Institute.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer said that the future work on this project is all of the exciting stuff, and they are looking forward to results coming out of these engines.

Reviewer 2

The reviewer indicated the project has a plan of tasks over four project years involving three engine platforms and catalytic methanol dehydration flow reactor experiments. The challenges indicated in the future work are similar to those noted in the approach. Having more specific metrics and targets for each of the engine configurations may be useful.

Reviewer 3

The reviewer suggested considering the delivery system and controls that are associated with the on-board DME device, including if a DME storage device is required. Ideally, water from methanol dehydration is used as a diluent for engine combustion instead of a new discharge stream.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer indicated that the project is extremely relevant to DORMA goals.

Reviewer 2

The reviewer commented that this is a very innovative approach using on-board DME from methanol for combustion assistance. The project team took a system approach considering all options and focusing on the tradeoffs of each approach.

Reviewer 3

The reviewer noted that methanol is a pathway to decarbonize the hard-to-electrify marine sector. It is relatively abundant and can be produced with a low carbon intensity. This reviewer encouraged the authors to quantify the GHG footprint from traditional means such as natural gas and biofuel sources. Technologies promoted in this project target efficient, clean, and durable operation with competitive diesel-like load capabilities.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer indicated the resources seem sufficient.

Reviewer 2

The reviewer noted that the DME production and storage system may take some time to build and requires some iterations before it will be ready for cold start and transient tests. This reviewer wished the team success.

Reviewer 3

The reviewer stated that the project aims to develop a methanol-based combustion system based on three possible approaches and engine platforms. The project has many challenges and unknowns as it moves forward. Some thought may be given as to how to maximize the effort, and if it makes sense to consolidate the effort on the two Caterpillar engines, at least with respect to the viability and merit of each of the pathways proposed.

Presentation Number: DORMA018
Presentation Title: SAF Combustion and Contrail Formation Research
Principal Investigator: Julien Manin, Sandia National Laboratories

Presenter

Julien Manin, Sandia National Laboratories

Reviewer Sample Size

A total of two reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 50% of reviewers felt that the resources were sufficient, 50% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

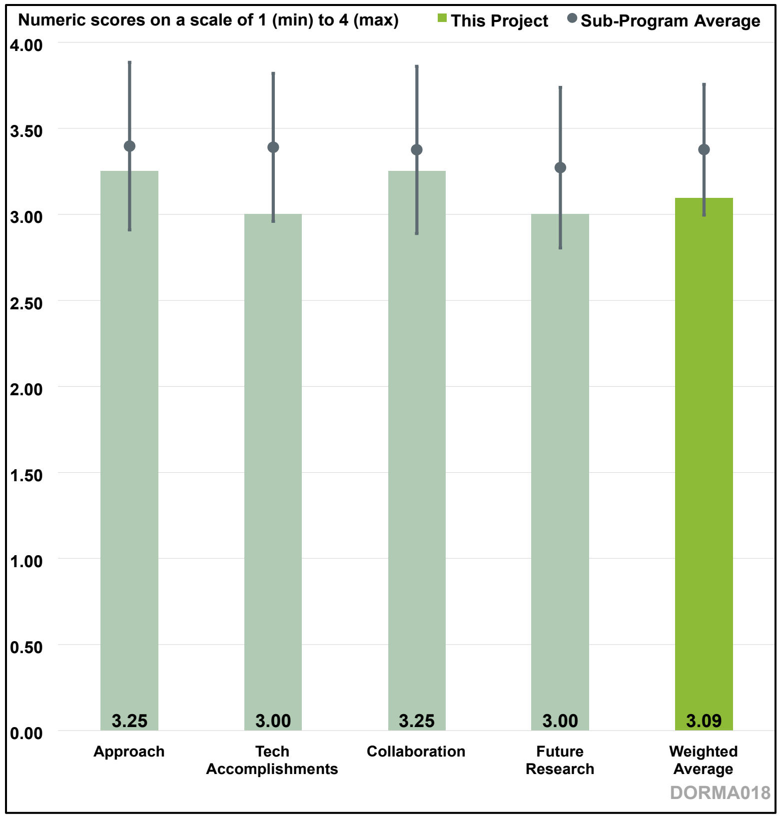

Figure 3-13. Presentation Number: DORMA018 Presentation Title: SAF Combustion and Contrail Formation Research Principal Investigator: Julien Manin, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The results of this work should contribute to all three of the bullets selected from the SAF Grand Challenge Roadmap. Several of the barriers are particularly challenging, specifically those related to vapor trail emissions and subsequent environmental impacts and will likely require an expanded effort. In addition, each year new (lower level) barriers are identified; hence the team has a strong, forward-looking perspective.

Reviewer 2

The effort focuses on a key research question regarding the understanding of fuel composition impacts on sooting propensity. The timeline and corresponding milestones are reasonably planned. The key milestones are the droplet nucleation altitude chamber and quantification of nucleation propensity for relevant sustainable aviation fuel (SAF) regarding fuel structure effect on sooting. Regarding the milestone on a standardized iso-paraffinic surrogate, this seems less critical and provides less unique research value given the many existing surrogate mechanisms. Differences between this work and prior existing work should be highlighted as part of this milestone.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The team has been coming up to speed to integrate themselves with the aero-engine community over the last several years. They have been doing that well and developed concepts for exploiting the fuel injection (pulsed) rig for reciprocating engines and applying it to conditions of interest (continuous combustion) to the aero-engine community. The success on simulation of the CFM combustor using reactor networks represents a new capability and an advancement to the state-of-the-art (SOA), although it remains to be seen how well this model extends to other combustor configurations. New capabilities regarding simulations using direct numerical simulation (DNS)-CFD and molecular dynamics for examining aerosol formation and plume generation are evolving well, although it will remain a challenge to validate such methods against experimental data sets resulting hopefully in new knowledge and strategies for reducing environmental impacts. The atmospheric chamber should help in this regard, but it will take a lot of work to fully characterize its capabilities and the chemical effects of different soots and sulfur on nucleation processes. The authors show in the back-up slides experimental/modeling comparisons of soot yields for different fuels. There is a substantial difference in the results for 1,2,4-trimethylbenzene (TMB). The reviewer said this discrepancy may warrant further investigation. The application of their tools to predictions near 3500 K is understandable due to computational costs etc., but there is a risk that reaction pathways may change at the lower temperatures applicable to aero-engine conditions.

Reviewer 2

The reviewer noted that accomplishments include results on the kinetics analysis of fuels on soot formation. The work aligns with previous work evaluating aromatics and other chemical classes. It is unclear what unique new knowledge this work provides or how it compares to previous studies. The work would be enhanced with these comparisons and clarifications. The other technical accomplishment on potential cycloalkane benefits on soot processes provides some value on fuel component comparisons. The work would be improved to have comparisons of this work to prior studies. Additionally, the comparison to “jet fuel with 20% aromatic” is not clearly making the case across all aromatics in fuels. Specifically, the synthetic aromatic kerosene from Virent has been shown to produce less soot than conventional aromatics. The study would be enhanced if a target blend representing the unique aromatic characteristics of potential synthetic aromatics was developed and analyzed. The results on the contaminant effect on water nucleation is a unique, valuable research effort documenting unique impacts from fuel impurities on water nucleation.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project has a great set of collaborations and utilization of their experience. Pacific Northwest National Laboratory (PNNL) is linked up with Washington State University (WSU), who are doing work with cycloalkanes. Raytheon Technologies Research Center might be a good contact (Miad Yazdani) regarding their Federal Aviation Administration (FAA) contract on contrail formation.

Reviewer 2

The reviewer said the effort seems to have broad collaboration across relevant industry, academic, and government institutions. The presentation notes the research partners and areas of work, but additional details throughout the documented effort would facilitate improved understanding of where various research partners are making specific contributions.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The researchers have identified a good set of specific tasks, although one or two might be missing. The first might be to characterize the soots from the “liquid fuel soot generator” and specifically how they change with different fuels to character (structure as well as hydrophobic/hydrophilic tendencies), number density, and size. A second might be to sort out the discrepancy in the soot yields from TMB. A broader topic for future research might be related to estimating the impact of different time scales (of the short-term nucleation processes for emissions from different fuels) on the longer-term climate forcing from the entire lifetime of the plume. These timescales are likely a function of local conditions (humidity, altitude, pressure, etc.) and probably variable, but ought to help focus future research efforts to the most critical needs.

Reviewer 2

The work outlines future research items with some detail on the purpose of the additional research. Additional information on the relative importance of future research would be beneficial to assess the value of the proposed work. While the proposed work includes tasks with experimental testing and sampling of flame stabilization and soot formation, it is unclear how the experimental work will be validated against available data from flight campaigns. Without proper validation, the reviewer is not clear if lab-scale experiments properly reflect real-world conditions. The reviewer said it seems likely that the proposed future work will be accomplished, but additional details are needed on the specific research objectives the proposed work intends to achieve.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The embedded links appear outdated, but the work is fully consistent for the SAF Grand Challenge Roadmap.

Reviewer 2

The project is relevant with regard to advancing new learnings for the sustainable aviation space. The reviewer commented that it was not clear from the linked VTO subprogram objectives which subprogram consideration this particular project addresses. Therefore, while the project may not clearly support a specific VTO subprogram objective, the project itself is enabling the understanding of fuel compositional effects on soot and contrail formation. This work is in a critical area as existing research gaps limit the understanding of contrail formation. Research to address these gaps may advance the ability to mitigate the global warming impact of persistent, warming contrails formed by aviation.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The project does not appear to be funded beyond FY 2024. The team has done well transferring their capabilities to SAF concerns and demonstrating that they can match or in some cases exceed the SOA. But to have a real impact, their work needs to continue further, and the experimental work needs to continue to support important model validation, with recognition that the experimental work is not cheap.

Reviewer 2

The project team seems to have sufficient resources to accomplish the milestones on schedule. The presentation did not indicate any resource constraints or concerns that would suggest otherwise.

Presentation Number: DORMA019
Presentation Title: Multi-phase flow studies of SAFs for industry-relevant conditions and geometries
Principal Investigator: Brandon Sforzo, Argonne National Laboratory

Presenter

Brandon Sforzo, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

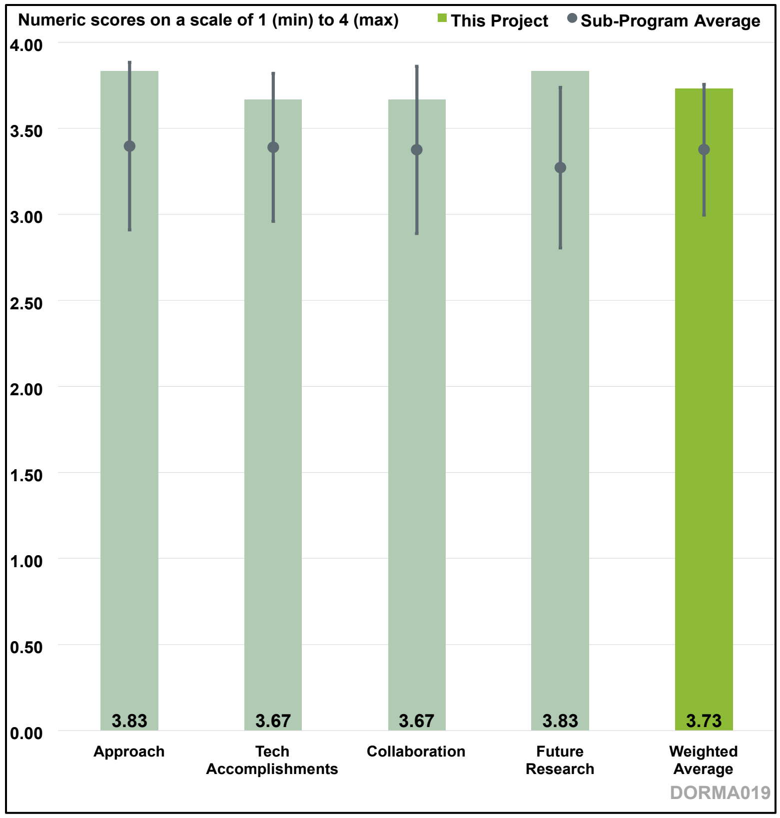

Figure 3-14. Presentation Number: DORMA019 Presentation Title: Multi-phase flow studies of SAFs for industry-relevant conditions and geometries Principal Investigator: Brandon Sforzo, Argonne National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project is providing unique measurements of the liquid fuel atomization process very near fuel nozzle exits using the using the high-flux X-ray source available at the Advanced Photon Source (APS) facility and is advancing the real fluid modeling of liquid injection and fuel-air mixing at elevated temperature and pressures where transition from two-phase flow to supercritical flow may occur. The testing and modeling include Jet-A and SAF fuels and are using non-proprietary injectors that use atomization techniques representative of current aircraft gas turbine engine fuel injectors. Testing at Phase 1 (1 atm, 25°C) conditions is underway with testing completed for one (pressure swirl + jet-in-cross flow) of the two 1 atm capable injectors provided under collaboration with the National Aeronautics and Space administration (NASA) and Woodward. Testing of the second (pressure swirl + pre-filming air blast) injector is somewhat delayed due to a one-year APS upgrade and the slower than expected time to get APS fully back online. Good progress was demonstrated on preparing for higher pressure (60 atm) and higher flow rate testing with window designs and rupture testing completed and hardware for higher flow rates assembled and undergoing safety inspections. CFD simulations of the first injector testing are making good progress and real fluid modeling has advanced beyond existing methods and has been demonstrated for single droplet evaporation including the National Jet Fuels Combustion Program (NJFCP) Category C fuels, C-1 and C-5. The X-ray phase contrast data very near fuel nozzle exits at any test condition is likely to help improve spray atomization modeling in general, but the largest benefit of this project is likely to come from the higher pressure and temperature testing where differences in Jet-A and SAF behavior may be more pronounced, particularly if transition to supercritical behavior occurs.

Reviewer 2

The major technical barrier that this project seeks to address is the limited available data and understanding concerning fuel-air mixing in a gas turbine engine close to the injector, with a focus on SAF. The project seeks to understand this mixing process using novel X-ray diagnostic methods and improved computational models. These models, validated through the experimental measurements, will improve understanding of SAF performance. This represents an important step towards 100% SAF adoption. The reviewer was impressed by the project's logical approach to the problem and the clarity with which this approach was presented.

Reviewer 3

This project addresses internal flow and atomization issues as relevant to fuel injection which has critical influence on the combustion and emissions generation processes in a gas turbine engine. The experimental part of this work leverages the capabilities of X-ray imaging to overcome drawbacks of conventional light sources to obtain significantly improved understanding of the spray breakup and atomization processes. A particularly key advantage of the X-ray imaging technique is the ability to understand the internal features of the injection hardware and its subsequent influence on atomization processes. The PIs correctly identify outstanding issues with predicting transcritical spray behavior as relevant to realistic gas turbine engine operating conditions. Through X-ray imaging of spray atomization and correlation of the same through quantitative measurements with fuel physical properties, key insights can be drawn that can be essential to designing the next generation of fuel injection hardware particularly for operation with 100% SAF. Further, the detailed data about early spray properties can be very effectively used as boundary conditions for spray modeling efforts and the highly resolved results from these experiments can provide a wealth of validation data for simulation efforts. The simulation effort undertaken by the PIs rigorously addresses development of real fluid models for the trans/supercritical conditions of interest. The reviewer noted that all of these details ensure that the project is addressing critical technical barriers of interest to the aerospace and combustion communities. The project is well-designed, and the 5- to 6-year timeline seems well suited to achieve all the project goals.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

Phase 1 testing and data analysis is making good progress. The project has completed X-ray tomography of the actual internal geometry of one non-proprietary injector (pressure swirl + jet-in-cross flow) and completed a series of X-ray phase contrast measurements for four fuels (Jet-A, SAF and high-viscosity fluid) for the Phase 1 testing (1 atm, 25°C) on one of the non-proprietary injectors. Detailed processing and analysis of the X-ray measurements has been completed for the primary fuel circuit (pressure-swirl) and is underway for the secondary fuel circuit (jet-in-crossflow). A strength of this project will be sharing the geometry, measurements, and information useful for CFD simulations (such as geometry and boundary conditions) in an open manner and the Box site is nearly ready to provide this information for Phase 1 testing of the Pre-Sec (pressure swirl + jet-in-crossflow) injector. The capabilities to perform Phase 1 testing of the second non-proprietary injector (pressure swirl + pre-filming air blast) are in place and are waiting on getting beam time in APS. The project is also making good progress in developing new capabilities to permit testing up to 60 atm and the corresponding higher flow rates needed for Phase 2 testing. Along with the higher-pressure testing capability, the project is developing real fluid modeling capabilities applicable to Jet-A and SAF. Validating these CFD models for hydrocarbon fuels with many components (such as Jet-A and SAF) is challenging. If the project can eventually perform Phase 3 testing (up to 60 atm and 700°C) the X-ray measurements may provide a unique data set for validating transcritical behavior for Jet-A and SAF under realistic conditions and with flow through realistic injector geometries.

Reviewer 2

The investigators have made excellent progress towards their objectives. Multiple atomizer configurations have been evaluated using X-ray imaging, revealing fuel atomization behavior at extremely high spatial and temporal resolution. The investigators have observed asymmetries in the fuel spray and have explained them by analyzing X-ray tomography images for atomizer defects. The PIs have characterized fuel effects on spray parameters, and their results compare well with those published in literature. The project team is developing boundary conditions for high-fidelity simulations that are accurate to the tomographic nozzle data and have a working single-phase simulation of gas flow in the atomizer. The PIs are also making progress towards models of SAF thermophysical properties and vaporization trends.

Reviewer 3

The PIs have acquired two non-proprietary atomizers. The PIs showed results for fuel effects on primary spray behavior for the Pri-Sec nozzle. The X-ray imaging very neatly shows the presence of a foreign object and helical grooves from the machining process. It is posited that the near-nozzle spray morphology is influenced by these features. There is a clearly observed asymmetry in the spray morphology resulting in variations in measured parameters including breakup length, sheet thickness, and cone angle. The PIs could have potentially tested more nozzles without these production artifacts or tested the same nozzle at different orientations to confirm their suspicions. The reviewer said it could be that X-ray imaging, given its demanding nature, made it hard for the PIs to conduct these additional tests. The PIs could add more effort to correlate their findings of the spray morphology parameters to the fuel properties through some physical underpinning of the underlying processes. The high-pressure windows needed for extending work to higher pressures seem to have been designed and tested and this should pave the way for the group to advance to transcritical conditions of interest. Upstream single-phase flows for both fuel and air have been successfully modeled. A comprehensive model for thermophysical properties of SAF has been developed using graphic processing units (GPUs)/machine learning approaches and its ability to predict properties in the transcritical region for both single component and blended fuels has been demonstrated. These efforts lay a solid framework for the proposed simulation efforts to be undertaken by the PIs.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The Aero-Spray Work Group includes members of aircraft engine manufacturers as well as other government agencies which benefits the project to acquire liquid fuel atomization data relevant to industry and next generation aircraft engine design. The project is also benefiting from some NASA funding supporting the design and delivery of non-proprietary fuel injectors for low pressure-temperature conditions and high pressure-temperature conditions. The National Renewable Energy Laboratory (NREL) testing of properties at higher pressure and temperature conditions will benefit the future CFD modeling of the testing at higher pressures and temperatures, as well as providing confidence in the lower pressure-temperature condition properties for current experiments. The real fluid modeling is a challenging area and experiments at higher pressure-temperature conditions with Jet-A and SAF being conducted by other DORMA projects may provide additional opportunities for validating the real fluid models being developed under this project. One example is the injection of Jet-A and SAF into higher pressure-temperature conditions performed in Sandia's constant volume rig.

Reviewer 2

Argonne leads the effort, performing experiments and simulations. The project relies on several partners across industry, government, and academia, for specific tasks, such as the design and fabrication of atomizers (Woodward) and the generation of fuel properties data (NREL).

Reviewer 3

The PIs are collaborating with a number of entities on this effort. This includes industry, national laboratories, and a university. The reviewer commented that there appears to be very specific contributions from each collaborator which is contributing to the success of this effort. The reviewer did not see the need for any more collaboration.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The project has a logical and achievable plan to complete the Phase I testing, analysis, and supporting CFD simulations. The project is also making good progress on developing capabilities for Phase 2 (60 atm, 25°C) testing and will have realistic non-proprietary injectors for that testing. The real fluid modeling has a reasonable plan to transition from existing cubic equations of state methods to a machine learning-based model. The largest benefit of this project is likely to occur if the project reaches Phase 3 (60 atm, 700°C) testing, but that goal may be outside of the current scope of this DORMA project unless funding outside of DORMA is provided. The unique spray atomization (or transcritical behavior, if that occurs) data collected very near the fuel nozzle exit at Phase 3 conditions for realistic injector designs is likely to provide new insights and validation data for fuel injection and atomization or transition to supercritical behavior for both Jet-A and SAF.

Reviewer 2

The proposed future work is well-defined and has a high likelihood of success. The investigators will first work on image processing for quantitative data, performing simulations on as-built atomizer geometry, and improving fluid models through FY 2025. Future phases of the project will expand beyond ambient gas conditions to higher temperatures and pressures in both experiments and simulations. A wider range of different SAF candidates will be investigated in a wider range of flow geometries.

Reviewer 3

The PIs have provided a comprehensive list of future research plans including experiments and simulations at elevated conditions of pressures and temperatures. These future proposed efforts are directly in line with the goals of the proposed research effort. The reviewer would strongly recommend adding a detailed investigation of any asymmetry effects to this list as the asymmetry would influence downstream mixing and combustion processes. Another item the reviewer would urge the PIs to consider is to add diagnostics for atomization and mixing as much as is allowed in the experimental setup. The reviewer commented that characterizing mixing quantitatively would yield very valuable information for the community.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The atomization of liquid fuels directly impacts the combustor operability and emissions since it directly impacts the location and uniformity of the fuel-air mixing. The X-ray phase contrast data very near the fuel nozzle exits provides unique data sets for improved modeling and understanding of the fuel atomization process. The most relevant testing and modeling will be at the higher pressure and temperature conditions where atomization for realistic injector designs is lacking, especially in publicly available sources. Additionally, the reviewer noted that comparisons of the atomization of Jet-A and SAF at higher pressure and temperature conditions were also lacking. In terms of real fluid modeling at higher pressures and temperatures, there are many approaches in the open literature for both ground-based and aircraft gas turbine combustor applications. The real fluid modeling developed in this project does add to the existing research. The big challenge is validating such real fluid models for realistic conditions, flow fields (or injectors) and relevant fuels (such as Jet-A and SAF). This project can potentially provide such validation data if Phase 3 testing is completed.

Reviewer 2

This project attempts to solve a problem that is key to SAF performance: understanding fuel-air mixing processes. The investigators do an excellent job explaining how X-ray diagnostics will bring about this understanding, promoting 100% SAF adoption, leading to economic and environmental benefits in the aviation industry. The reviewer stated that the project was very relevant to VTO objectives.

Reviewer 3

The project and its deliverables absolutely support the objectives of the DORMA subprogram. Spray atomization and mixing significantly affect the combustion and emissions processes. Results generated from this effort which is fine tuned for operating conditions as relevant to real engine operation will provide a wealth of knowledge for researchers. Particularly the early spray morphology and effects of nozzle internal geometry are significant inputs generated by the X-ray imaging technique. The effort to develop a model to incorporate real fuel effects at transcritical conditions and make it available to researchers is very notable. The strong collaboration with industry and NASA is very noteworthy and will ensure the results of this work are of high practical relevance.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

There are sufficient resources to complete Phase 1 and Phase 2 testing, data analysis and CFD simulations of those experiments, and sufficient resources for the development of real fluid models. The reviewer commented that it is uncertain whether there will be sufficient resources for the Phase 3 (60 atm, 700°C) experiments which may have the largest impact liquid fuel atomization modeling for Jet-A and SAF.

Reviewer 2

The excellent experimental and simulation results that this project has so far produced demonstrate that the investigators have all the required resources to execute the planned work. The reviewer commented that project milestones are very likely to be completed on time. The budget for this project is expensive but this expense is well-justified by the X-ray diagnostic results.

Reviewer 3

The reviewer said resources, including physical and financial resources as well as collaborative support, seemed sufficient.

Presentation Number: DORMA020
Presentation Title: Sustainable Aviation Fuel (SAF) Contrail Modeling
Principal Investigator: Matt McNenly, Lawrence Livermore National Laboratory

Presenter

Matt McNenly, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

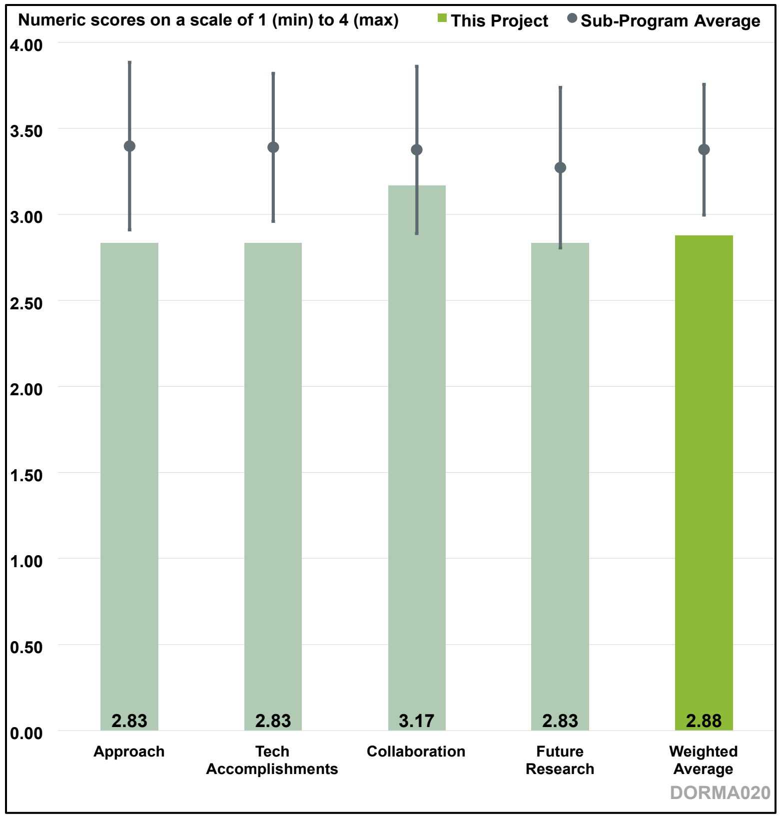

Figure 3-15. Presentation Number: DORMA020 Presentation Title: Sustainable Aviation Fuel (SAF) Contrail Modeling Principal Investigator: Matt McNenly, Lawrence Livermore National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

There are two barriers identified, the first of which is extremely vague so that any project in the general area might be sufficient. The second is much better, although very challenging. The researchers have identified critical work on understanding causes of hydrophobic and hydrophilic properties of soot as well as soot shape and surface chemistry as phenomena to be examined.

Reviewer 2

The project demonstrates DOE’s strong expertise related to fuel chemistry and impacts on particle emissions. Contrails form on aircraft engine exhaust particles, and the project will connect the fuel-soot model to contrail formation via a microphysical model. It is currently thought that contrail cirrus clouds have a climate impact that is comparable to the cumulative emissions of aviation CO_2. This is an important research topic, and the project demonstrates a clear understanding of the motivation for the work.

Reviewer 3

The project outlines the two key technical barriers being addressed: insufficient data and tools for SAF performance metrics and SAF effect on contrail formation. While the proposal outlines milestones to FY 2024, the documentation indicates the project's anticipated end of FY 2027. The reviewer said it was unclear what the FY 2025-FY 2027 milestones are or what research goals are anticipated. The reviewer also said It was not clear how the planned milestones will be expanded for the variety of SAF pathways. The broad variability of SAF pathways require modeling and data for more than Jet-A and the C-1 fuel of the NJFCP. The proposed future research does not include a plan to address the still present barrier of lack of experimental data for analysis, as identified by the presentation.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The application of ab-initio molecular dynamic simulations to analyze the hydrophilic character of (flat) graphene sheets with defects based on different functional groups is interesting and is a good fundamental contribution to science. The results of this theoretical work will need to be extended to soot particles, with agglomerated structures and curved surfaces. The microscale phase field modeling for ice crystal formation is a good development and should be useful in subsequent modeling of contrail evolution. Insufficient details of the Zero order Reaction Kinetics (Zero-RK) model were provided to assess its ability to model the ice nucleation and cloud models, nor compare/contrast its advantages with respect to other possible approaches.

Reviewer 2

The reviewer said the project appears to be on track to complete the major milestones on time. Fuel chemistry accomplishments to date are excellent; however, the bulk of the contrail modeling heavy lifting remains to be done. The reviewer also said it was important that the project team connect with an atmospheric science/cloud physics subject matter expert early in this process to ensure that the contrail modeling approach is realistic.

Reviewer 3

The project notes that work is mostly on track, with one delay for the testing of the coupled multi-scale ice nucleation model. The project activities and accomplishments thus far are key fundamental experimental and simulation efforts that will serve as foundational starting points for subsequent work. The work will need to demonstrate its ability to integrate these early results into more applicable tools that can be validated with real world data. Otherwise, this work runs the risk of being limited to a purely theoretical exercise with no ability to inform the direction of SAF development or contrail mitigation.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer commented that the collaborations and contributions from other DOE funded groups seem well established, but the predicted sooting levels as shown in the back-up slides seem to be for fuel components of gasoline fuels rather than for SAF, perhaps suggesting that the coordination with collaborators is not sufficient. The Computational Chemistry Consortium (C3) is a great resource, and such interactions certainly should be continued.

Reviewer 2

The reviewer stated that the collaboration and coordination at Lawrence Livermore National Laboratory (LLNL) and with outside institutions seems strong. The team has a strong skill set regarding turbulent reacting flows, kinetics, and soot formation; however, there is not an obvious collaborator with expertise in plume-scale contrail or atmospheric modeling.

Reviewer 3

The effort highlights the project team members and their contributions across the various tasks. The extent of the collaboration could be further explained by highlighting specific contributors on the relevant slides where the work is shown. Otherwise, the extent of collaboration was not fully apparent to the reviewer.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The description of the high-level objectives is good, but there are many pieces to come together to make all of this happen. The research direction might benefit from an analysis estimating the impact of different timescales (of the short-term nucleation processes for emissions from different fuels) on the longer-term climate forcing from the entire lifetime of the plume. These timescales are likely a function of local conditions (humidity, altitude, pressure, etc.) as well as soot particle size, structure and character, and probably variable, but ought to help focus future research efforts to the most critical needs.

Reviewer 2

Future work will focus heavily on connecting the modeled soot particle size distribution and properties to ice nucleating properties. This is an interesting research question with climate-relevant importance via natural cirrus formation pathways; however, the relevance of ice nucleation to contrail formation was not clear to the reviewer. Typically, contrail formation occurs in a two-step process within less than 1 second after leaving the engine exhaust plane. In the first step, the plume mixes with the atmosphere, which cools and dilutes the exhaust species. If, along this mixing line, the plume exceeds saturation with respect to liquid water, then liquid water will condense onto the soot and/or volatile particles forming small water droplets (the so-called Schmidt-Appleman criterion). Then, it is thought that these water droplets freeze homogeneously to form ice crystals that are sometimes assumed to be spherical or droxtal. Thus, the ice nucleating properties of the emitted particle are not relevant to near-field contrail formation. However, these emitted soot particles can influence the formation of natural cirrus clouds via traditional heterogeneous ice nucleation pathways, and it has recently been suggested that aviation soot might even have a climate-cooling impact by serving as ice nucleating particles and suppressing homogeneous nucleation in natural cirrus (this is highly speculative and uncertain!). Consequently, the ice nucleating properties of realistic aviation soot (less than 30 nm diameter) are relevant to answering these downstream aerosol-cloud interactions questions (even if the role of soot as ice nucleating particles is not relevant for direct contrail cirrus formation). There are also interesting questions that the model could be used to answer regarding the role of fuel sulfur and surface oxygenation in making the aviation soot particles hydrophilic/hydrophobic, which might be relevant for the early contrail water condensation process. In sum, the future potential of the model is significant for addressing important questions related to SAF and cloud formation. The project would benefit from including collaborators with atmospheric science and/or contrail modeling expertise to complement the outstanding DOE fuel combustion modeling expertise.

Reviewer 3

The project clearly outlines the future work but lacks defining the purpose of the future work in addressing the technical barriers. The reviewer stated it was likely that the work will be able to achieve the targets it has set for proposed future research. However, clearer connections between the proposed future research and the broader research objectives are needed.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The embedded links appear outdated, but the work is fully consistent for the SAF Grand Challenge Roadmap.

Reviewer 2

The project is highly relevant to VTO. SAFs are a cornerstone of future aviation industry efforts to mitigate environmental impacts. The fundamental research outlined within this project represents an end-to-end approach linking fuels to combustion modeling to emissions modeling to contrail modeling.

Reviewer 3

The project is relevant but could be improved with a clear plan to ensure the applicability of the final work. This requires more robust data resources to validate the work to a more varied set of fuel types. It was not clear to the reviewer where the project fits under the VTO subprogram objectives.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

Based on the progress thus far (in two years) which seems to be more on the fundamental side, the team will need to start exploring modeling complications and data needs for validation and extension to practical concerns. The remaining timeframe (three years is reasonable) ought to be sufficient to (at least partially) achieve the stated goals assuming funding support for this and aligned projects are sustained.

Reviewer 2

The reviewer stated that the project resources appeared to be commensurate with the proposed effort.

Reviewer 3

The project notes that there are research collaborators across a multidisciplinary team. The team resources seem sufficient to meet stated milestones. The reviewer said it was important that the team does additional work with and beyond the current team to gather sufficient experimental data on SAF fuels for adequate model validation.

Presentation Number: DORMA021
Presentation Title: Simultaneous Greenhouse Gas and Criteria Pollutants Emissions Reduction for Off-Road Powertrains
Principal Investigator: James McCarthy, Eaton

Presenter

James McCarthy, Eaton

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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

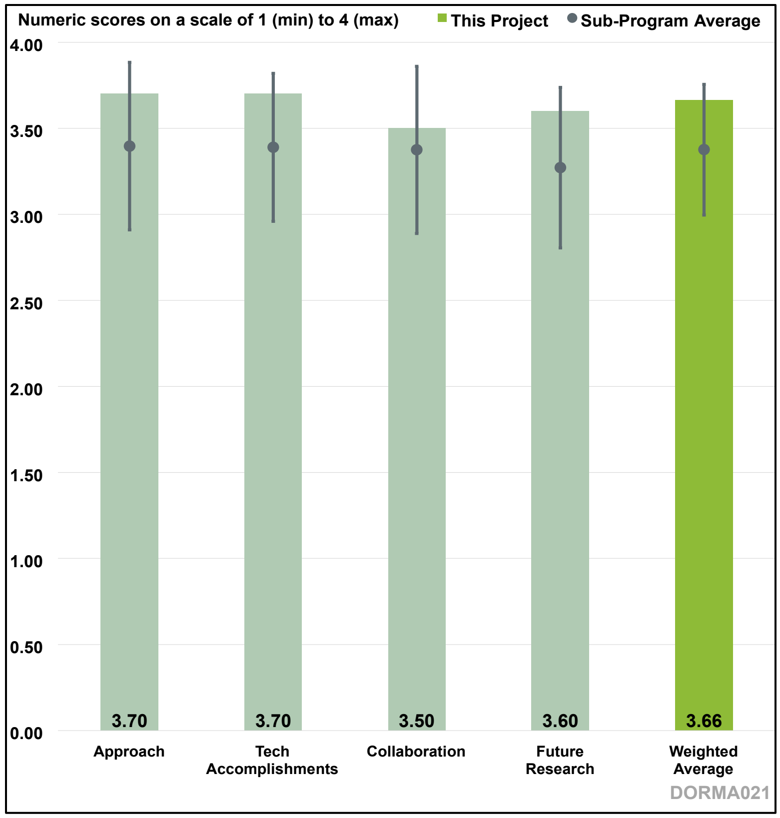

Figure 3-16. Presentation Number: DORMA021 Presentation Title: Simultaneous Greenhouse Gas and Criteria Pollutants Emissions Reduction for Off-Road Powertrains Principal Investigator: James McCarthy, Eaton

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The NO_x and GHG emissions from diesel engines are the two barriers determining the future of the diesel engine in on-road and off-road applications. This project is well designed. The timeline is well planned. The testing schedule is very tight but the reviewer was confident team would make it. The test work proposed for ORNL may be challenging with the unit DOE lab environment in consideration, but the reviewer is sure this team has had a plan in mind if ORNL has difficulty in completing the research work assigned as scheduled.

Reviewer 2

The reviewer commented that the presentation was excellent, explanations were clear, descriptions were detailed, and overall, really nice. The review suggested following the review format (look at ORNL presentations as an example) to make it a little easier on reviewers. The approach to achieve the project goals is solid and on a reasonable time scale. The project schedule is reasonable and on track and there is a strong plan for multiple publications (which is fantastic and not something most PIs plan).

Reviewer 3

The project clearly addresses technical barriers related to the development of next-generation, high efficiency off-road engines. The desire to develop modular aftertreatment systems means focusing on single path scenarios is a necessity. While modest CO_2 reduction is targeted, significant NO_x breakdown is a goal. Importantly, it is also a target to quantify NO_x and GHG emissions in the systems, effectively establishing baselines for these engine of the future scenarios. As there are no current standards, this is a key part of the effort to further set the stage for the field.

Reviewer 4

The project has a very comprehensive approach toward improving efficiency and reducing emissions. There is good characterization of the varying duty cycles of the different agricultural tractor uses. The reviewer said multiple aftertreatment approaches were being considered.

Reviewer 5

The reviewer said the overall technical strategy was sound. The team is implementing the plan accordingly and reference data have been generated.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

This team has made significant progress in project deliverable as demonstrated in the presentation. The work prosed for Budget Period 1 (BP1) has been completed as planned.

Reviewer 2

The reviewer stated there was strong progress in both BP1 (the focus of this review) with the first paper presented at SAE WCX 2024, and into BP2. Even the baseline engine emissions were below Tier 4. The comparison between the on-road and off-road low load cycles was particularly interesting.

Reviewer 3

In general, the structure of the effort is very logical and rationally guided. In the first work period, a design and testbed build phase was completed, followed by testing in the current phase, and ending with an optimized demo build testing various aftertreatment configurations. The presenter mentioned a no cost extension for a few months will likely be requested to complete the project. Milestones generally seem to be on track, with a configuration already in hand that seems promising to make the 10% CO_2, 90% NO_x targets. The team has a clear trajectory to the Budget Period 2 (BP2) go/no-go point. The reviewer appreciated the detailed project schedule and the goal to have multiple publications result from the effort. The reviewer stated it was important to disseminate the information from the testing to establish the gold standard for quantifying the emissions in these systems. The work seems carefully done, with baseline CO_2 correctly considered. Mitigation efforts are well considered and potential issues impacting the work are adequately anticipated. The aftertreatment configurations pursued seem logical and will provide valuable data for various scenarios. This can be a good way to leverage and connect on-road and off-road data for researchers. The reviewer appreciated the cost model comparison toward the end of the presentation as it provided some idea of the scale of costs for both engine systems. While the reviewer thought lining up the five additional publications is a great way to extend the potential impact of the studies to the broader community, some more detail on these later in the presentation would have been nice, just to provide a little more detail on the topics and demonstrating the community value.

Reviewer 4

The project has done a good job mapping out the potential of the various components going into the efficiency gains as well as the aftertreatment configurations for NO_x reduction. The reviewer commented that the cost analysis was good to see, but difficult to evaluate without disclosing the baseline numbers.

Reviewer 5

Baseline emission data shown on Slide 11 does not include engine out NO_x, while emission data shown on Slide 16 does. The reviewer questioned if the indent of researchers was to keep the engine out NO_x the same for comparison of GHG with the “future” engine. The review said it appeared to create confusion with the EGR pump reducing “NO_x by 33%” from 9-6 g/kWh. It was not clear to the reviewer what the stock engine CO_2 grams per kilowatt-hour was. For the emission data shown on Slide 16 with aftertreatment (AT), the researchers did not state if the AT is the stock production configuration of diesel oxidation catalyst (DOC)-SCR. The reviewer also recommended researchers elaborate if an EGR cooler is installed or the EGR pump is meant to function as “hot EGR” without a cooler. If possible, the reviewer would encourage the team to report engine CO_2 and CO_2 from diesel exhaust fluid (DEF) moving forward. Reducing engine out NO_x requires less DEF therefore less CO_2 from DEF. For the “future” engine emission results without AT on Slide 16, PM emissions are 0.4 g/kWh which is very high. The reviewer suggests double checking the result. No explanation was provided on differences of cycle work when tested at Southwest Research Institute (SwRI) vs. ORNL (Slide 16). The reviewer commented that a comparison of torque curves of baseline versus “future” engine would have been useful or there may be a lab-to-lab variation. Slide 21 appears to have an error of about “>=90% lower GHG.”

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

This team has a well-organized collaboration consisting of Eaton, SwRi, Fiat, ORNL, and Tenneco. The hardware needed for this project has been made available. The inclusion of industry partners such as the Fiat Powertrain (FPT) in this project is significant. The reviewer is sure SwRI has made significant contribution in technology development beyond test work.

Reviewer 2

The reviewer stated there was strong collaborations with Fiat, ORNL, Tenneco, and SwRI but would have liked to seen university participation.

Reviewer 3

Overall, the team is comprised of a diverse set of entities that bring singular skill sets to the project. Given the many moving parts in a project like this, it is obvious that experts in engines and their optimization, catalyst testing, and aftertreatment are needed. The partners from the various companies and the national lab group bring these needed skills and appear to be working together well to complete the various milestones in a timely manner.

Reviewer 4

The reviewer said the project team seems to have all the relevant aspects of the project covered. The reviewer also said It was difficult to tell specifically what the contributions were from Fiat, however, engine testing was clear between SwRI and ORNL.

Reviewer 5

The report reflects strong collaboration among team members for hardware design, controls, tests, and cost analysis. The project has a very broad scope with many variables. The reviewer stated to keep up the good work and collaborations.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The project has clearly defined the purpose of future work. With the deliverable completed in BP1 and the work proposed in BP2, the reviewer is confident that the future work will highly likely achieve the goal of this project.

Reviewer 2

The future work for BP2 seems reasonable, but what earns this project the score of outstanding is the recognition that the BP3 plans may need to be revisited based on the data.

Reviewer 3

The path forward for the project is clear with a series of aftertreatment configurations needing to be tested, the results disseminated in the publications to some degree, and an optimized system tested and further tuned. There appear to be no major hurdles at this stage to completing the work in BP2 and BP3.

Reviewer 4

The team seems confident that the go/no-go target for BP2 will be achieved, however, it seems the BP3 goal may need some re-direction to achieve.

Reviewer 5

The reviewer was concerned on time/resource of testing different configurations and recommended the team to consider simulations moving forward. For cost analysis, the reviewer recommended the team show a boundary diagram with what is included in the analysis and what is out of scope. For example, the reviewer questioned if a 48 V electrical system or a battery was included in the cost analysis. The predicted cost reduction of -6.7% with added aftertreatment content of a diesel particulate filter (DPF), dual dosing, e-heater to a stock production system DOC-SCR appeared to be optimistic to the reviewer and recommended further cost refinement.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This project is closely relevant to advanced engine and fuel technologies, and it supports the overall VTO subprogram objectives in NO_x and GHG reductions.

Reviewer 2

The review commented that the project is relevant to VTO goals.

Reviewer 3

The project goals and approach are well-aligned with VTO interests in developing new engine and exhaust configurations for off-road applications that reduce GHG emissions and keep NO_x conversion high. Beyond the information on the new systems, the careful baselining of multiple configurations is of value to the research community.

Reviewer 4

A 10% GHG reduction and a 90% NO_x reduction does fit the VTO objectives. The reviewer suggested modifying the GHG reduction goal to get closer to 50% for more relevance towards the U.S. National Blueprint for Transportation Decarbonization.

Reviewer 5

The project addressed both CO_2 and emission reductions. The project further considers the CO_{2eq} contribution of nitrous oxide (N_2O) and CH_4 and feasibilities of meeting them individually. They are aligned with California Air Resources Board (CARB) Tier 5 regulations which has limits for N_2O and CH_4. This team is thinking very comprehensively including future emission regulations.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

With strong support from FPT, SwRI and ORNL, this project has excessive resources for them to complete the research work proposed. The reviewer felt that this project was under-budgeted, this team may have spent more money or has more hardware support from their partners.

Reviewer 2

The reviewer said the project has sufficient resources.

Reviewer 3

Given the diverse skill sets of the partners and that they cover all the areas needed to develop the engine and aftertreatment configurations and test them fully, all needed resources were present.

Reviewer 4

The reviewer stated that the resources seemed appropriate for a project that does not require a machine demonstration.

Reviewer 5

The reviewer was concerned on the team's ability to test all hardware combinations which would further include calibration optimizations.

Presentation Number: DORMA022
Presentation Title: Development of a Flex-Fuel Mixing Controlled Combustion System for Gasoline/Ethanol Blends Enabled by Prechamber Ignition
Principal Investigator: Adam Dempsey, Marquette University

Presenter

Adam Dempsey, Marquette University

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

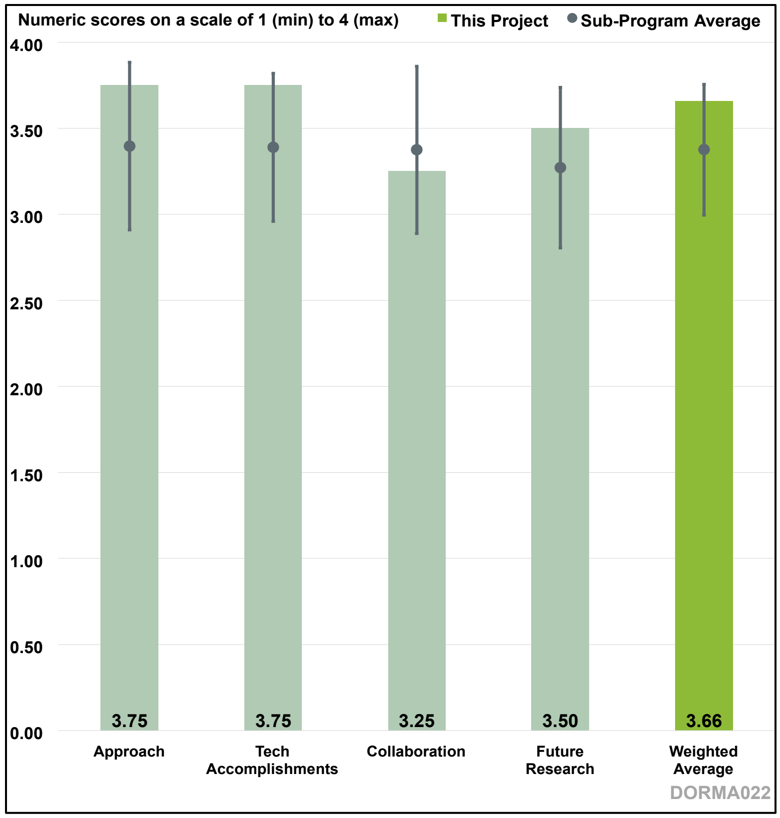

Figure 3-17. Presentation Number: DORMA022 Presentation Title: Development of a Flex-Fuel Mixing Controlled Combustion System for Gasoline/Ethanol Blends Enabled by Prechamber Ignition Principal Investigator: Adam Dempsey, Marquette University

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer said this is a well laid out project in which the tasks are being executed as planned. The modeling tasks are clearly being used to guide the design and implementation. Moving from modeling to single-cylinder experiments to multi-cylinder experiments is the right level of scale-up and design. The fact that the prechamber system is operating as predicted by the modeling is a major success for the project team.

Reviewer 2

The project addresses key questions and barriers linked to prechamber ignition. The project is also designed well to address translating the engine design from a low technology readiness level (TRL concept to higher TRL. The analysis of cylinder head fatigue is a great approach to address applicability of technology in a production environment. The intended total cost of ownership (TCO) assessment tasks were also important for commercial acceptance of the technology.

Reviewer 3

This project has a well thought out approach, starting with the modeling, single-cylinder engine, and validation with the multi-cylinder engine. The reviewer was unclear on how the CFD modeling of the rapid compression machine (RCM) fit in for mechanism and surrogate selection and that the timeline seemed to indicate that work would be part of this review period.

Reviewer 4

The reviewed commented that the research was outstanding on ethanol prechamber enabled mixing-controlled combustion (PC-MCC) combustion. The reviewer said CFD modeling and single-cylinder engine testing was very good and that the results have been analyzed and presented in a very good format. This project is very well designed and is important in reducing GHG emissions.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project team is collecting experimental results from custom hardware and the design and implementation of the custom hardware was guided by the modeling studies conducted early in the project and function as expected. The reviewer said this demonstrates that the project is answering the technical questions that are needed to develop this combustion strategy to implementation. The studies being conducted have both a scientific curiosity component and are pragmatic. For instance, the approach taken to understand the effect of equivalence ratio on prechamber stability laid out the tradeoffs that one could expect in a much better way than had been seen before. Thus, the reviewer's understanding of this effect is greatly improved, as is the practical nature of what needs to be done from an engine operation standpoint.

Reviewer 2

The completion of CFD modeling for the design and combustion strategy development has been conducted in a timely manner and the results are very promising. Fabricating the prechamber components is a key milestone of the project as it is a very critical element of combustion control. The start of single-cylinder testing is also an impressive accomplishment. The reviewer was not clear on the combustion stability with PC-MCC combustion in 98% ethanol, 2% gasoline (E98) fuel or what the IMEP comparison between -20° and +4° spark was for PC-MCC.

Reviewer 3

This project team has made quite a lot of progress and a large number of accomplishments. The team showed great results demonstrating the benefit of prechamber over conventional spark ignition.

Reviewer 4

The reviewer commented that there was great progress on CFD modeling, single-cylinder engine testing, and analysis.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project team includes a second university (University of Wisconsin-Madison [UW-Madison]), an off-road OEM (John Deere), as well as Clear Flame Engines and Missouri Corn Merchandising Council. Thus, there is good representation across a spectrum of perspectives. However, the project seems to be driven by Marquette with relatively minor contributions from the other stakeholders. For instance, it was not clear to the reviewer what Clear Flame Engine is bringing to the project other than serving as a location to test the multi-cylinder engine. However, more collaboration may not be necessary to accomplish the project goals.

Reviewer 2

The presentation did not clearly mention the coordination process and specific tasks accomplished by the various partners. Project partners that include MAHLE and John Deere are excellent, but the reviewer noted specific inputs provided by these partnerships would be useful.

Reviewer 3

It was not clear to the reviewer how the UW-Madison task is linked in with regard to the surface temperature measurements. The reviewer said it appears to be an experimental task, but it was not clear what engine is being used or if it was the same CAT C9. The reviewer also questioned what differences there will be in moving to the John Deere 9.0-liter platform.

Reviewer 4

The reviewer commented that the overall results show good collaboration between project team members.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The future proposed research consists of additional single-cylinder engine experiments at higher load and then moving the concept to a multi-cylinder engine with heavy involvement from an OEM. This is the right development path to be able to introduce a new technology and have an impact on the industry in a short timeframe.

Reviewer 2

The future tasks planned are highly relevant and provide a complete overview of the pros and cons of this strategy.

Reviewer 3

The reviewer was not clear on whether the validation tests were planned to be done only on a dynamometer or in a vehicle (Clear Flame Engines). The reviewer noted some of the connections between tasks got lost in the presentation.

Reviewer 4

The reviewer stated there were clear targets on future research tasks including multi-cylinder engine testing and technology assessment.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This project is directly aimed at off-road decarbonization by enabling the use of a low carbon fuel in compression ignition engines.

Reviewer 2

This project addresses a highly relevant topic of using low lifecycle GHG fuels in existing engine platforms. The modifications of existing engine architecture to prechamber to maximize the efficiency is a novel approach and the project is well designed to address critical barriers.

Reviewer 3

The project is a nice demonstration of lowering the carbon intensity using mostly conventional engine technology.

Reviewer 4

The project is clearly relevant by supporting VTO objectives in reducing CO_2 emissions for off-road vehicles.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said the project appears to be well-resourced and on-track. There is no evidence of a lack of resources, nor is there any evidence of an overabundance of resources.

Reviewer 2

The reviewer commented that academia and industry collaboration provided the necessary resources for the project.

Reviewer 3

This team is getting great output at the current funding level.

Reviewer 4

The reviewer stated the project seems to have sufficient resources for completing required tasks and project plans.

Presentation Number: DORMA025
Presentation Title: Fully Electric Powered Hydraulic Assisted Compact Track Loader
Principal Investigator: Perry Li, University of Minnesota

Presenter

Perry Li, University of Minnesota

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

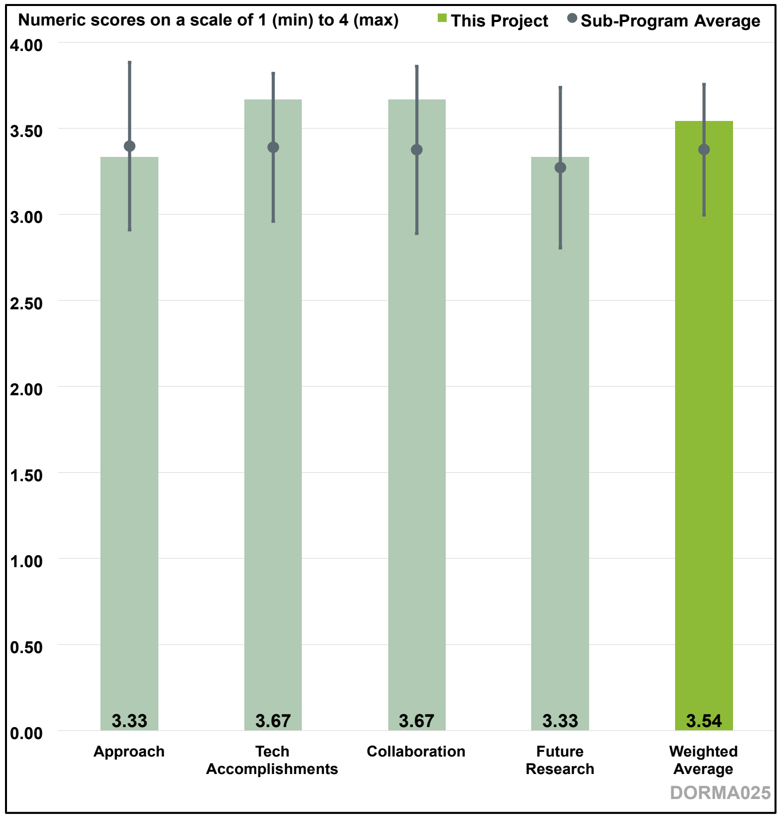

Figure 3-18. Presentation Number: DORMA025 Presentation Title: Fully Electric Powered Hydraulic Assisted Compact Track Loader Principal Investigator: Perry Li, University of Minnesota

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The overall effort in designing the hybrid hydraulic-electric architecture system and overcoming technical challenges compared to the baseline track loader is good.

Reviewer 2

The project shows all around fantastic work. The project is well-designed, and the timeline is reasonably planned. The reviewer appreciated the novelty of this technology and due diligence by the investigators with regards to the implementation in compact construction equipment. The critical commercialization challenges with regards to battery size selection to reflect realistic customer duty cycles, controllability of the switching digital displacement pump, and scalability of this technology are being investigated in a comprehensive and well thought out manner. The reviewer also said the project was well done.

Reviewer 3

The approach of this project is to selectively improve off-road electrification efficiency by significantly improving the hydraulic portion of the vehicle by maximizing the effectiveness of the electrification. This approach makes a lot of sense and has already demonstrated significant improvement in improving the electrification efficiency of the vehicle by essentially doubling the battery in-use time from 1-2 hours to 3-4 hours. The project uses advanced hydraulic valves and an advanced control scheme algorithm to optimize the ability of the vehicle to adapt to real-time changes in vehicle operation and use. This is an important aspect to this project. There is uncertainty that the in-use operation of a typical 75 kWh battery will ever reach the desired 8+ hours, which is a major challenge in electrifying this market segment. At the moment, there is no engine-hybridization option being explored. There is risk that even if the project is very successful, the end-goal of a “day’s work” using only the battery as energy storage may not be achieved. There may be some merit in exploring additional differentiation between the work circuit and the propel circuit and their relative power and energy sources.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project showed good progress on improving energy efficiency over e-motor replacement design.

Reviewer 2

The technical progress that has been made compared to the project plan has been impressive from the baseline machine performance testing, estimation of energy saving potential and battery charge duration, feasibility evaluation of alternate electric assist approach, construction of laboratory work circuit and propel testbed, real-time rail-selection and rail-filling algorithm, rail-switching loss minimization and component sizing, as well as sourcing for the demo machine. The reviewer encouraged the PI to keep up the good work. The reviewer looks forward to the results from the demo machine.

Reviewer 3

Effectively doubling the in-use time of the battery is a significant achievement. The novel approach has allowed for significant technical progress to occur. Additional work on the control scheme and further investigating the external assistance scheme (as shown in the presentation as external levers/linkages driven by the e-motor), in addition to the hydraulic pump assistance is a good idea.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer commented that all members of the project team seem to work together effectively.

Reviewer 2

The reviewer said the collaboration and coordination between the partners which include academia, OEM, and critical component suppliers are well documented.

Reviewer 3

There are excellent partners in this project. CNH is an OEM that has provided significant access to their machines and test facility. Parker and Danfoss are industry leaders in hydraulic technology. The University of Minnesota has shown to be a leader in controls and hydraulic actuation technologies.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

Base goals are listed in the future research slide. The reviewer suggests adding one or two stretch goals to further improve battery life compared to a diesel compact track loader.

Reviewer 2

The proposed future research is reasonable with clearly defined purpose and the investigators are very likely to achieve the project targets based on the consistent progress that has been made on this project over the years.

Reviewer 3

Future work aims to improve efficiency further by improving valve switching speed and reducing pressure losses. This should provide assistance in additional improvement in energy efficiency. However, these improvements alone are not likely to result in an additional “doubling” of battery in-use run time, from 3-4 hours to 6-8 hours which is the desired outcome.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said this project is extremely relevant to improving efficiency and CO_2 reductions of off-road tracked vehicles.

Reviewer 2

The project introduces a novel architecture to address cost and power density challenges with electrification of off-highway equipment which supports the overall VTO subprogram objectives for decarbonization of difficult-to-electrify sectors.

Reviewer 3

This project definitely supports the DOE goal of improving energy efficiency of off-road vehicles and decarbonization of same. The technical progress is quite good to this point. This type of optimization work will be applicable to a variety of off-road technologies. The primary concern of the reviewer is that the scale of operating the vehicle on the battery is still too low to really be impactful in this marketplace. Either additional battery capacity would need to be explored, or the possibility of a downsized engine hybrid mixed with the electrical system may need to be explored.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer commented that the resources seem to be sufficient in meeting project targets and timeline.

Reviewer 2

The project is on track to meet the milestones outlined in the project scope with the current funding levels.

Reviewer 3

The resources allocated to this project appear to be sufficient to support achieving the target goals.

Presentation Number: DORMA026
Presentation Title: Articulated Dump Truck (ADT) Electrification—Greenhouse Gas Reductions and Commercialization of New Technology
Principal Investigator: Brij Singh, John Deere

Presenter

Brij Singh, John Deere

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

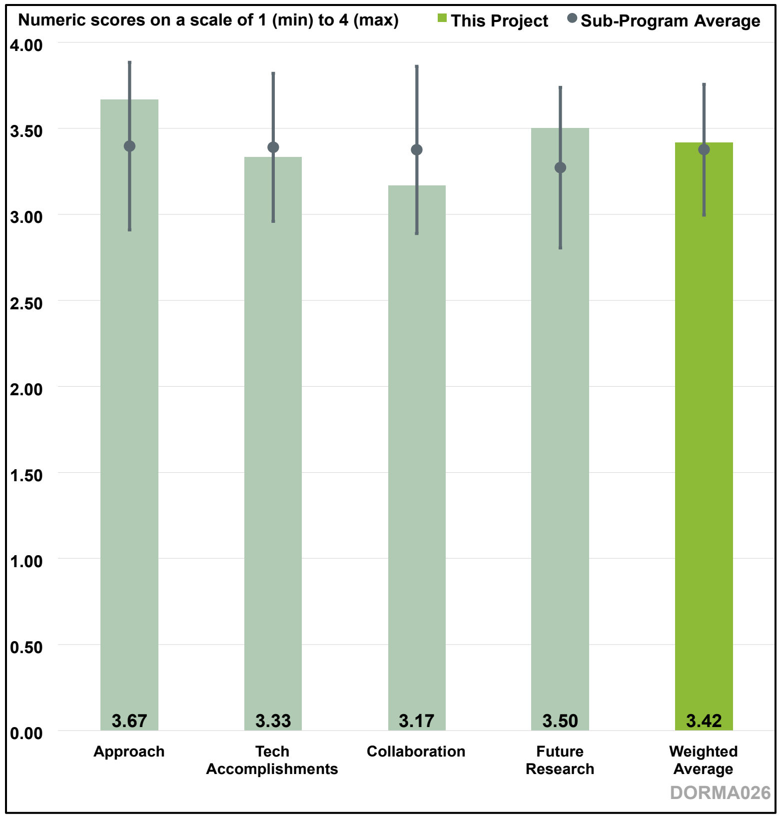

Figure 3-19. Presentation Number: DORMA026 Presentation Title: Articulated Dump Truck (ADT) Electrification—Greenhouse Gas Reductions and Commercialization of New Technology Principal Investigator: Brij Singh, John Deere

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

This project is sharply focused on vehicle-level integration to achieve a diesel-hybrid (electrified diesel) ADT in order to reduce the GHG emissions associated with the large (78%) idle times experienced by the vehicle. Eliminating ADT idling is challenging, as it requires replacing the conventional hydrostatic drivetrain with a diesel-electric hybrid powertrain, which does not currently exist, and make the design shock-proof for the rugged environment. To create this novel diesel-electric hybrid (which has further application beyond just the ADT) requires integration of a silicon carbide (SiC) inverter, SiC non-isolated direct current-to-direct current (DC-DC) converter, SiC/SI isolated DC-DC converter and a battery pack in order to accomplish a dual path for power flow between the downsized engine and traction system. To accomplish this, the team is making use of dynamic system modeling to represent the ADT test bed drivetrain, optimizing the design of both power inverters, doing a life assessment of the 700 V Li-ion battery pack, doing durability analysis of the new hybrid ADT powertrain, and defining the specifications for the necessary power electronic components. This process is well-designed to accomplish the project goals. By taking a pre-existing production vehicle and designing the electrified ADT architecture to integrate into the existing system, the project team are leveraging past work and not spending excessive timing designing from the ground up. The reviewer said while this might cause some integration challenges, it seems like a smart and efficient approach.

Reviewer 2

The reviewer commented that in Budget Period 1, concentrating on identifying the components needed for the powertrain with a focus on the shortcomings of available inverters is a sound approach.

Reviewer 3

The reviewer stated the approach is sound by using a downsized engine with an electro-assisted infinitely variable transmission and a battery pack. Parallel flow power is also a good approach that optimizes each system based upon power demand. Reaching for technology advances in inverter and DC-DC converter technology is also a favorable aspect to this project. The reviewer noted one uncertainty is that SiC inverter/converter technology will be scalable in time for the project goals and needs. There is a sound backup plan to use conventional insulated-gate bipolar transistor technology if SiC is not ready in time.10 kW SiC machines are a good starting point but not imminently close to the 100 kW or 200 kW SiC inverters that would be preferred. The fact that this work is at a university and not an inverter supplier implies that it is further out technology than imminent. The reviewer said it was a good risk to take, but it is a risk. There is also some slight risk in using nickel manganese cobalt (NMC) cylindrical batteries instead of other chemistries. NMC batteries tend to have shorter cycle lives and tend to need extensive immersion cooling (which is provided here) to operate safely and sensibly. Even though the project partners may not have immediate access to other battery types, it may be worth exploring lithium iron phosphate-based chemistries for cost, cycle life, and reduced cooling demand purposes.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

Despite several reviewer questions, it was not clear how much the success of this project relies on the SiC technology working out. While the team has a backup plan that will allow them to accomplish the overall goal of hybridizing, it is unclear how much that would impact the efficiency or GHGs associated with the project.

Reviewer 2

The reviewer said the project looks good but there still appears to be significant risk on the scaling up of the soft-switched SiC inverter. The reviewer suggested to focus more on making significant progress with that.

Reviewer 3

The project has achieved all relevant milestones for the budget period. The project is on-track to accomplish all the target goals of the project on its current trajectory.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

Each of the university partners has a task to focus on and work closely with Deere on. The reviewer noted that this seems like an excellent way to leverage these resources.

Reviewer 2

The reviewer said it was hard to judge the effort that goes into collaboration within the Deere organization. The universities appear to have well-defined roles and are contributing nicely to the project.

Reviewer 3

The primary participants in the project are different portions of John Deere. There are two universities, the University of Arkansas and North Carolina State University, working on the electrification portions of the project. These universities appear to be making excellent progress in their respective technical areas. However, there is no partner with experience mass-producing inverters and DC-DC converters involved. There is some risk that even if SiC breakthroughs occur, there may not be the right partner involved to capitalize upon those breakthroughs.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer noted there are anticipated challenges.

Reviewer 2

The reviewer commented that it was good to see that the team had identified innovation needs for the inverter technology.

Reviewer 3

John Deere is using an excellent approach to downsizing the engine, providing modest electrification, and pushing inverter/converter technology to improve the efficiency of multiple types of vehicles/devices. This approach is likely to be effective in multiple market segments. The project team has a fallback plan if the SiC technology is not ready by the required time and the overall project goals are highly likely to be accomplished. The reviewer said the future work looks very promising.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The project supports the overall VTO goals for reducing GHG emissions in off-road vehicles.

Reviewer 2

Electrification of the ADT will lead to significant decarbonization since this application has significant energy recovery opportunities under its prevalent duty cycles.

Reviewer 3

This work leverages known benefits of downsizing engines and adding electrification to improve overall vehicle efficiency. This project is very relevant to DOE goals to improve GHG emissions in the off-road sector. The project is using the correct approach and technology suite to help DOE achieve these goals.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The resources for this project seem to be sufficient, though additional DOE investment could help accelerate the timeline of deliverables and the number of pieces of equipment that the novel hybrid system could be applied to.

Reviewer 2

The significant delay in BP1 makes it hard to evaluate the resources but the reviewer assumed that it was not due to lack of funding (Federal or cost share).

Reviewer 3

The resources appear to be sufficient for the project to accomplish the intended goals.

Presentation Number: DORMA027
Presentation Title: Control of aldehyde emissions from alcohol-fueled non-road engines
Principal Investigator: Sreshtha Majumdar, Oak Ridge National Laboratory

Presenter

Sreshtha Majumdar, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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

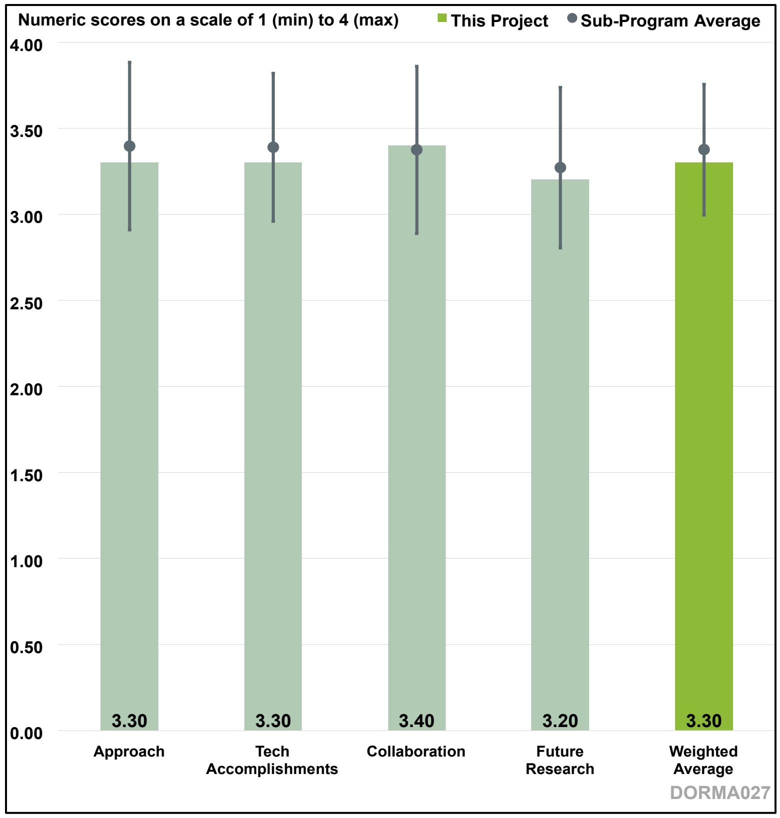

Figure 3-20. Presentation Number: DORMA027 Presentation Title: Control of aldehyde emissions from alcohol-fueled non-road engines Principal Investigator: Sreshtha Majumdar, Oak Ridge National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project clearly addresses obtaining insights into technical barriers associated with partial alcohol oxidation in engines for off-road applications. The need to evaluate aldehyde emissions in particular is made clear from the presentation. Fundamental insight into the nature of these intermediates is key to developing ways to mitigate their formation. In general, the system design to monitor reactivity using advanced infrared methods (diffuse reflectance infrared Fourier transform spectroscopy [DRIFTS]) is appropriate. The reviewer said it was also gratifying to see close interaction with industrial partners to ensure the types of catalysts and conditions used mimic as closely as possible conditions in the real systems.

Reviewer 2

The findings and detailed data on formaldehyde formation from methanol and acetaldehyde formation from ethanol are necessary to look further in how to improve the system. The range of tools used, including DRIFTS, is a very wise plan. The reviewer is hopeful to see the DRIFTS data in a future presentation.

Reviewer 3

The reviewer said that a good range of fuels are being tested and there was a good use of Clean Energy Emission Reduction protocols. The reviewer also said there was a good combination of DRIFTS, flame ionization detection, and Fourier transform infrared (FTIR) spectroscopy for gas analysis and that the development of the aldehyde introduction system was impressive.

Reviewer 4

The project goals include further understanding of LLCF, with a specific interest in MeOH and ethanol (EtOH), reactivity over emissions control catalysts and identification of catalyst formulation to mitigate aldehyde emissions. Upon reviewing the presentations from 2022, 2023, and 2024, the reviewer noted that the technical work appeared exploratory in nature. Clear and measurable goals and therefore the metrics that should help to achieve these goals were not obvious to the reviewer. Going forward, defining success criteria of what it means by “further understanding” and “identification of a catalyst” should be attempted. Specific strategies for identifying alcohol and aldehyde mitigation were not obvious to the reviewer. The reviewer suggested examples including identifying commercial formulations, working with suppliers to develop formulations based on the insights generated, identifying conditions for optimal performance to enable engine-based controls to mitigate the pollutants, or generating quantifiable insights (kinetics) to select right design for the catalyst package/formulation (PGM contents/ratio) etc.

Reviewer 5

This project addresses aldehyde emissions issues from alcohol-fueled engines. Aldehyde emissions is not a new topic as it has been discussed for decades when alcohol research was conducted before 2000. This project is not well-designed. The reviewer noted the research should focus on the methodology mitigating aldehyde emissions other than aldehyde formation in the DOC. The project milestone was also not well-designed. The reviewer stated the milestone should be technical achievement rather than submitting a publication.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

Progress has been significant towards the goals. The equipment and data have been well done to advance for great results in the coming year. The reviewer commented that it will be great to see the paper that will be submitted soon.

Reviewer 2

Commercial DOC technologies were used and oxidation of alcohols and aldehydes were carried out. The reviewer recognized the challenge of handling aldehydes in the lab and how ORNL overcame this hardware challenge. However, from the technical studies that addresses the intent of the project, the presentation did not highlight what was the unique or impactful technical insights that were not already known. From conversion and selectivity data such inhibition signature was not obvious. The reviewer was unclear on what specific data led to the statement “Highly stable acetates or formates on the catalyst during alcohol oxidation can inhibit aldehyde and alcohol oxidation.” The reviewer also noted that this is limited research work to theorize the underpinnings of inhibition. Potential constraints and feasibility of specific solutions derived from this project in overcoming the barriers were not obvious.

Reviewer 3

The project team found that oxygenated fuels unfortunately form stable aldehyde intermediates on the conventional oxidation catalyst formulations which are difficult to get rid of and can block catalyst sites and disrupt activity.

Reviewer 4

The reviewer said milestones appeared to be on track though it would have been good to see metrics from other FYs for reference. The general setup appears well designed, with a flow reactor system that allows testing of a range of catalysts that have been varied in their aging conditions and composition. The reviewer also said it was clear care was taken with replication of experiments and the data presented was top notch. The systems are clearly well characterized and provide reproducible platforms to study these intermediates. The reviewer stated DRIFTS seems like the perfect tool to interrogate surface functionalized organics in the course of the reaction. The reviewer also noted the development of a high part per million formaldehyde delivery system is not a trivial technical accomplishment given the difficulty in handling of the reagent. Examination of the surface species and understanding of their stability under operating conditions will certainly help in the design of next generation catalysts. While the current capabilities are good, there is also a heavy reliance on DRIFTS. The reviewer suggested expanding to other techniques to provide additional information on intermediates or how the catalyst changes over time. In particular, the reviewer noted that imaging of catalysts before and after might be beneficial to understand the impact of the surface intermediates seen by DRIFTS on the catalyst structure (migration of sites in the formulation, etc.). Several presentations on the work were good, though the reviewer questioned listing internal quarterly DOE program updates in this section. The reviewer noted that providing more details on the progress and status of the publication was a missed opportunity.

Reviewer 5

Some progress has been made in characterizing the impact of the current DOC in producing aldehyde and aldehyde oxidation in the DOC at different temperatures. Progress was well aligned with the milestone but the milestone was not well developed. The submission of one paper should not be a milestone assessing the progress of this project.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The collaboration has been mainly limited to discussion, guidance, and assistance. Caterpillar provided the catalyst sample. The new catalyst provided by Johnson Matthey is the key to the success of this project. The reviewer suggested ORNL has further discussions on aldehyde emissions control especially the new catalyst which can oxidize aldehyde at lower temperature.

Reviewer 2

Caterpillar and Johnson Matthey appear to have been excellent partners in that Johnson Matthey provided a catalyst to test and Caterpillar provided focus on the aldehyde formation from alcohols.

Reviewer 3

Collaborations with Caterpillar and Johnson Matthey are good, but the reviewer would have liked to have seen involvement of a university partner or at least summer interns.

Reviewer 4

Overall, the team is comprised of a small but diverse set of entities that bring singular skill sets to the project. ORNL supplies the catalysts and characterization expertise while the two companies provide key insights on aging conditions and catalyst composition to provide the most "real" conditions possible that mimic industrial catalysts. The partners from the various companies and the national lab group bring these needed skills and appear to be working together well to complete the various milestones in a timely manner, given the amount and quality of data provided.

Reviewer 5

The reviewer commented that the partners were relevant. More partners may not be required, however, the reviewer could not tease out their active contributions from the generic statement of "Discussions, guidance and catalyst sample." Listing specific and concise contributions of collaborators will help in better assessing the effectiveness. The reviewer suggested examples such as: Collaborator 1 helped in defining and shaping up specific technical barriers and defined real-world operating conditions based on which relevant evaluation protocols were developed; Collaborator 2 designed the catalysts for the targeted reactions and conditions as defined by Collaborator 1; and all collaborators reviewed the progress on periodic basis and collectively decided on the metrics for success of this project, etc.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

Future research should focus on the technology/catalyst improving the oxidation of aldehyde. The research of biodiesel fuel seems not necessary with the future market in consideration. The resources and time are limited. The mitigation of aldehyde should be the focus of this project.

Reviewer 2

The reviewer stated future plans look excellent. One of the main variables so far has been comparing catalyst formulations and finding the platinum (Pt) + Pd catalyst had the lowest temperature light-off for alcohol oxidation and aldehyde formation, but the Johnson Matthey methane oxidation catalyst was better for aldehyde conversion at lower temperatures. The reviewer noted that it would have been nice to know why, possibly from the DRIFTS studies. The other variable that does not appear to have been tried, which is easier, would have been to change the gas feed of some species. In 2012, this ORNL group published a paper where NO concentration was varied and it appeared to affect the temperature of aldehyde formation and conversion. NO and other species could be increased or decreased in a few experiments to see if they have any impact in future studies.

Reviewer 3

The plan to evaluate alternative catalyst formulations is good, but based on the presentation, the reviewer did not see any evidence for rational design of these materials. Right now, it seems as if this project lacks a clear end goal.

Reviewer 4

In general, the provided plans were adequate. The team plans to examine other catalysts and a range of other organics that would likely be part of fuel formulations and study in analogous fashion how they degrade and the surface intermediates involved. Given the prior success outlined in the presentation, the reviewer has no doubt of the success of these studies. The reviewer would have liked to seen a little more detail and insight on the rationale of new catalyst formulations that might be pursued. Even if only broad strokes are provided, some idea of how the catalysts might be changed would be valuable.

Reviewer 5

Using alcohols as fuels is a pertinent project under LLCF. However future work must define specific research activity, not a generic high-level description. The reviewer suggested identifying the pragmatic fuel (for example, MeOH or EtOH) and developing an approach, activities, and project success metrics and deliver the outcomes in support of such plans.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This project is relevant to advanced engine and fuel technology. The research will help industry to solve the aldehydes emissions issues from alcohol-fueled engines.

Reviewer 2

As stated in the slides and talk, LLCFs like those studied here will be useful and important in powering off-road, marine, and rail applications and are relevant to this project's goals. This is especially true towards the end of project that is getting excellent data from the new directions seen in the project.

Reviewer 3

The reviewer said the project is relevant to supporting low carbon fuels.

Reviewer 4

The project goals and approach are well aligned with VTO interests in understanding emission profiles from engines that run non-standard fuels derived from biodiesel or other sources. Understanding the emissions will be critical to eventually gaining certification for use of such systems broadly. The focus on the catalytic intermediates and evolution of the catalyst will also be helpful in the design of next generation formulations.

Reviewer 5

The project is relevant to overall VTO subprogram objectives. Projects such as this present a great opportunity for enabling reduced emissions, energy security and transition to renewable energy sources, and play a significant role in achieving a more sustainable transportation solution.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This team has sufficient resources needed to complete the research work proposed.

Reviewer 2

This group at ORNL has sufficient access to the tools it needs.

Reviewer 3

The reviewer stated that the resources appear sufficient.

Reviewer 4

Given the diverse skill sets of the partners and that they cover all the areas needed to probe relevant catalysts, along with having the necessary instrumentation in place to study key catalytic intermediates, all required resources were present.

Reviewer 5

The performance evaluation hardware developed at ORNL, the advanced characterizations tools that exists at ORNL, and catalyst development capabilities from suppliers and research expertise from all the participating collaborators are more than sufficient to define and achieve the milestones in a timely fashion, especially that are needed to identify practical solutions with solid underpinnings.

Presentation Number: DORMA028
Presentation Title: Comprehensive Integrated Simulation Methodology for Enabling Near-Zero Emission Heavy-Duty Vehicles
Principal Investigator: Andrea Strzelec, University of Wisconsin-Madison

Presenter

Andrea Strzelec, University of Wisconsin-Madison

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

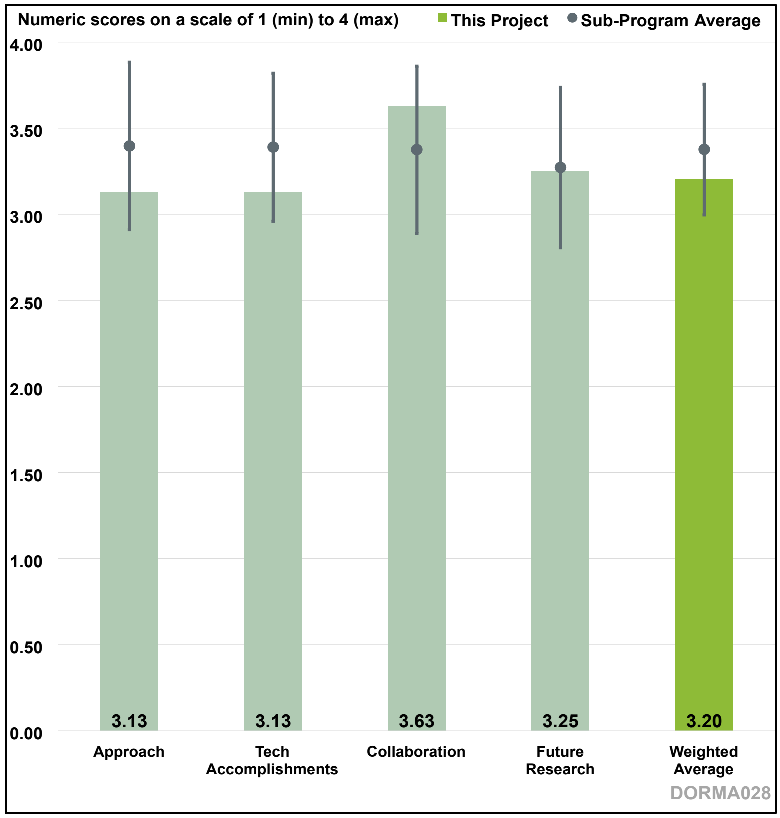

Figure 3-21. Presentation Number: DORMA028 Presentation Title: Comprehensive Integrated Simulation Methodology for Enabling Near-Zero Emission Heavy-Duty Vehicles Principal Investigator: Andrea Strzelec, University of Wisconsin-Madison

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

One of three key innovations (“Introduction of VoFLE methodology to provide unprecedented levels of validation to reduced-dimensional aftertreatment models”) was dropped due to computational cost.

Reviewer 2

The reviewer said it appeared that the urea spray modeling was being done at a much higher fidelity than the rest of the aftertreatment system model. The reviewer also said it was hard to tell from the presentation that this effort is indeed producing a better result. “Objective of this work is to determine the concentration of ammonia at the SCR inlet plane for different engine exhaust conditions.” The reviewer questioned if that was presented at a previous Annual Merit Review. “Unprecedented levels of validation” are claimed, but that was unclear to the reviewer.

Reviewer 3

This is a great project to have an integrated simulation tool in GT-POWER. In the presentation, it was stated the SCR model was a single Cu-zeolite formulation. The reviewer commented that it may be an improvement to add other formulations such as vanadium and was not sure if these models are available to import into package.

Reviewer 4

The project is well designed with clear plans laid out on tasks by the partners. The PI is an excellent integrator and communicator for tasks.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

Actual/planned completion dates are not fully populated in the tables so the reviewer could not tell if the project is on time or behind. Large eddy simulations replaced Volume of Fluid and Lagrangian Eulerian (VoFLE) due to computational cost. The SCR model has been validated and shows good experimental agreement. The integrated GT-POWER model (aftertreatment + engine) is completed. There were limited comparison results presented between GT-POWER and experiment due to availability of data at the time of presentation submission. The reviewer noted that load vs. speed vs. error plots should have been shown as well as space velocity vs. temperature vs. error plots. Error (of unknown magnitude) should have also been shown between the model and experiment for hydrocarbon (HC), CO, and NOx conversion efficiency. Further calibration work is planned that may address conversion error but could also over-calibrate the model to one engine. It was not clear to the reviewer how the model will stay architecture general in nature.

Reviewer 2

The reviewer was happy to see the aftertreatment model in GT-SUITE working and is looking forward to the validation of the optimized models.

Reviewer 3

The reviewer commented that there was good progress on meeting targets and plans.

Reviewer 4

The reviewer said good progress has been made on all fronts. Computational work complements experimental work well. In situations where experimental data is unavailable, higher fidelity computations are being used to train the 1D approach in GT-POWER.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project work is well dispersed across industry and academic laboratories. Isuzu is providing the engine and aftertreatment hardware, FEV is conducting engine testing, and Marathon is providing the fuel. ORNL is providing bench testing for SCR aging.

Reviewer 2

This is an impressive team organization for this sized project. The reviewer commented that there was great coordination.

Reviewer 3

All project team members seem to work together to create a simulation tool package and meet project targets.

Reviewer 4

The reviewer said the project team was excellent. The roles and responsibilities of each team member were clearly laid out.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

Model calibration form engine testing will no doubt help improve the model. The reviewer questioned how the model will stay general to all architectures and which architectures were in consideration. The reviewer assumed that SCR will be needed for all of them but there are different types of SCR catalysts, DPFs, and DOCs. The reviewer also questioned if the DPFs would be catalyzed to oxidize HC or if DOCs would be left out in some architectures. It was unclear to the reviewer if the large available library of architecture allows for this project to be completed by the end of the year or what metric is needed to meet near-zero emissions.

Reviewer 2

The reviewer said the project looks to be on track to finish out in the next few months and that future work is on target.

Reviewer 3

The reviewer stated there was a clear list of future research tasks. The low NOx concept demonstration will be a great test on the usefulness of the simulation tool. The reviewer also stated additional SCR models would be a good goal to target.

Reviewer 4

The future work is well laid out. The general applicability of the model for different fuels and engine platforms was also addressed. Follow-on Coordinating Research Council (CRC) funded work is also encouraging to see.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The project supports VTO subprogram objectives to minimize the formation of emissions.

Reviewer 2

Improvement in aftertreatment optimization supports VTO DORMA subprogram goals through better, more predictive modeling.

Reviewer 3

The project clearly supports VTO DORMA subprogram targets and objectives.

Reviewer 4

The project supports the deep decarbonization objectives of the DORMA subprogram.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer commented that there seemed to be only one student at UW-Madison providing engineering support. Putting models and data together from the collaborators is a very large task. The reviewer suggested that more students be added to the project to support calibration and check the model architecture.

Reviewer 2

The project has been on target the entire time with the current resources.

Reviewer 3

The reviewer stated the project seemed to have sufficient resources to meet project targets and timeline.

Reviewer 4

The reviewer said resources were sufficient and there was good leveraging of cost-share as well.

Presentation Number: DORMA029
Presentation Title: Fast Simulation of Real Driving Emissions from Heavy-duty Diesel Vehicle Integrated with Advanced Aftertreatment System
Principal Investigator: Hailin Li, West Virginia University

Presenter

Hailin Li, West Virginia University

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 67% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 33% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

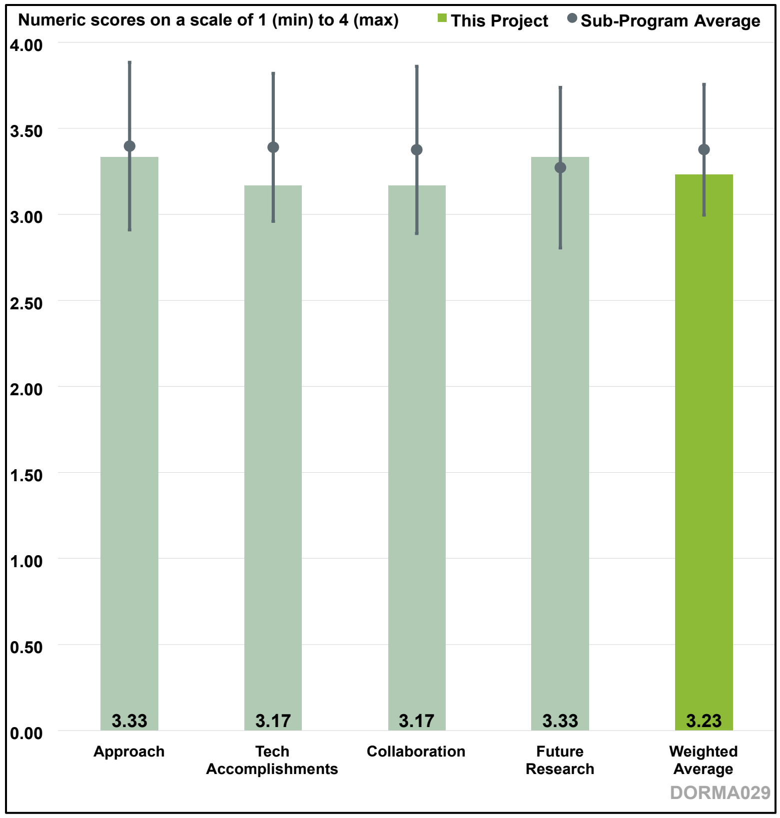

Figure 3-22. Presentation Number: DORMA029 Presentation Title: Fast Simulation of Real Driving Emissions from Heavy-duty Diesel Vehicle Integrated with Advanced Aftertreatment System Principal Investigator: Hailin Li, West Virginia University

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The research plan encompasses both experimental and modeling accomplishments on a complicated system. The reviewer said that it appeared to be well laid out with about a year to go on a project that is two years in.

Reviewer 2

The overall approach to the project is sound, but the specifics of the implementation seem to be fighting against some of the project goals. For example, the reviewer noted that if the eventual model platform is GT-SUITE, which does pair with CONVERGE, it seemed like extra work to develop a high-fidelity 3D CONVERGE CFD model, only to have to reduce it to a reduced order model in the simulation platform to avoid excessive computational times. The reviewer also noted that it seemed that just developing a 1D model in GT-SUITE would have moved the project along more quickly. Certainly, there is value in the CONVERGE model (for student learning if nothing else) but it did not make sense to the reviewer as part of a 3-year project that will end with a 1D system simulation. It was unclear to the reviewer what SCR catalyst formulation was being used. Quasi-steady circuit splitter appears in both system simulations projects that GT-SUITE is part of. The reviewer was curious about how GT-SUITE is able to leverage both projects. The reviewer thought there was a lack of planning on aftertreatment system aging. Hydrothermal aging can be done in a relatively short period of time by a number of suppliers. The reviewer questioned if the project would get to a demonstration of near-zero NOx.

Reviewer 3

The project focus is on combined simulation of a heavy-duty diesel engine (15 L from Navistar) with exhaust aftertreatment system (EAS). This is a legacy project (ACE172) that primarily addresses on-road applications.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

A great range of results are already in that show many areas are well covered. The aftertreatment modeling and results seem to match well, especially for the transient response. Having detailed mixer ammonia uniformity studies developed is harder to find, but it could be improved.

Reviewer 2

Overall, a lot of work has been done, but it was hard for the reviewer to correlate that to achieving the overall project goals. The project is behind schedule, mostly related to negotiations being delayed. However, there is also work going on (i.e. CFD) that seems to be a bit of a side stream rather than contributing to achieving the project goals.

Reviewer 3

The project team was finally able to generate data from the Navistar engine and EAS in the test cell. Data was collected spanning the full speed and load range for the engine and tabulated steady-state engine-out results. The ANL team has validated the combustion CFD model for the engine, including NOx formation, and are fitting the model to the experimental data. The technical progress for the current budget period seemed good to the reviewer, especially given the disruption in the test facility availability.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The partners are very supportive given the many results. The relationships with modeling partners are strong and captured in the results. The reviewer commented that it was hard to evaluate the contributions of equipment and approaches to experimental systems, but that it appeared to be working well also.

Reviewer 2

The reviewer said there was good collaboration with Gamma Technologies and ORNL, but it was not clear to the reviewer how much the other partners were involved.

Reviewer 3

The ANL team did engine CFD. Gamma Technologies supported development of the EAS model, including SCR system models at varying levels of detail (i.e., 1D, two-dimensional [2D], 3D) and the urea injection model. West Virginia University (WVU) is primarily working with ANL and Gamma Technologies. Convergent Science is in more of a vendor role. Navistar provided the engine, dyno harness, and controller and has been consulting/providing technical support as the team works with the engine.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

All of the items appear responsive to indicators from previous results, so future plans look reasonable. The reviewer noted that completing them in about one year will be a challenge.

Reviewer 2

Future work does not include demonstration of project goals being achieved. Machine learning for adaptive aftertreatment system simulation (and control) seems to be computationally expensive and as the PIs note, have significant barriers remaining.

Reviewer 3

The team wants to understand the uniformity index for the urea distribution over the front face of the SCR catalyst. To that end, the team has removed and scanned the static mixer to be able to use CFD to evaluate its performance in radial mixing.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The relevance strongly supports VTO’s and DOE’s interest in improving fuel economy and reducing greenhouse gases.

Reviewer 2

The reviewer said the project was relevant to VTO goals.

Reviewer 3

The reviewer stated the project was relevant, especially considering when the project started.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

This group of partners is well provided with the equipment to carry out this project.

Reviewer 2

Based on the project resources expended to date (40% of total project after two budget periods), the reviewer questioned if perhaps the project estimates were incorrect or if the project team could not access the resources and testing that they originally planned.

Reviewer 3

The reviewer commented that it was a major setback for WVU to offload their engine laboratories from the university to an external organization. The overall budget seems sufficient otherwise, though. The team has sourced used EAS hardware from a vendor that works with Navistar trucks.

Presentation Number: DORMA030
Presentation Title: Opposed-Piston 2-Stroke Hybrid Commercial Vehicle System
Principal Investigator: Ming Huo, Achates Power

Presenter

Ming Huo, Achates Power

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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

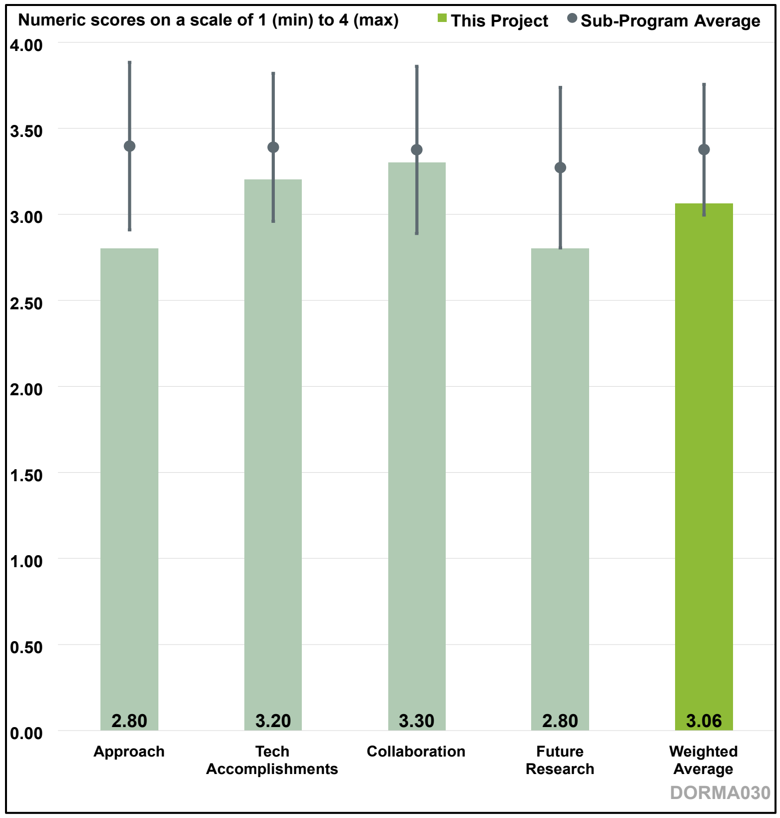

Figure 3-23. Presentation Number: DORMA030 Presentation Title: Opposed-Piston 2-Stroke Hybrid Commercial Vehicle System Principal Investigator: Ming Huo, Achates Power

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project is confusing and is difficult to rate because there are really two separate efforts. The original project scope seemed to be centered around developing a hybrid electric strategy for the opposed 2-stroke engine, including all of the milestones, but there is a substantial amount of unrelated hydrogen work. On the hybridization work, the project team is developing a hybrid strategy from the ground up. It was not clear to the reviewer how much of this is unique to the opposed piston 2-stroke engine (OP2S) architecture and how much could be ported over from existing hybrid trucks. Further, the motivation for using reinforcement learning seemed to be lacking. On the hydrogen engine work, the team has done a lot of work and got an experimental engine working on hydrogen direct injection with a diffusion combustion system. The reviewer commented that is a big deal and did not want to understate it. However, the team's approach did not seem to be sufficiently focused on emissions, as no emissions results from the OP2S engine were shown.

Reviewer 2

The approach to the work is technically sound and the use of modeling capabilities to achieve the objective is a cost-effective approach to develop a hybrid powertrain. The reviewer questioned if there was there any other metric like brake specific fuel consumption, boost response, etc., used as a validation of GT-POWER and experiments in addition to fuel economy or if there were any special considerations for modeling an opposed piston using GT-POWER. The reviewer also commented that hydrogen combustion in an opposed piston engine is an excellent approach.

Reviewer 3

Achieving the dual goal of meeting ultra-low NO_x ($ULNO_x$) and demonstrating hydrogen combustion on this relatively new platform provides significant complexity. This project will provide confidence and insight into the maturity of this specific approach to opposed piston 2-stroke engines. The demonstration of emissions over key legislation cycles appears to show compliance though the effect of hybridization requires more repetition than shown to allow the storage at cycle-initiation to be understood. Also, the reviewer noted that the condition of the aftertreatment at the start of cycles may not be consistent due to the hybrid system and should be shown as well. The steady performance of hydrogen operation is an excellent accomplishment.

Reviewer 4

The approach to hybridize a truck has some merit to create the lowest possible fuel consumption. However, hybrid trucks are most effective in the medium-duty (MD) space, not HD. The closer the vehicle operates to an automobile, the more likely hybridization is to help. However, MD vehicles are extremely cost sensitive and paying for both a high voltage electrical system (batteries, motors, inverters, etc.) and an expensive engine system with aftertreatment (even if it is a slightly reduced cost engine and aftertreatment system) is a major challenge for commercial vehicle OEMs. Potentially a spark-ignition engine (natural gas, in particular) could have a use case in hybrid, but compression ignition (CI) engines almost all need some form of $ULNO_x$ aftertreatment. The reviewer questioned what a hybrid MD truck has that a battery electric truck does not. Range and payload are not major concerns on MD trucks. Battery electric MD trucks can operate in zero emission vehicle zones and provide carbon credits. Hybrid electric MD trucks are significantly more expensive. The fuel savings will not likely overcome the substantial initial cost differential compared to a conventional powertrain and offer no real advantage compared to a battery electric truck. The OP2S engine is likely better applied to Class 8 and vocational trucks where conventional powertrains are used. Electrical hybrid systems on trucks tend to be very unattractive due to cost, complexity, and modest return on investment. The reviewer noted that perhaps the off-road market may be a better application of this approach. The hydrogen work is novel, if only for the use of CI. If successful, it could pave the way to more extensive use of CI hydrogen in the future. There are significant challenges, however, and this project has only begun to address them. NO_x and transient performance are likely to be very difficult to get control of in this combustion system.

Reviewer 5

The reviewer stated that progress was being made to achieve the project goals. There has been some slips in the timeline but the plan for getting on track was noted by the reviewer. The coordinated approach is good on a high-level but the lack of details of how the work was performed made it difficult to link the approach to the barriers.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project team has done a great deal of work with the opposed piston 2-stroke hybrid architecture development. The team compared simulated cycles to experimental cycles with engine-in-the-loop testing. It was not clear to the reviewer if there were any unique battery or power electronics requirements for this system, as the team viewed their hardware role to be exclusively limited to the engine. On the hydrogen engine development side, getting the engine to operate on direct injection hydrogen is a big deal. The reviewer would have liked to have seen some emissions plots, as there is a great deal of concern with NO_x emissions with hydrogen and a stratified charge.

Reviewer 2

The technical accomplishments to a large extent depend on the accuracy of the engine model. The reviewer would have liked to known what specific steps were taken to model the opposed piston accurately in the vehicle model. The results show only a fuel consumption comparison and not a comparison of other parameters such as boost pressure, IMT, etc., to assess the engine performance with a different hybrid strategy. The reviewer questioned if there were any critical changes to the airpath to deliver the required air flow for hydrogen combustion, especially during transients, or if the project team expects any pre-ignition in the opposed piston design.

Reviewer 3

A sound plan and goals were put forth to address the barriers. At completion, insight into the applicability of this approach to internal combustion propulsion will be better understood. The challenges of packaging, durability, and the operational implications to aftertreatment from both approaches will still need to be investigated. The reviewer stated this is solely due to the departure from traditional engine arrangements for the opposed piston and departure from conventional operating characteristics driven by the hybrid system and not a comment on the architecture.

Reviewer 4

With the stated goals provided, the technical progress has been quite good. The engine has demonstrated significant progress toward the project goals. The hybrid work appears to show some potential for fuel consumption improvement. The hydrogen engine also shows some promise in a CI combustion system.

Reviewer 5

The technical progress supports the project plan, objectives, and milestones. The reviewer noted there was a lot of detail missing in how the accomplishments were actually performed. Questions about the calibration starting up in a catalyst heating mode instead of hot mode were not addressed. Questions about the measurements made during the engine-in-the-loop testing were also not answered. The link of the Markov training to the more targeted speed and load points was also not clear to the reviewer. No information about the hybrid setup, the size of the engine, details of powertrain or energy storage were provided. The quick coverage of the CFD accomplishments made it hard for the reviewer to link to the project plan objectives.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project team consists of an OEM (Isuzu) and two universities working with Achates Power. This project has all of the required participants. And although they are not officially a partner on the project, Argonne National Laboratory is a contributor. While it was clear what Clemson University and UW-Madison contributed, as well as Argonne National Laboratory, the reviewer would have liked to have seen Isuzu have a bigger role in the project as it appears they are mainly consultants. The reviewer questioned if Isuzu had any plans to put either the hybrid system or the hydrogen engine into a vehicle.

Reviewer 2

The reviewer stated the project had excellent collaboration between industry and academia.

Reviewer 3

The use of the team has provided a satisfactory range of input but perhaps not comprehensive from a commercial vehicle application (starting point) and the shift to off-road applications was not addressed. Input from an off-road OEM would be useful as a reaction to the shift in focus of the VTO's advanced engine area. The public entity contributors and academic institution seem to be providing excellent service.

Reviewer 4

Several collaborators were listed (Clemson University, UW-Madison, ANL) and it appears that each organization supplied valuable input to the work as a whole. The project appears to be well-coordinated, with each partner providing results that build upon the others. For the vehicle portion, the reviewer noted it would have been beneficial to have a commercial vehicle OEM on the team, particularly for any hybrid drive work.

Reviewer 5

The reviewer said it seemed like there was good coordination with existing collaborators. The nature of collaboration with ANL was not clear in the presentation or even noted in Slide 18 on collaborations. The actual collaboration on each task was not clear in the presentation.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The next steps listed are logical given where the team is with the project and the fact that this project will wrap up later this year.

Reviewer 2

The work planned for the future does address many of the questions that the reviewer put forward. Overall, the work yet to be completed is interesting and much needed for the success of the project.

Reviewer 3

For future work, addressing the barriers to implementation is needed. The reviewer questioned what that looks like in agricultural or construction equipment applications and what the operating cycles for those applications emphasizes. The reviewer also wanted to know if those applications result in any new hurdles. Continued investigations as to the enablers of efficiency for hydrogen combustion in the OP2S engine are called out and extremely important. Simulation-led development of combustion systems leveraging current work will be very interesting.

Reviewer 4

Investigating hydrogen CI parameters and performance will be critical to enabling this type of combustion system. The reviewer was uncertain that the hybrid portion of the project will deliver on the promise of improved fuel consumption, particularly since no HD OEM is involved.

Reviewer 5

The proposed future research is inline with meeting project milestones but the link to achieving project targets and overcoming the barriers was not clear to the reviewer and seemed more focused on the hydrogen portion of the project. The expected gains from the reinforcement learning-trained control strategies for meeting the challenges were also noted by the reviewer. The discussion of NO_x

mitigation strategies included hydrogen SCR as a potential path forward but it was not clear to the reviewer if there is even the ability to source a prototype system for use in the project.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

This project, and the hydrogen piece in particular, directly contributes to the decarbonization goals. This application is somewhat smaller than most of the other goals for the DORMA subprogram, but hydrogen combustion is of keen interest.

Reviewer 2

The project is highly relevant for the decarbonization goals of DOE as well as accelerating new powertrain technology for hydrogen engines.

Reviewer 3

New approaches that promise increases in efficiency though prediction or initial demonstration are important to investigate all the way through the expected lifecycle. The approach that is being taken will build confidence in the direction of the selected approach but will still leave questions about many aspects of applying this approach in the field.

Reviewer 4

The reviewer noted that this work may be a bit more applicable to off-road vehicles that may benefit more from hybridization than on-road trucks. Hydrogen engine improvement certainly supports DOE’s goals of decarbonization. The quality of the work appears to be quite good, just perhaps a bit misapplied in terms of market segment.

Reviewer 5

There is general relevancy to increase efficiency, reduce NO_x emissions, and utilize a low-carbon fuel like hydrogen. However, the reviewer said there were no clear links to the subprogram objectives from when the project started.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said resources would have been excessive if the project was solely a hybrid effort. With the hydrogen piece added, the reviewer said the resources seemed about right.

Reviewer 2

The industry and university partners have all the testing and simulation capabilities for the project. For the future hydrogen work, it was unclear to the reviewer if testing capability has been identified for hydrogen engine testing.

Reviewer 3

The reviewer commented that more investigations into the in-vehicle performance of this OP2S approach are needed and would be very interesting. The reviewer also said that it appeared as if the engine alone with appropriate aftertreatment was viable. The hybrid approach was novel and brings the questions from light-duty applications to heavy-duty applications relying on aftertreatment in different ways and different operating regimes.

Reviewer 4

The reviewer said the resources appear to be sufficient to accomplish the goals of the project.

Reviewer 5

The reviewer stated the resources seem sufficient for the project and did not impact the milestones.

Presentation Number: DORMA032
Presentation Title: High Efficiency Ultra Low Emissions Heavy-Duty 10L Natural Gas Engine Project
Principal Investigator: Tim Lutz, Cummins

Presenter

Tim Lutz, Cummins

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

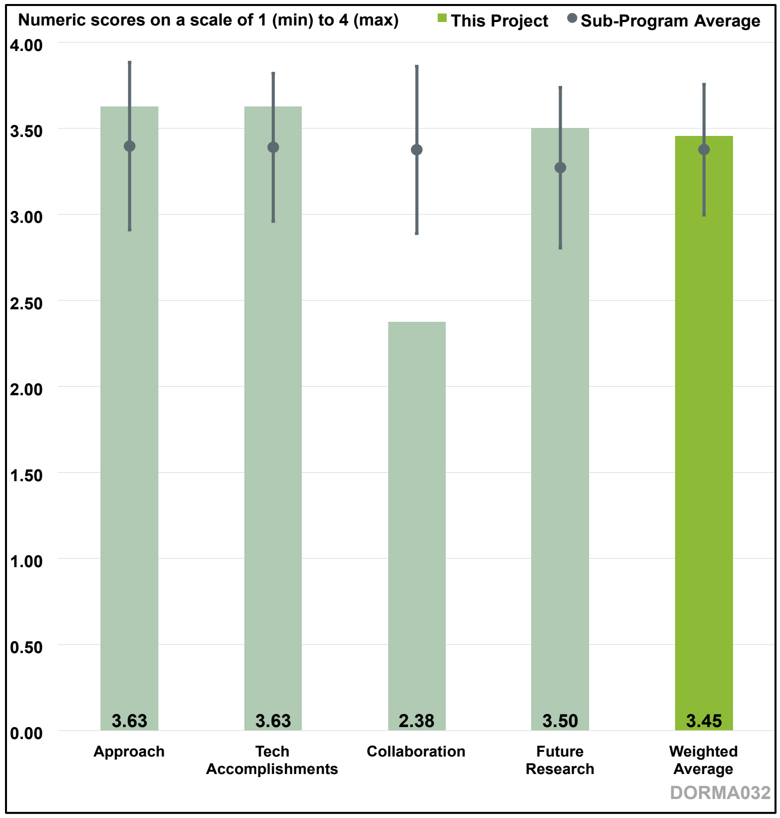

Figure 3-24. Presentation Number: DORMA032 Presentation Title: High Efficiency Ultra Low Emissions Heavy-Duty 10L Natural Gas Engine Project Principal Investigator: Tim Lutz, Cummins

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer approved of the approach to design an engine specifically for natural gas combustion rather than just adapting a diesel (CI) engine for SI natural gas use. The reviewer assumed the previous years' reports spoke to the details of what was done. Given that the project is running on schedule, the timeline was definitely reasonable.

Reviewer 2

The barriers are well-defined, and Cummins has a well-planned approach to resolving them.

Reviewer 3

This project does an effective job at addressing some of the previous challenges with compressed natural gas (CNG) engines, an engine designed from the start to be SI and gaseous fueled. Proper cylinder head geometry, the elimination of EGR, and other design choices make this project rather innovative in approach. There is likely still some work to be done in cylinder-to-cylinder lambda control to take full advantage of these opportunities, particularly for low NO_x. The reviewer said it was an intelligent decision to keep the NO_x target at 0.02, even in light of recent regulatory changes.

Reviewer 4

The project has a complete and comprehensive development and testing plan and includes aggressive application of CNG with cost savings and industry satisfying brake thermal efficiency (BTE). The reviewer also commented that the project was on track.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project seems to be running ahead of schedule and the team has started work on Budget Period 3 tasks. The reviewer said that the results to date seem very promising, although some important gaps remain between what has been demonstrated and what remains to be delivered. The team is using intake cam phasers to implement variable valve timing (VVT) for Miller cycle late intake valve closing to reduce the effective compression ratio at high load to mitigate knock and improve overall efficiency. The team has demonstrated 41% BTE with fixed cams, so reaching 42% BTE with VVT seems achievable. The engine needs premium exhaust system materials because natural gas combustion exhaust is hotter than diesel exhaust. The intent is to use a combined close-coupled and underfloor three-way catalyst (ccTWC + ufTWC) for criteria pollutant control. Cummins does not want an EGR loop in parallel with a high-temperature nickel-alloy exhaust manifold. Thus, no EGR is a better solution for the targeted power density. Cummins will evaluate a stainless steel exhaust manifold option to mitigate costs.

Reviewer 2

This team has made excellent progress with first engine firing 18 months from the project start. It was unclear to the reviewer how far along this new engine was in its development prior to the start of this project, but the efficiency “out of the box” was very impressive.

Reviewer 3

Building a new engine is a costly undertaking. The progress made thus far is excellent. The engine has already fired and has demonstrated excellent efficiency numbers right out of the gate. The modeling was even close, which probably was a bit surprising to all involved. This bodes well for the ability to hit the target in the future. The reviewer also said the preliminary performance results were very encouraging.

Reviewer 4

The project team has made good progress with a low-cost, single injection point method while still meeting NO_x requirements. Though CNG combustion has CO_2 as by-product, it is lower than diesel and the GHG production is far less. There is a fuel sourcing issue with renewable CNG, but this work helps to solve the vehicle side factors. The initial engine test results indicate that the team should be able to meet BTE targets when additional hardware testing allows for optimization of combustion (new cam phasing, etc.).

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

Cummins is apparently the only funded partner on this project. The reviewer was disappointed, especially since their cost share is under 50%, and are not a national laboratory.

Reviewer 2

The reviewer would have liked to have seen some other entities brought into this project. The reviewer suggested some modeling expertise at a university or national lab that could help with the poor knock prediction by using a higher fidelity simulation. DOE had a consortium with the national laboratories (Partnership for Advanced Combustion Engines) that had a focus area on knock modeling.

Reviewer 3

Cummins is a big and very capable company with lots of experience in CNG engines and development. The reviewer suggested that a university or national lab could have investigated some of the knock issues given their improved tools and work purpose for this type of research.

Reviewer 4

Predictions from modeling seem to match well with early test results but the reviewer would have liked to seen some materials development to help with any issues that may arise from high temperature combustion or possibly any aftertreatment concerns that arise after lengthy durability testing.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

No results were presented that showed current engine-out NO_x values, so it was difficult for the reviewer to gauge how challenging the brake specific NO_x target would be. The knock control seems like it will be especially challenging for this engine given the non-linear onset of knock. The team needs to “upfit” the engine with cam phasers for VVT and the EAS (three-way catalysts) for Budget Period 3 tasks. To mitigate damage from knock, the reviewer noted that Cummins could perform modal analysis of the vibrations caused by knock if using an accelerometer to detect knock, although challenging. Ideally, the reviewer suggested having a cylinder pressure sensor to measure the knock more directly. Cummins will also look to change the piston material from aluminum to steel. The aluminum piston transfers heat well, so the face stays cooler until knock starts. Thus, the onset of knock is quick. Steel pistons will be hotter in the bowl, but cooler around the perimeter because of the piston cooling jets. In addition, the steel piston crown will be more robust to knock pressure spikes than aluminum is. Excellent air-fuel ratio (AFR, or λ) control is key to achieving low engine-out NO_x levels and high BTE. However, the reviewer noted it was tricky to mitigate cylinder-to-cylinder variation in AFR given the air flow and fuel variability. Additional challenges for a natural gas-fueled engine are that three-way catalysts require relatively high PGM loading to oxidize methane and that the natural gas fuel system is very expensive. The reviewer questioned if the Cummins team could evaluate other ignition systems (e.g., pre-chamber, plasma) that might help mitigate knock conditions better than spark plugs. The reviewer recommended conducting CFD studies first to evaluate potential benefits.

Reviewer 2

The work proposed in the final budget period will produce the milestone deliverables of 42% BTE and 0.02 g/hp-hr brake specific NO_x over the Federal Test Procedure and ramped mode cycle Supplemental Emissions Test cycles.

Reviewer 3

Lambda control and NO_x prediction/mitigation are the heavy hitters that potentially limit the impact of this project. The reviewer was happy to see them both explicitly addressed as the next steps to come. Again, the right partner here may have been useful.

Reviewer 4

As the project enters Budget Period 3, the team has a running engine with solid initial results. As discussed with the PI, there do exist other applications for this powerplant once the research effort is converted to commercial products. Port injection variations may also be investigated in the future to understand the sensitivities to load balancing and to combat predictive detonation but would drive project cost.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

Natural gas is one part of a decarbonization strategy, especially if there are renewable, non-fossil sources for methane available at scale.

Reviewer 2

A high-efficiency, alternative-fueled internal combustion engine meets the VTO DORMA subprogram objectives. The reviewer was glad to see the planning for hydrogen fueling for future decarbonization work.

Reviewer 3

This project definitely addresses DOE goals for CO_2 reduction. The reviewer said there was an opportunity to use CNG, renewable natural gas, and even hydrogen as the project progresses.

Reviewer 4

The project is extremely relevant to decarbonizing efforts in difficult to electrify sectors. The results of this work may have multiple applications as natural gas strengthens the options to decarbonize without going full electric.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said the project definitely seemed to be running on budget. Given that Cummins has a line of natural gas-fueled engines in production, the reviewer would have expected this project to have had a 50% cost share requirement.

Reviewer 2

The reviewer commented that the resources seemed reasonable with the costs of prototype hardware for an engine demonstration project.

Reviewer 3

The reviewer stated that the resources allocated appeared to be sufficient for this project to accomplish the goals.

Reviewer 4

The project has progressed well against the planned timelines, and the funding available should allow the team to complete engine upgrades and future testing.

Presentation Number: DORMA033
Presentation Title: High Pressure Fast Response Direct Injection System for Liquified Gas Fuels Use in Light-Duty Engines
Principal Investigator: William de Ojeda, WM International Engineering

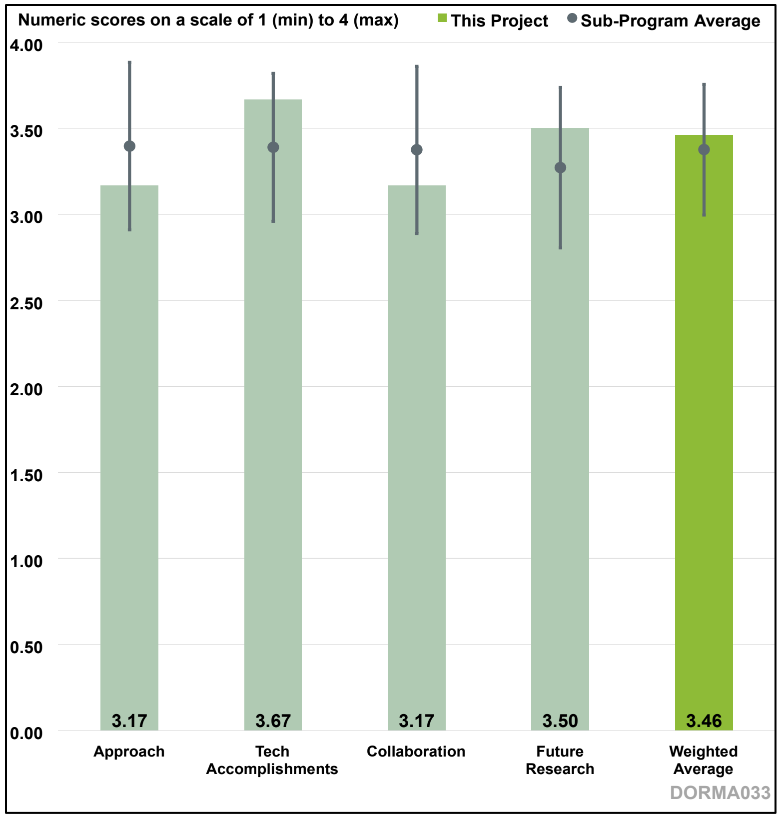

Figure 3-25. Presentation Number: DORMA033 Presentation Title: High Pressure Fast Response Direct Injection System for Liquified Gas Fuels Use in Light-Duty Engines Principal Investigator: William de Ojeda, WM International Engineering

Presenter

William de Ojeda, WM International Engineering

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

67% of reviewers felt that the project was relevant to current DOE objectives, 33% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 100% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project is well-executed to develop a DME and propane capable light-duty engine. However, while propane/DME have technical possibilities to reduce GHG emissions, as demonstrated in the project, their practical impact on GHG emissions reductions is minimal, and the project does not significantly contribute to technical barriers identified by DOE to the commercial utilization of lower carbon intensity fuels.

Reviewer 2

This project team took a sound approach to identify the difficulties with fuel handling equipment (pumps and injectors), which is one of the main difficulties with DME and propane, and focused on solving the associated technical challenges. In the case of the pump in particular, the project team made major modifications to the state-of-the-art and proved it was durable. The reviewer also applauded using a multi-cylinder engine for the engine testing and brake efficiency measurements.

Reviewer 3

The approach of the project clearly addresses the main challenges associated with developing a high-pressure fuel system for liquified gas fuels. The project has adopted the necessary steps to design a fuel system, demonstrate the durability, and then conduct engine optimization to deliver GHG reduction.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project has made outstanding progress, achieving all technical milestones on time.

Reviewer 2

The project team has designed, fabricated, and tested new fuel component hardware for proof of concept and durability. The team has also performed engine testing in a way that allows potential engine calibration (e.g., mapping out the EGR and emissions space). The reviewer noted that the team has done a lot.

Reviewer 3

The reviewer stated that comparison of a high flow injector with baseline flows and the benefits of the new design was a good accomplishment for combustion stability. The reviewer also stated that nozzle design for quicker injector closing was an excellent design change.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The team has identified technical partnerships, however it seemed to the reviewer that the partnerships did not have major impacts on the project.

Reviewer 2

The project team consists of WM International to do the majority of the development work, as well as Argonne National Laboratory to do the spray imaging and durability testing. Diversified CPC was providing the fuel. It was not immediately clear to the reviewer what role Illinois Tech was playing. Regardless, the team appeared to be well integrated and was making progress towards their goals.

Reviewer 3

The task of the university partner was unclear to the reviewer. It was also unclear to reviewer if any tasks were delivered by Illinois Tech or if they were part of future work.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The project's proposed future research aligns with project goals and has a clearly defined purpose to deliver on remaining project commitments.

Reviewer 2

The project is roughly 67% complete, and the team is well poised to be able to successfully conclude the project goals with the remaining planned work.

Reviewer 3

The reviewer said future work related to engine testing and project demonstration will be an important part of this project.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

Use of low carbon domestic fuels is critical for energy security and this project directly focuses on increasing the use of propane-DME mixture for transportation applications.

Reviewer 2

The project was relevant when it was initially funded. However, since this project has shifted to decarbonization the off-road, rail, marine, and aviation sectors, the project goals of using mixtures of propane and DME in a 2.2 L engine seem less relevant than when the project was initially awarded.

Reviewer 3

The project does not substantially support overall DOE VTO subprogram objectives, and therefore is not relevant. Combustion of DME/propane in an automotive-type engine does not advance DOE objectives of increasing utilization of lower carbon intensity fuels in off-road/marine/rail (“hard to abate”) sectors.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer commented that the project’s budget was sufficient for the scope of the planned work.

Reviewer 2

The project team has made good progress on their project goals and seems poised to successfully conclude the project. At the same time, the team has done a lot of work and achieved a lot. The project resources seem about right.

Reviewer 3

WM International is highly experienced in fuel system development and their collaboration with ANL and Illinois Tech provides them visualization and modeling capabilities.

Presentation Number: DORMA037
Presentation Title: Sustainable Aviation Fuel Characterization
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 felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 80% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 20% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

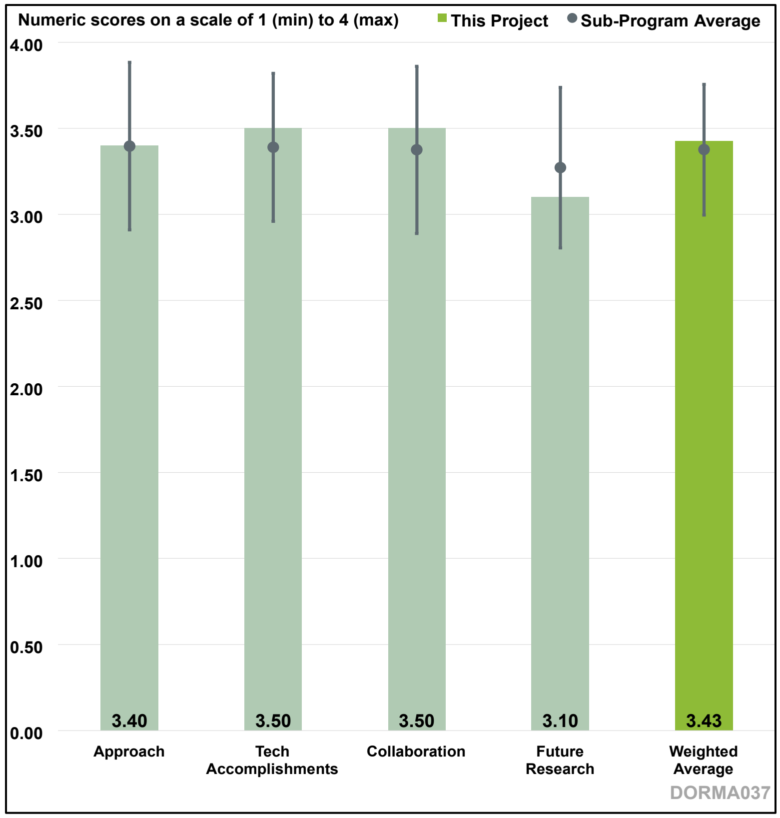

Figure 3-26. Presentation Number: DORMA037 Presentation Title: Sustainable Aviation Fuel Characterization Principal Investigator: Gina Fioroni, National Renewable Energy Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project's approach to reducing barriers to the utilization of SAF through a data-driven program is providing high-quality data to industry and industry committees, speeding the process to further SAF approvals.

Reviewer 2

Four barriers are listed, all pertinent, and the team has a good project plan to address them. However, one of the barriers listed is just a start. To address this barrier, specific further identification of the "remaining barriers that constrain current fuel property requirements" are required. Engagement of OEMs or ASTM committee members should help. Although it is clear the team is generally aware of some of the issues (and is addressing them), the reviewer said it would have been good to call these out clearly and talk about which of these the team is addressing, and which are beyond the teams control. Regarding the property measurements of fuels at a range of engine conditions, the reviewer suggested the team might engage OEMs to define the key property needs at what conditions, and to what accuracies. This will help ensure the team does not miss a critical need by the aero-engine community.

Reviewer 3

The project is well designed to address the noted technical barriers with proper goals set across a reasonable timeline. The project tasks include key fuel property measurements needed to address the stated technical barriers.

Reviewer 4

The approach presented was confusing to the reviewer because it included a wide range of focus areas. The approach makes connection of work in this area to the bigger picture, but it really does not seem to connect to the technical accomplishments. The reviewer commented that it would have been beneficial to streamline the language so that reviewers can connect approach to technical accomplishments and future work.

Reviewer 5

This is a large project with a comparatively large budget that includes PIs from national laboratories and academia. The subjects covered are among the most important that can be envisioned for selecting alternative fuels and simulating their performance in combustion engines. The properties selected for measurement are relevant and the methodology and data appear outstanding. There are also a lot of data on surface tension using other methods. The presentation could do a better job of comparing their pendant drop data in the context of alternatives, though the Wilhelmy plate method is mentioned that shows “good agreement.” It was not clear to the reviewer what that meant or what liquid was being referred to. The reviewer thought the pressure effect on surface tension was interesting. Corresponding states correlations do not consider it. The reviewer questioned if there was an effect for incompressible liquids. The reviewer suggested the team scrutinize their data to try to develop a correlation that includes a pressure effect. There is an opportunity here for the team to make a useful contribution to bring in the pressure effect in a correlation of surface tension. It was not clear to the reviewer why the PIs selected cryogenic temperatures for their measurement conditions in some cases. Distillation data for POSF# 10325 show temperatures ranging between 177°C (T10) to about 245°C and average boiling points of about 270°C. An oxidation mechanism is being developed for a SAF which will be validated by RCM data, which is very important. The broader applicability of the validated mechanism to the engine environment should be considered. Transport can affect a kinetic mechanism by its influence on distributing the gaseous species throughout the combustion zone in different ways for different combustion configurations with different transport. Since data for validation obtained from laboratory scale configurations include transport conditions that are very different than in an engine (e.g., 1D for laboratory scale vs. 3D transport in the combustor environment), the reviewer suggested some thought should be given to the broader question of what “validation” means. The reviewer said it was best to try and use data from three or four configurations to develop a sort of averaged mechanism that provides the best fit to several configurations. The configurations that are modeled the greater chance of a broader applicability. The reviewer noted that the surrogate for hydroprocessed esters and fatty acids-synthetic paraffinic kerosene (HEFA-SPK) and how it was determined was not specified in the presentation. The reviewer recommended that a review be undertaken of the governing transport equations for simulating combustion in engines to identify the properties of greatest importance in simulation engine combustion. The reviewer noted that measurements of binary diffusion coefficients for species ‘i’ and ‘j’, thermal diffusion coefficients for species ‘i’, specific heat at constant pressure, gas and liquid thermal conductivities among others were not included in the research. For some of these properties, data do not exist at temperatures relevant to combustion and significant extrapolations to operational conditions are required which can create inaccuracies. The reviewer also noted that some discussion of mixing rules in property correlations would have been useful.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project is delivering a number of technical accomplishments that directly support the increased utilization of SAF, furthering DOE goals. Providing high-quality data on physical properties of jet fuel and SAF samples across a range of temperatures and pressures allows for a direct comparison of where SAF is indistinguishable from today’s jet fuel, and where measurable differences occur. One key watchpoint for this work is to recognize that jet fuel varies substantially from producer to producer, and therefore a range of jet fuel samples must be obtained and measured in order for comparisons with SAF to be meaningful.

Reviewer 2

The team started nearly three years ago, has made good progress, and even has started sharing results with the pertinent ASTM committee on fuels. Further, the team has successfully acquired or fabricated experimental equipment to make measurements of a variety of hydrocarbons over a range of conditions, much of which was not available before. Extensions of these studies to more SAFs and a range of different jet fuels would be a big contribution to the literature. Much of the data were lacking uncertainty bars, although the numerical data for density suggests five decimal points of accuracy, yet no accuracy level is claimed. The reviewer commented that such information should have been reported.

Reviewer 3

The project is making good progress according to the document project plan. The four top level milestones are all complete or on target. It was unclear to the reviewer what milestones are projected beyond FY 2024 given that the project end is set for FY 2027.

Reviewer 4

Critical fuel properties for simulations to accelerate fuel qualification is a unique area that DOE is having a large impact. The results of this accomplishment were well presented and interesting. There should continue to be investment and technical work in this area. All technical accomplishments are well presented and are impactful to the community. The reviewer noted that it would have been helpful to connect the approach language to the technical accomplishment language to know where each of these tasks/working areas fit.

Reviewer 5

The PIs have reported a lot of data which have the potential to be very useful. The data reported appear to be quite accurate for surface tension, liquid density, and kinematic viscosity. Given that it will be a POSF# 10325 surrogate that would be simulated, the reviewer noted that measurement of mixture component properties may need to be carried out. Mixing rules will be necessary which is especially true for development of an equation of state. Many such rules exist, and the reviewer suggested that the team should try to identify those that will yield the most accurate mixture “rules” from measurements of component mixture properties.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project leverages a range of collaborations with DOE laboratories (Lawrence Livermore National Laboratory and Argonne National Laboratory), universities, and industry committees in order to increase the value derived from this project.

Reviewer 2

The reviewer said collaborations and coordination amongst groups appears to be working very well. The team is engaging WSU in one area. Given that there is substantial overlap with the group at WSU headed by Prof. J Heyne with funding by the FAA, the reviewer encouraged increased collaboration and sharing of information.

Reviewer 3

The project clearly identifies project team partners alongside roles and responsibilities. The project notes the contributions made by industry partners (General Electric), national laboratories (LLNL, and ANL), federal partners (U.S. Navy), and academia (WSU, Princeton, and Georgia Tech).

Reviewer 4

Collaboration was presented as working with Georgia Tech, WSU, and ANL but the actual work within these collaborations was not clear to the reviewer. The reviewer understands that the presentations are short and it is hard to highlight all of the areas, but this is an area that is important for understanding how the DOE work integrates into the general community and has impact. Several questions were based on this topic. The reviewer noted that it was great to see engagement with ASTM and CRC.

Reviewer 5

The collaborative team is excellent for the properties being investigated in this project. The team has significant expertise from their past work for making accurate measurements of the properties selected. The effort to obtain data at elevated pressures is particularly challenging and the team has done a good job to obtain data at the pressures considered in the project. Development of the kinetic mechanism and equation of state for POSF# 10325 is highly relevant though the broader applicability of the mechanism being developed may be a concern.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The project's plans to leverage ongoing work to support ASTM ballot measures, increase experimental capabilities, and support contrail work being developed at other DOE laboratories clearly identifies technical barriers and proposes effective measures to overcome these barriers.

Reviewer 2

Regarding the 2D gas chromatography (GC) method for SAF analysis, the reviewer encourages comparing/contrasting this work with that of WSU (J. Heyne) and Purdue (G. Kilaz), who have been doing similar research for several years. The reviewer noted that pressure-enthalpy curves for the different fuels would be useful as well as collecting and reporting data on critical points for the different fuels. The reviewer also noted that limited details were provided about the jet stirred reactor to examine the impact of different fuels on sooting characteristics, but if the research is done well, it will be well-received by the community. Given the demonstrated ability to measure physical properties of liquid hydrocarbons over a range of conditions, a major contribution by this team could be made by studying and documenting properties of binary and tertiary mixtures. Subsequent studies on theoretical simulations of such fluids could result in significant advancement in the science of mixtures and intermolecular forces amongst dissimilar molecules. Given the immense number of possible combinations, some thought into targeting certain mixtures will be required. Tahe reviewer stated that coordination with members of the ASTM approval committees and OEMs would be very useful to target certain properties at selected conditions and for which fuels. The reviewer also noted that it would be useful to characterize liquid properties of the “worst” and “best” jet fuels as defined in the NJFCP studies for comparison to the SAFs (existing and future).

Reviewer 3

The project has clearly defined future research tasks with noted purpose for tasks outlined in FY 2024 and FY 2025. The reviewer said that it would have been helpful to have the proposed tasks more clearly linked to overarching research targets but noted that it is very likely that the project will achieve the targets for proposed future research.

Reviewer 4

Proposed future research in enthalpy and GC seem in line with relevant and impactful work. The reviewer was not sure what the jet-stirred reactor soot generation-characterization for contrail formation was, but that it did not seem to align with other future research areas.

Reviewer 5

The reviewer said the focus on reactor design, model validation of burner experiments, and kinetic mechanism development for future work was good. The PIs also want to “broaden collaborations” for model development which was also good. For the continuing work, some consideration should be given to such properties as diffusion coefficients, gas thermal conductivity, and mixing rules for combining mixture component properties in a way that results in accurate data for the mixtures which will be relevant to the equation of state that is planned for development. Surface tension and liquid density are important to processes relevant to liquid jet and spray injection, but liquid phase properties will not factor into the burning of fuel vapors once the liquid has completely vaporized and transport dynamics take over to control and maintain the fuel burning process. The reviewer noted consideration should be given to developing correlations for some of the properties developed such as a pressure (and temperature) effect for surface tension. Adding new properties may mean scaling back other properties but can be worth the effect if the property being added is especially useful to modelers. In the process of validation of a kinetic mechanism, for example the reviewer commented that the plan for dealing with discrepancies between measurements and simulation was not discussed for future work. With the kinetics, there are many rate constants to consider and not all of them will be known with unquestioned accuracy. The reviewer stated that a strategy should be developed for closing the gap between measured and predicted data used for validation.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The project directly supports DOE’s goal of increasing SAF utilization to reduce the carbon intensity of commercial aviation. The project’s results will aid in the adoption of SAF by reducing concerns over SAF variability, refining of SAF specifications over time, and the eventual elimination of the SAF blendwall.

Reviewer 2

The embedded links appear outdated, but the work is fully consistent with the SAF Grand Challenge Roadmap.

Reviewer 3

The project is relevant and clearly set its tasks against identified research needs under the SAF Grand Challenge Roadmap. The reviewer noted that the linkage to a specific VTO subprogram objective was not clear given the linked VTO subprograms.

Reviewer 4

Work presented in the package centered around fuel characterization is incredibly relevant to the community and helps fill in a gap that is critical for future fuel qualification.

Reviewer 5

This project touches on many of the most important problems that will limit simulation of SAFs in engines: property database development; equation of states of a SAF (POSF# 10325 being chosen here); oxidation kinetic mechanisms; surrogates for POSF# 10325; validation of the simulation, data and oxidation mechanism, etc.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The project's resources are excessive compared to other DOE VTO projects, program goals and technical accomplishments.

Reviewer 2

Resources appear to be healthy, although the reviewer recognized that developing and running such experiments are costly. The reviewer noted that it would be a shame to create these capabilities and not get the required data sets for a few extra dollars. The reviewer also commented that it was important to note that the cost of further development of the jet reactor, assembling its diagnostics, characterizing its performance, and running a variety of pertinent conditions and fuels will be costly.

Reviewer 3

The resources are well suited to achieve the project's stated milestones in a timely manner. The project has a diverse research team to support the tasks and deliver the research objectives.

Reviewer 4

A budget of $4.05 million across three years seems like a significant amount of funding for the tasks laid out in this project.

Reviewer 5

The project is large, incorporates many collaborators and organizations, and covers an important topic. It is envisioned that additional topics as noted in the review could have been incorporated which would require more resources (e.g., additional property characterization and data processing, other burning designs for validation, etc.) although some could be scaled back to incorporate new properties.

Presentation Number: DORMA038
Presentation Title: Towards Accurate Combustion and Emissions Modeling of Sustainable Aviation Fuels
Principal Investigator: Debolina Dasgupta, Argonne National Laboratory

Presenter

Debolina Dasgupta, Argonne National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

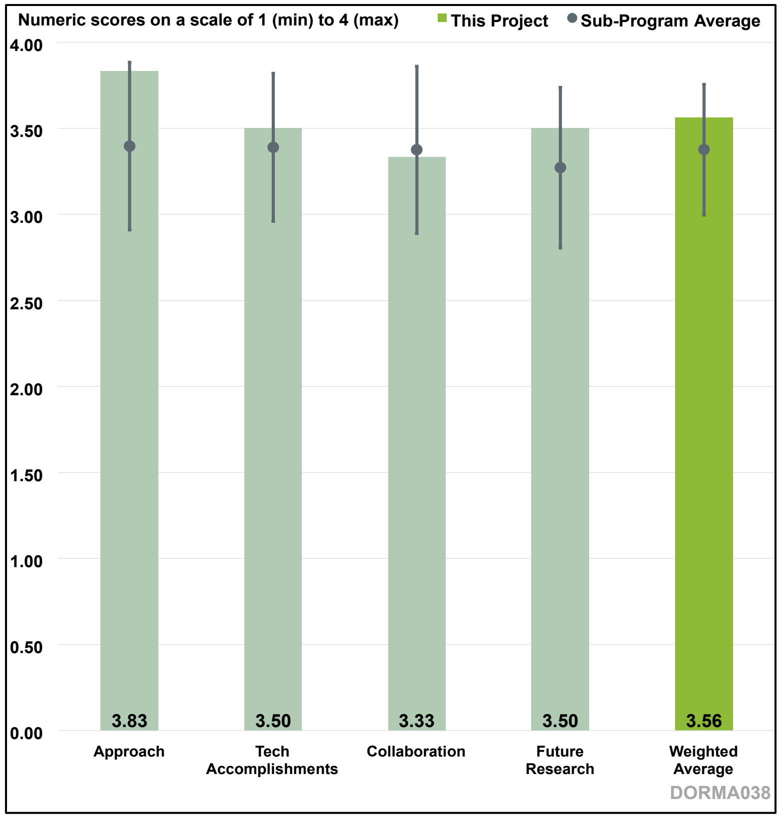

Figure 3-27. Presentation Number: DORMA038 Presentation Title: Towards Accurate Combustion and Emissions Modeling of Sustainable Aviation Fuels Principal Investigator: Debolina Dasgupta, Argonne National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The project is performing simulations that address fuel impacts on combustor operability (lean blowout and ignition) and is performing modeling work (wall-resolved LES) to improve the wall-modeled LES simulation of combustor operability. The project has also started work in two challenging areas that are important to quantifying and reducing aviation's impact on climate: soot modeling and contrail modeling.

Reviewer 2

This project aims to address two major SAF technical barriers: a lack of 100% SAF blends that meet conventional fuel performance and safety standards, and a lack of understanding of fuel formulation effects on engine performance and emissions. The project aims to do this with a three-pronged approach. First, high-fidelity combustion simulations will be developed, validated using optical diagnostics, and used to create sub-models that describe relevant flows. Second, these sub-models will be implemented in engine performance simulations which will be used to investigate the stability and sensitivity of SAF-burning engines, with comparison to a Jet A baseline. Third, the simulated engine performance will inform a computational investigation of soot behavior and contrail formation.

The proposed approach is sound, and the three focus areas create a logical division of interrelated tasks. The timeline is well-planned, with all milestones either complete or on track for completion.

Reviewer 3

This work focuses on development and use of simulations for assessment of SAF at realistic engine conditions. The PIs aim to develop reliable tools for predicting ignition, heat transfer, combustion instabilities (including LBO), and emissions/contrails over the range of operating conditions to be expected on a gas turbine engine. The duration for the proposed scope of activities (2022-2027) appears to be sufficient. Milestones for the current year's work are well laid out and the PIs seem well on their way to achieving them. Tasks dealing with LBO, cold-start ignition with plasma discharge modeling, and contrail formation are well delineated. The use of two combustors (Army Research Combustor [ARC] and referee rig) was a bit confusing to the reviewer. The reviewer questioned if it was because soot emissions were only available from the ARC combustor. In any case, validation of results for two combustor rigs is certainly a commendable effort. The collaborations with entities who can provide experimental data and validation support are well established. Overall, the project and proposed goals have the potential to make a significant contribution to the combustion and aerospace community as well as related industry partners. The focus on extending knowledge to engine performance on 100% SAF is also noteworthy.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

For improved LES modeling of LBO and ignition, the project is performing a limited set of wall-resolved LES (WRLES) for the ARC-M1 combustor. Non-reacting WRLES have been completed and compared to particle image velocimetry (PIV) velocity measurement in the ARC-M1 combustor and reacting simulations are underway. The details of what wall models will be developed based on these WRLES simulations was not presented other than noting these will address combustion and heat transfer modeling near the walls. There are challenges in having an efficient GPU-based spray solver and less stiff chemistry mechanisms for these WRLES (or near DNS) simulations. The progress is reasonable, but the reviewer believes it was uncertain whether improved wall models for wall-modeled LES (WMLES) will be available in time to impact to WMLES simulations for LBO or ignition. WMLES simulations of LBO in the Air Force Research Laboratory (AFRL)/University of Dayton Research Institute (UDRI) referee rig for individual and combined fuel property variations relative to the average Jet-A baseline have been completed for a limited set of property variations (density, viscosity, heat of combustion) and there are plans to extend such LBO studies to HEFA fuel and the ARC-M1 combustor (which is similar in combustor design to the AFRL/UDRI referee rig). The method for approaching LBO in the simulations appears similar to that followed in NJFCP (a set of step reductions in global equivalence ratio, sufficient flow through time simulated at each new global equivalence ratio [GER] and monitor time variation of global heat release rate at each new GER). It was not clear to the reviewer if GER was reduced in a constant step wise fashion after GER of 0.096 and 0.090. The reviewer was expecting GER values of 0.085, 0.080, 0.075, etc., for each property combination until LBO was reached. The reviewer was also surprised at the 10-12% difference in LBO GER predicted with only changes in heat of combustion and one or two other properties (density and/or viscosity) but using a fixed chemistry mechanism and spray injection conditions since the NJFCP experiments with average Jet-A (A-2) and Gevo alcohol-to-jet (C-1) had only a 8% change in LBO GER (0.0806 for A-1 versus 0.0869 for C-1 at the same starting conditions as these simulations).The project made some progress on the soot modeling goals by developing a

Jet-A mechanism with polycyclic aromatic hydrocarbon (PAH) chemistry using HyChem for A-2 and King Abdullah University of Science and Technology for PAH chemistry and comparing the large molecules from this 126 species mechanism with the more detailed LLNL mechanism for Jet-A with PAH. The project also completed some evaluation of existing soot models and performed some validation of core and bypass flow mixing typical of a jet-engine exit for a simple experimental geometry. These activities provide a reasonable start to efforts on soot and contrail modeling.

Reviewer 2

Two out of five and a half years of this project are complete, and the technical progress made so far is excellent. LES compares well to non-reacting PIV measurements of an optically accessible combustor. Initial engine performance simulations demonstrate significant sensitivity to fuel properties, as demonstrated by changes in flame shape, droplet distribution, and LBO equivalence ratio. The investigators have developed a soot mechanism and are building the computational framework needed for the third focus area of the study.

Reviewer 3

The PIs have presented results from reactive and non-reactive LES calculations conducted on a GPU-ported code for the ARC combustor from the University of Illinois. The influence of perturbing fuel physical properties (within ASTM spec limits) was investigated individually and in a combined fashion. Downstream effects on flame shape and symmetry (or lack thereof) was investigated. Correlations between observed flame shape/asymmetry were made with regard to perturbed fuel properties and are consistent with what would be expected intuitively from changes induced in atomization and combustion processes. Droplet size distributions and their effect on flame stabilization are presented. The reviewer said it would be very worthwhile to compare droplet size distributions to measurements if available. The reviewer also noted that some more effort to understand the reasons for flame asymmetry would be good and any possible comparison to experimental results through imaging/planar laser-induced fluorescence/etc. LBO was investigated for the various cases using a set simulation approach. The reviewer commented that comparison of LBO phi to those from experiments would have been good to have. Attempts to further correlate LBO phi to cetane number which has been recognized as a marker for fuel sensitivity to LBO is recommended. A soot and contrail modeling framework has been established. The reviewer said it was good to see the PIs leveraging efforts at LLNL and Sandia National Laboratories on this aspect. A key question would be pressure and temperature effects on the soot modeling and fuel chemical kinetics and to what extent validated kinetics models for SAF in particular are available as needed to conduct the LES calculations.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The project has good collaboration and access to test data for previous referee rig experiments conducted under NJFCP and experiments using the ARC-M1. Soot modeling is an area that would greatly benefit from increased collaboration among the DORMA projects especially for simulations of soot evolution using Jet-A and/or SAF fuels. The work on contrail formation near the jet engine exit and contrail evolution in the far field are both challenging areas for LES simulations. It was not clear to the reviewer how much experience the team has to start this effort so any collaboration within DOE or with other research groups actively engaged in LES simulations of contrails would greatly benefit this project. Validating such simulations is also challenging. The reviewer commented that comparisons to previous LES simulations for a particular aircraft and flight conditions may be beneficial or at least provide a longer-term target of some final set of simulations.

Reviewer 2

A very large number of groups collaborated on this project. Argonne National Laboratory leads a group of several national laboratories performing computational fluid dynamics tasks. Experimental results are provided by AFRL and The University of Illinois Urbana-Champaign. There is coordination with another DORMA project (019) that is providing experimental and simulated multiphase flow results. It is to be commended that this project brings together many different groups to tackle an incredibly difficult and multifaceted problem. However, the reviewer commented that the specific responsibilities of each group were left somewhat unclear. Computational fluid dynamics efforts are billed as a coordinated effort between five different laboratories. It was unclear to the reviewer, for example, what exactly ORNL will contribute to, as they are not mentioned elsewhere.

Reviewer 3

The PIs are collaborating with industry, a university, and other government laboratories. The reviewer noted that there does not appear to be a need for more collaborations. The collaboration with experimental groups to get data for validation and geometry/boundary conditions/etc., is key to this effort. The collaboration with other groups working on soot and contrail models is also very strategic and will help the project move faster to achieve their goals.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The proposed research is addressing important simulation capabilities: fuel impacts on LBO and ignition; soot modeling for jet fuels; and contrail formation and evolution. The reviewer said the proposed work on contrail modeling appears very broad and with the resources available may need to narrow its focus to achieve meaningful results in the next few years.

Reviewer 2

The proposed future work for this project is well-defined, likely to succeed, and fits well with the work that has already been accomplished. Direct numerical simulations will be developed to model combustion with improved resolution and fidelity over current large eddy simulations. Combustor simulations will move to HEFA fuels with a comparison to experimental rigs. Advanced soot models will enable high-accuracy contrail and cirrus formation simulations. This research contributes directly to the goals of the project and is achievable in the stated timeframe.

Reviewer 3

The project has identified key tasks related to high fidelity simulations, fuel and combustor performance simulations, and contrails modeling for future research. These activities are in line with the technical barriers that the project seeks to address. In particular, the DNS simulations and their ability to inform and improve the LES modeling efforts will be very useful. The PIs could also refer to ongoing DNS work from Souza-Soriano and Chen and their findings in this project. Evaluating SAF like HEFA and others will be of very high interest to the combustion community. While sensitivity to LBO to perturbing fuel physical properties is interesting, the PIs could potentially also generate a lot of interesting information about near-blowout dynamics through their simulations. The impact of droplet size distributions (which other investigations in DORMA have shown to be asymmetric and/or influenced by nozzle internal geometry), turbulence-chemistry interaction, multi-modal flame propagation phenomena, turbulence backscatter, etc., are very interesting and these simulations are ideal for examining such effects. Plans for contrail modeling in the near and far field are discussed and also in line with overall project goals. Potentially other emissions, particularly NO_x, could be incorporated within the framework of this effort.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The project is developing capabilities that address combustor operability fuel sensitivity, soot modeling, and contrail modeling. These are all important simulations capabilities for understanding and minimizing aviation’s impact on climate.

Reviewer 2

This project directly supports VTO objectives. It aims to create predictive simulations that can screen SAF candidates, enable SAF adoption, and analyze SAF combustor performance and emission effects. Achieving these goals will decrease the cost of SAF adoption, mitigate aviation environmental impacts, and enhance aircraft engine performance.

Reviewer 3

The relevance of this project to DORMA is supported through the stated goals of this work to develop predictive modeling capabilities that can provide a pathway for 100% SAF adoption. Further, through the efforts of this work to model emissions including soot and examining contrail development, metrics other than safety relevant ones (LBO, cold start) will be evaluated which have received less attention in past work. Development of improved heat transfer and combustion modeling techniques through the overlapping DNS and LES portions of this work will be beneficial to the community as a whole.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

For the milestones to be completed in FY 2024, the resources are sufficient. And for future work on wall-resolved LES, wall model development, and further LBO simulations, the resources are sufficient. The reviewer was concerned that the current resources may be insufficient to complete future plans to develop a simulation framework for high altitude relight predictions and predicting contrail formation and evolution for Jet-A and SAF. Those are very challenging efforts that likely require more than a few people working the effort.

Reviewer 2

The investigators have sufficient resources to carry out the project and the budget is reasonable. Collaborators have demonstrated that they have the experimental and diagnostics framework to produce high-quality validation data for simulations. Investigators at Argonne have demonstrated that they have the computing infrastructure and expertise necessary to perform the proposed simulations.

Reviewer 3

The reviewer said resources, personnel and financial, appear to be sufficient for this work.

Presentation Number: DORMA040
Presentation Title: Optimized Low Carbon Fuel Range Extender (HyREX)
Principal Investigator: Jon Dickson, Cummins

Presenter

Jon A. Dickson, Cummins

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

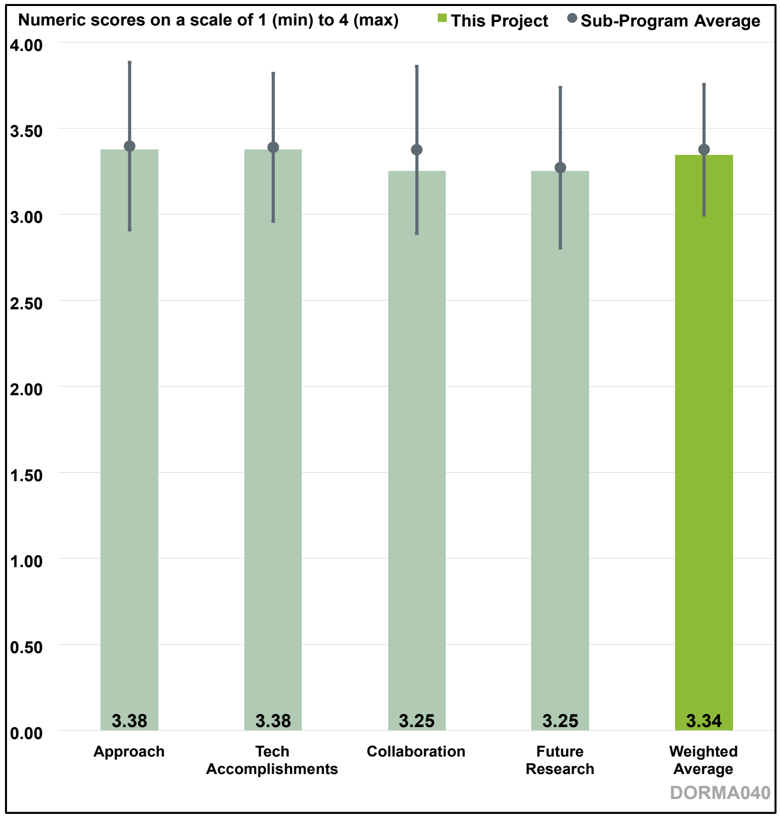

Figure 3-28. Presentation Number: DORMA040 Presentation Title: Optimized Low Carbon Fuel Range Extender (HyREX) Principal Investigator: Jon Dickson, Cummins

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

This project has just begun (15% complete) and is in its first budget period. The overall approach is good, but details will be defined as the data is collected. In BP1, the team plans to 1) define the simulation approach for technology evaluation, by defining the model requirements, architecture, interfaces, tools, machine types, power range, duty cycles and design space; 2) identify the low carbon liquid fuel (LCLF) pathways for techno-economic analysis by providing data on current market LCLF volumes, planned expansions and potential future volumes; 3) determine the layout of the motor-generator (MG) and inverter components, and finalize the MG topology and coolant strategies; and 4) define the base range-extended electric vehicle architecture and power-generating unit size for the range-extender and power-generating unit. The reviewer said this was an appropriate approach to defining the overall project.

Reviewer 2

The reviewer commented that the project plan seems reasonable for the scope of work. The project is still in an early phase, so there have not been many opportunities for setbacks or similar that would affect the schedule. The reviewer had some concerns about the schedule for the design, build, and demonstration phases, given that the design has hardly been started. If successful, the project will definitely address the barrier of decarbonizing non-road applications.

Reviewer 3

A range extender hybridized powertrain provides a very flexible approach to adapting to multiple offroad applications, particularly those with hydraulic power needs that can be electrified. Identifying the hydraulic power partner soon will be important to the success of the project.

Reviewer 4

The project relies on a lot of factors to fall into place and be defined during the final year of the project. Ther reviewer said this approach seems to have high risk associated with it. If successful, the approach would address the technical barriers that the team strives to overcome which is increased low carbon fuel adoption and demonstration of a 50% reduction in GHG. The reviewer noted that the lack of specifics in the presentation made it difficult to assess the likelihood of success.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The project is at 15% completion so at this point only the first milestone has been achieved. The reviewer commented that the timeline appeared reasonable, development of the optimization pathway was in process, and analysis on closed cycle, open cycle and mechanical efficiencies were ongoing. The reviewer also noted that the powertrain roadmap workflow was well-defined. Evaluation of range options, selection of machines, and duty cycle gathering is complete. Model development and cost input gathering are in progress and on-schedule. The TCO ranking approach has also been identified.

Reviewer 2

The reviewer questioned how a series hybrid configuration was different from a typical non-road equipment diesel-electric powertrain. For example, it was unclear to the reviewer what the opportunities for energy recovery were. The reviewer noted that energy recovery options were limited, and very application specific. The main benefit comes from aggressive powertrain optimization and from the use of lower-carbon fuels. The team is using an EAS solution from Cummins Emission Solutions to meet CARB Tier 5 non-road emissions requirements (NMOG+NO_x) that also accounts for the effects of fatty acid methyl ester biodiesel on the EAS. The goal is to narrow the operating range of the engine in the series hybrid configuration, hence the redesign of some engine components (Slide 9 in the presentation). The Cummins team is building a series hybrid system for demonstration, but they are evaluating other options as well in its modeling work.

Reviewer 3

The reviewer commented that it was very early in the start of this project, so most tasks were just getting underway. The reviewer would have liked to have seen more information on the machines and duty cycles that have been selected. The reviewer noted that the maps on Slide 21 did not provide enough information about the energy recover opportunities.

Reviewer 4

The project is effectively just getting started and is thus far meeting the proposed milestones.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

Collaborations with a university (Ohio State University), a national lab (NREL), and other partners seems well aligned, though the team is still working on selecting a hydraulic system partner which will have strong impact on the energy efficiency of the overall system.

Reviewer 2

The reviewer said that it looked like the overall collaboration was good among the team. The reviewer did not see a lot of engagement from Manitowoc yet but assumed that will come in later phases of the project. The reviewer was concerned that the team did not yet have a hydraulics supplier engaged on this project yet.

Reviewer 3

The reviewer commented that a hydraulic systems partner was needed.

Reviewer 4

The reviewer noted there were good partners and collaborations which seemed to be engaged at this point.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

Results from the first budget period will help to further define the follow-on work with the MG and inverter designs being the key portion of the work. From there, the remaining tasks will be able to be more fully defined.

Reviewer 2

Building a demonstrator is going to be one of the more challenging tasks of this project with lots of risk to the budget and schedule. The reviewer questioned what the team’s stretch target for GHG reduction was. The key innovation from this work is the high-temperature motor-generator and high-temperature inverter that will work well at 105°C, a typical temperature for engine coolant.

Reviewer 3

The reviewer said that the project plan looked good.

Reviewer 4

The stated that the proposed future work was too open-ended to fully evaluate for appropriateness. With further questioning, it was determined the project is focused on one or two fuels.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer noted that a 50% reduction of lifecycle analysis-GHG was an incredibly aggressive target. Additionally, there are a number of technological advancements proposed in this project that are definitely benefiting from DOE funding.

Reviewer 2

The project does support the VTO objectives since it is focused on decarbonizing non-road machines, both for agriculture and construction. Cummins is a reasonable lead for getting this series hybrid powertrain into production.

Reviewer 3

A 50% reduction in GHG emissions in addition to meeting CARB Tier 5 NO_x limits meets the DOE VTO subprogram objectives.

Reviewer 4

This effort supports decarbonization technologies and is thus relevant.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

At this time, the resources seem sufficient, but the project is only 15% in. The reviewer imagines that as the project progresses, there may be a need for additional funding.

Reviewer 2

The project has a budget of nearly $9 million, but it does involve building a demonstrator system and testing it. The reviewer was more concerned about the schedule than the budget.

Reviewer 3

The reviewer said the resources seemed appropriate, but most of the expense would be in building the demonstration machine.

Reviewer 4

The reviewer commented that the funding level from both DOE and Cummins was adequate for this project.

Presentation Number: DORMA041
Presentation Title: Low greenhouse gas NO_x control
Principal Investigator: Dhruba Deka, Pacific Northwest National Laboratory

Presenter

Dhruba Deka, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 60% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 40% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

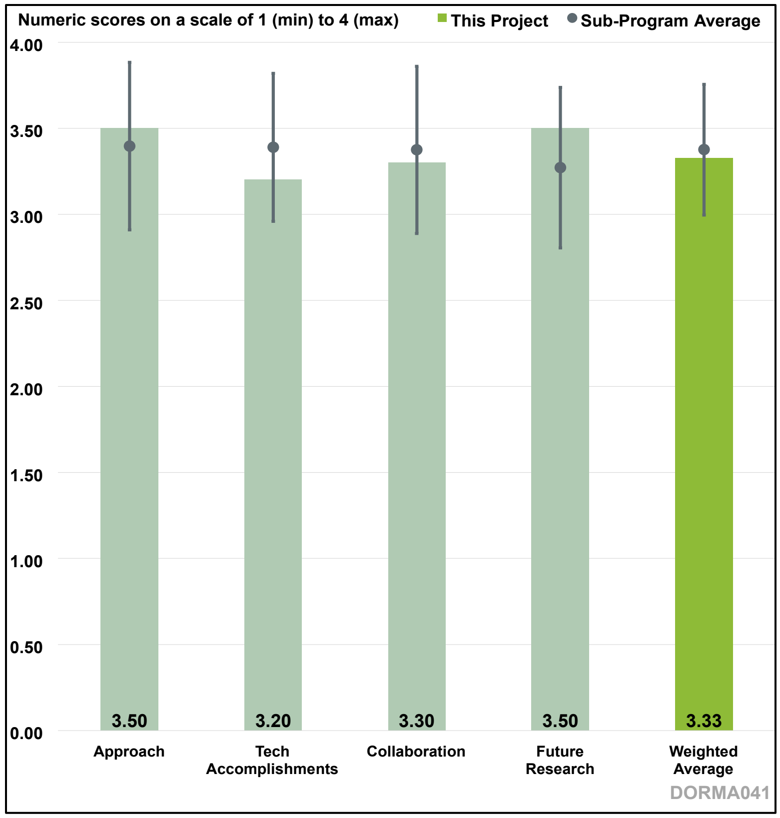

Figure 3-29. Presentation Number: DORMA041 Presentation Title: Low greenhouse gas NO_x control Principal Investigator: Dhruba Deka, Pacific Northwest National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer stated that the project clearly addresses the fundamental science that underpins technology barriers related to development of active exhaust catalysts that operate at low temperature, minimize GHG emissions, while minimizing N_2O formation. The mechanistic focus and emphasis on exploring a broad range of catalysts to interrogate effects of various structural and electronic motifs seems like a logical way to develop design overarching principles to help guide future catalyst development.

Reviewer 2

The reviewer commented that the project focus is solidly on reducing both criteria pollutants and GHG emissions from diesel exhaust aftertreatment systems.

Reviewer 3

The reviewer noted that this project address the N_2O formation mechanism in SCR and mitigation methodology, which addresses the GHG topic of diesel engines in both on-road and off-road applications. This project is well designed, and the timeline is well planned. The project team has completed the work as scheduled; however, research on nitrogen dioxide (NO_2) mitigation technology could be very challenging, so the team will need more efforts in next budget period.

Reviewer 4

The reviewer articulated the project technical goals as understanding the mechanism behind N_2O formation and identifying opportunities to reduce GHG emissions. Considering the approach to performing the work and progress, it appears that the two goals cannot be completed. This is understandable as the challenge is technically complex. However, the approach has to be revisited on a periodic basis and adjusted accordingly to increase the success chances of reaching the goals. Setting up specific quantifiable key performance indicators might help in achieving impactful outcomes. The feedback in other fields should provide a few relevant details.

Reviewer 5

The reviewer commented that the approach seems to be “cook and look” rather than following a hypothesis driven rational design (or at least this was not explained). Despite the amazing resources available at PNNL, the project team really is not set up for high throughput screening of materials; that seems to be better done at the supplier. Additionally, it was not clear that the experimental conditions represent real exhaust; zeolites can be particularly sensitive to those conditions.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer remarked that this team has made excellent progress in characterizing the NO_2 formation mechanism, and confirmed the sensitivity of N_2O formation to temperature, NO_2 pool, and the formation of N_2O through ammonium nitrate, which helps industry to develop the technology mitigating N_2O emissions from SCR.

Reviewer 2

The reviewer appreciated the work that has gone into developing the dual-bed SCR system, an iron-chabazite (CHA) SCR catalyst brick followed by a composite of a selective catalytic oxidation (SCO) catalyst blended with a copper (Cu)-CHA SCR catalyst, and noted good work with the accomplishments in this fiscal year (FY). A focus is on lower-temperature N_2O formation, in the 180° to 300°C range, since high-temperature N_2O formation greater than 450°C) comes from ammonia oxidation. It appears that there is not one single mechanism for N_2O formation on all catalysts. The project focus is then on Cu-CHA catalysts, since that is a common commercial SCR catalyst. Catalyst cost and complexity, especially the mixed SCO and Cu-CHA, will be a barrier to adoption.

Reviewer 3

The reviewer stated that the focus on mitigating N_2O formation seems appropriate, given industry identifying this driver for further investigation. Milestones have been completed or appear on track, including the specific goals of understanding the catalyst active site, the role of the zeolite support, and identifying opportunities to mitigate N_2O selectively which seem like key areas to study to make impacts in catalyst design. The approach generally seems rational with studying a range of Cu-exchanged small pore zeolite catalysts, and allowing various parameters such as metal loading, acid site density, and aging protocols to be tuned. The work has clearly demonstrated that multiple mechanistic pathways are operative and intermediates are less stable than the ammonium precursor result in N_2O formation, insight that can be used in future catalyst design. Using the knowledge gained from the mechanistic studies to move toward a multi-component system demonstrates the power of the approach. The resulting hybrid catalysts appear promising to break down NO_x with low levels of N_2O production.

In general, the reviewer appreciated the amount and depth of results presented. Despite this wealth of data, a slide focused more on the overall discrete mechanistic picture of what is going on in the systems would be very instructive; some elements of this appear in places (Slide 13), but a complete picture that covers the full catalytic cycle is not presented and would further enhance the work. While a multitude of techniques were mentioned such as transmission electron microscopy, electron paramagnetic resonance (EPR), X-ray, and nuclear magnetic resonance spectroscopy, these did not really appear as significant components of the data presented. This seemed like a missed opportunity and could be exploited more heavily in future studies.

Reviewer 4

The reviewer commended the really impressive number of samples screened, and some good insights that were able to come from this work regarding the stability of the intermediates that can lead to N_2O formation. However, there appears to be no mechanistic insight possible from this array of samples which do not appear to follow a single pathway. Perhaps it is too early in the project to evaluate the usefulness of the data and accomplishments.

Reviewer 5

The reviewer questioned information presented on Slide 6. How much variability or noise should be expected in the activation energy (AE) for N_2O, given the fact that they are very small numbers and that also measured in the regime is either high NO_x conversion, is limited by reactant availability, or in the measurement noise ratio? Regarding the Y axis for N_2O, is it rate of N_2O formation or converted parts per million (ppm) into logarithmic scale? If it is ppm converted to log scale, is it expected it to show a different AEs? SCR and N_2O formation do not share the same intermediate, therefore how is this conclusion derived? If they share the same intermediate, is the same AE expected? The project team does not have to form ammonium nitrate (AN) for N_2O; it is AN-like species on the catalyst surface that decomposes to N_2O. Were there any tests to confirm whether it is surface species or bulk-like AN; did the project team do any low levels of AN deposited on the catalyst followed by its decomposition and calculate the AEs?

Regarding Slide 7, the project team's technical objective is to understand the mechanism behind N_2O formation. If a single mechanism does not explain the N_2O formation, what is the path forward to resolve it, especially given there is almost no time left in this project? Without such understanding how can the formulation be optimized or the N_2O emissions quantified?

Regarding Slides 8-12, NO_2-containing feed gas reactions at low temperatures for example below 150°C certainly form bulk ammonium nitrate deposits and interfere with various reactions and decomposition processes. An overarching question is were such scenarios considered during the analysis and interpretation of the data in coming up with proposed reaction schematics? These are going to be important to create kinetics for quantifying in the application space.

Regarding Slide 14, the reviewer suggests the primary focus of solutions should be decreasing N_2O formation on copper (Cu) SCRs. Hybrid systems are not preferred due to application robustness challenges. Also, it will not solve the fundamental challenge of N_2O formation on CuSCR, a most widely used technology.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer stated that the team is comprised of a diverse set of individuals and institutions who generally bring unique expertise to the project. A project of this type clearly needs expertise in zeolite synthesis, active site modelling, characterization, catalysis, and reactor engineering. The roles of each institution were described sufficiently.

Reviewer 2

The reviewer identified a diverse collaborative team including OEMs, two catalyst suppliers, and two universities.

Reviewer 3

The reviewer remarked that PNNL has the state-of-art facility for the project team to complete this project. The support from BASF is critical for the project team to succeed. The reviewer is not sure of the role that John Deere and Cummins have played in this project. Overall, the project team has enough support in PNNL and from industry. There should be more funding made available to this project as N_2O is so important in this area, especially when a hydrogen engine is to be deployed as N_2O will be the key GHG emitted from hydrogen engines.

Reviewer 4

The reviewer commented that the project team is PNNL only, although the PNNL team is informally consulting with external partners on this project. Collaborations to date have been informal, involving soliciting information from commercial partners about what the key needs are. This feedback focused the project team on mitigating N_2O formation from SCR catalysts. The reviewer recommends collaboration with partners who could commercialize the SCR catalysts evaluated on this program.

Reviewer 5

The reviewer noted relevant partners and indicated that more partners may not be required. However, the reviewer could not tease out collaborators’ contributions from the generic description on Slide 15.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer stated that the N_2O formation mechanism has been well understood in literature and the research in this project. The key issue is how to mitigate N_2O emissions from SCR. The future work proposed in this project is well aligned with the critical problems needs be mitigated. The reviewer is sure the project team can and will make significant progress in this area.

Reviewer 2

The reviewer commented that the proposed future work is a logical continuation of the work to date. The goal is to set up a formal CRADA with external partners to help foster commercialization of the SCR catalyst concepts evaluated here.

Reviewer 3

The reviewer noted that the future work clearly builds on the technical achievements described in the presentation. Remaining challenges/barriers are adequately identified. However, some degree of defined metrics on the future slides, even if more qualitative, would be desired and is a bit lacking. Even for a more exploratory project of this nature, attempting to align with some semi-quantitative goals could be productive.

Reviewer 4

The reviewer stated that the proposed future work items are open-ended, in that the success criteria for generated knowledge use is not obvious. For example, generated knowledge will be codified into a model and the model will be validated, or the generated knowledge will be used to generate recommendations to address the low carbon fuel strategies to minimize or avoid excess N_2O formation and other metrics.

Reviewer 5

The reviewer commented that it was not clear, based on the earlier data showing that there are multiple mechanisms in the mix, which of them this work will focus on. Based on the work so far, will there be a down selection of materials?

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer noted that the project goals and approach align with VTO interests in developing improved catalysts or formulations for exhaust systems while reducing GHG emissions in the process. In this reviewer's view, the connection between performance and understanding at the atomic level of composition and dynamic behavior is an important aspect of the research.

Reviewer 2

The reviewer stated that this project is well aligned with the advanced engine and fuels area. There should be more funding made available in this project so that the project team can develop the methodology mitigating the N_2O issues from future carbon-free engines such as hydrogen engines and ammonia engines.

Reviewer 3

The reviewer commented that the project is relevant to overall VTO subprogram objectives. Projects such as this presents great opportunity for enabling reduced GHG emissions, and a smoother transition to renewable energy sources.

Reviewer 4

The reviewer remarked that one of the challenges of urea-SCR is that it forms N_2O from the NO_x in the exhaust. N_2O is a potent GHG, with a warming potential of about 300 times that of CO_2. Thus, finding copper zeolite SCR catalysts that have a very low selectivity for N_2O is necessary to make sure that a criteria pollutant problem does not become a GHG problem.

Reviewer 5

The reviewer commented that the project is relevant to VTO objectives.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer remarked that given the diverse skill sets of the partners and that they cover all the areas needed to prepare a range of catalysts, assay them in catalytic reactions, model active site behavior, and adequately characterize them, the appropriate amount of resources appear to be allocated across the partners.

Reviewer 2

The reviewer noted that the performance evaluation and other advanced characterizations tools exist at PNNL and catalyst development capabilities from suppliers and research expertise from all the participating collaborators are more than sufficient to define and achieve the milestones in timely fashion especially that are needed to identify practical solutions with solid underpinnings.

Reviewer 3

The reviewer commented that this team has an extensive research facility in PNNL to conduct the research work proposed in this project.

Reviewer 4

The reviewer commented that a FY 2024 budget of $300,000 seems sufficient for the bench-scale testing and associated analysis that the project team looks to do. This project is part of a series of single-year projects.

Reviewer 5

The reviewer stated that the resources appear more than sufficient.

Presentation Number: DORMA042
Presentation Title: Unforeseen challenges with renewable fuels
Principal Investigator: Konstantin Khivantsev, Pacific Northwest National Laboratory

Presenter

Kenneth G. Rappe, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 67% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 33% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

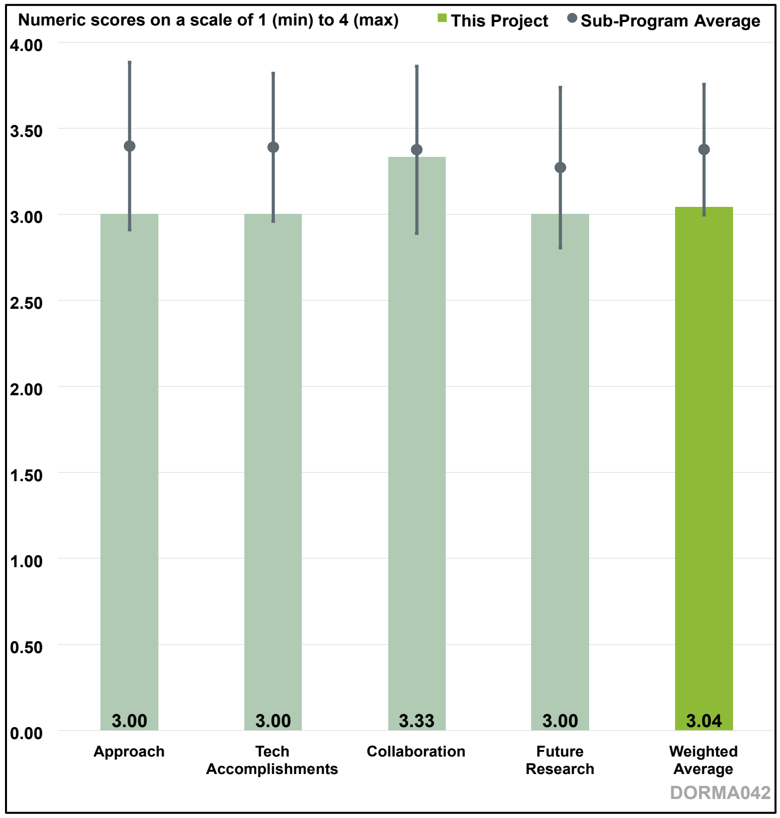

Figure 3-30. Presentation Number: DORMA042 Presentation Title: Unforeseen challenges with renewable fuels Principal Investigator: Konstantin Khivantsev, Pacific Northwest National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer stated that the study focuses on impact of renewable fuels on aftertreatment systems, specifically biodiesel. Has a survey of biodiesels across the country been conducted? Phosphrous has been identified as a target species to study; is there any background on the levels of phosphorus in market fuel?

Reviewer 2

The reviewer commented that the project clearly addresses core research and development guided toward technology barriers related to challenges associated with H_2 ICE emissions and improving durability of ammonia (NH_3) SCR catalysts. It is less clear from the presentation the connection of the studies to the on track goal related to aldehyde oxidation. Even if dealt with in another presentation, more explicit mention of the connection should be provided in the slides. The lower-end TRL work is needed to clarify challenges in these areas and look for general principles to guide potential solutions in next generation catalyst design, striving for low temperature, durable catalysts that remain effective in their role. Understanding the fundamental issues that arise in emissions streams from various contaminants (phosphorus, water, and certain organics) is certainly a topic of value, given that it was also mentioned in the presentation as being suggested from industry feedback.

Reviewer 3

The reviewer identified the project technical goals in support of a hard to electrify sector and in using next generation renewable biodiesel and hydrogen fuels to be identifying or clarifying the challenges and removing the barriers such as minimizing the detrimental effect of poisons derived from renewable fuels.

The approach to performing the work selected phosphorus contaminant for studying biodiesel-derived contaminants; the rationale for the selection of this contaminant for the study are not obvious. Major challenges using biodiesel are trace level of contaminants like potassium and quantifying its impact and potential mitigation strategies based on sound science. Similarly, the fuel properties like sharp but high boiling point will bring additional new, unique or difficult engineering issues and how these species interact with catalyst components in a quantified (kinetics) way are still a gap. Such important aspects were not considered in the approach. The approach did not indicate plans for removing the barriers. The approach must focus on specific fuel; without such consideration the studies will be superficial and incomplete.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer commented that given the nature of the catalyst systems involved, which are complex multi-atom alloys, the need for molecular level insight into how these catalysts operate and change during reaction is very important to guide future catalyst design. General milestones seem completed or are stated as on track. Valuable results have been obtained in the view of this reviewer. For one, the effects of water and phosphorus have been explored and given the differences in catalyst behavior from commercial and in house versions with phosphorus contaminants, it is clear great care is needed when baselining and drawing conclusions from batch to batch. This further demonstrates the need to work out and understand these discrepancies in a controlled environment.

The advanced tools brought forward by the project team to characterize the systems is a clear strength. The advanced microscopy and elemental mapping are critical to the effort, along with X-ray methods very useful to see changes in the NH_3-SCR catalysts and the role of hydrogen (H_2) as a partial reductant. A potentially promising H_2-SCR catalyst has been developed that reduces Pt loading, while the multi-stage concept also seems interesting with shunting of NO_x to a low temperature reactor bed allowing high temperature NH_3-SCR to still occur. It was a little difficult for the reviewer to see how the economics of this type of system might work in practice, but it is still critical to develop lower TRL concepts like this if they indeed accomplish the goal of negligible N_2O emission so they are ready if the time is ever right for scaling. The reviewer was surprised at no mention of publications. For a lower TRL research and development effort, this is pretty disappointing not to have a discrete plan for some dissemination of the very carefully performed studies. The reviewer would hope some part of the in house/commercial material story behaving differently in the presence of phosphorus could be of great value to the community. This seemed like a missed opportunity not to have some degree of focus on broader distribution of the work.

Reviewer 2

The reviewer stated that the impact of water on N_2O formation is a very interesting result, specifically 0% water exhaust where the N_2O formation window is shifted. The implications for a hydrogen engine is significant at the low temperature window. Should engine calibrations target a higher engine out temperature to around 300° C SCR temperature to get higher NO_x conversion as well as lower N_2O formation? N_2O formation in H_2-SCR appears to be a significant problem; are there mitigation strategies being researched? The combination of H_2-SCR and NH_3-SCR is an interesting approach, complexity of system could be a barrier for packaging reasons for off-road applications.

Reviewer 3

The reviewer commented that for the DOC study, it was not obvious what the technical outcome means to the path forward. Were the commercial DOC technologies studied under this project representative of next generation DOCs, in other words state of the art DOCs? If not, it is strongly suggested to work with catalyst companies to procure the latest technologies which could be advanced designs whose chemistry and physics of interactions are expected to be different. The underpinnings of contaminant impact on such technologies are critical for identifying advanced solutions.

On slide 9, what does the ratio of N_2O rate to NO_x conversion rate convey? In addition, there were no insights into the important observation of N_2O increase with increase in H_2O concentration through the studies.

Regarding Slide 10, the impact of H_2 on long term NO_x conversion is an important nuance. However, the technical rationale provided to explain the nuance is substantiated with limited characterization information, if any. Such impactful findings are expected to be followed upon with solid experimental evidence such as operando copper species characterization or other specific probing techniques. It is also expected for the project to provide technical insights under long term exposure to H_2-containing feed gas, under practically relevant conditions but such attempts were not made.

Slide 11 reiterates known technical challenges and no major nuanced insights and solutions. What would be the recommendation from these studies on the H_2-SCR TRL?

Regarding Slide 12, the question is what the expectations from this study were, given the practical application of the proposed technical approach as a solution and the intricacy associated with it (requiring H_2 fuel, safety, sensors, valves etc.) makes it difficult if not impossible.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer appreciates the breadth of industrial collaborations. This is an absolute necessity in a lower TRL, more research and development environment to be able to identify the key issues and bottlenecks various parts of industry encounter and need help solving. Access to the expertise across catalyst formulation, engine, and system design is critical to the effort focusing on the types of issues that advanced characterization methods can shed the most insight on and to ultimately maximize impact of the research.

Reviewer 2

The reviewer noted relevant partners. More partners may not be required, however, the reviewer could not tease out current collaborators' active contributions from the generic statements on Slide

13. Listing specific and concise contributions of collaborators will help in better assessing the effectiveness.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer stated that there are solutions such as Clearflame technologies that are developing E98 fueling for compression ignition engines. The reviewer thinks the impact of E98 type fuels on current SCR formulations would be interesting to focus.

Reviewer 2

The reviewer remarked that in general, the future areas seems reasonable and binned in ways that can provide impact and insight from additional characterization of the systems, explore further designs of systems involving H_2 SCR and NH_3 SCR improvements, as well as examining oxygenates further. It was a missed opportunity to at least have a slide on the final topic, as there was little or no reference to this milestone in the deck.

Reviewer 3

The reviewer commented that the breadth of proposed future work will not allow focused identification of specific critical challenges, technical underpinnings and solutions. The project teams needs to select a specific fuel for the hard to electrify sector and address challenges and identify solutions. Oxygenated fuels are also studied at ORNL for a couple of years; what different and additional technical aspects will be addressed by PNNL? The project team needs to identify synergy between PNNL's proposed work and ORNL's current project work and must avoid redundancy. For H_2 ICE work, without understanding the technical underpinnings, for example N_2O increase mechanism, how is it possible to identify solutions as indicated by future plan? The reviewer suggests revisiting such proposal and comprehensively address scientific reason behind the increase in N_2O with increase in water (H_2O) and similarly other nuances.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer stated that the project goals and approach are well aligned with VTO interests in understanding the challenges with use of biodiesel streams in engines and exhaust catalyst systems. The work here can give key insight into the issues that arise with various contaminants and the ways they can be mitigated, either through separations on the front end or use of new catalyst designs. By understanding the change in catalyst structure over time, it should be possible to identify when major problems will arise and potentially impact catalyst durability and provide a path to potentially circumvent such issues by innovative reactor design or reformulation of catalyst.

Reviewer 2

The reviewer remarked that the impact of renewable and low-carbon fuel on engine and aftertreatment is highly important understand to develop mitigation strategies for pre-mature component failure. This will directly help in adoption of renewable fuels into current powertrains with minimal modifications.

Reviewer 3

The reviewer commented that project is relevant to overall VTO subprogram objectives. Projects such as this present great opportunities for enabling reduced emissions, energy security and transition to renewable energy sources and play a significant role in achieving more sustainable transportation solution.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer noted that the performance evaluation and other advanced characterizations tools exist at PNNL; catalyst development capabilities from suppliers and research expertise from all the participating collaborators are more than sufficient to define and achieve the milestones in a timely fashion especially that are needed to identify practical solutions with solid underpinnings.

Reviewer 2

The reviewer stated that given the diverse skill sets of the partners and that they cover all the areas needed to identify the types of contaminants that need to be studied and the characterization tools required to understand the systems of interest, all required resources were present.

Presentation Number: DORMA043
Presentation Title: Low-load cycle emission control
Principal Investigator: Yong Wang, Pacific Northwest National Laboratory

Presenter

Yong Wang, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 60% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 40% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

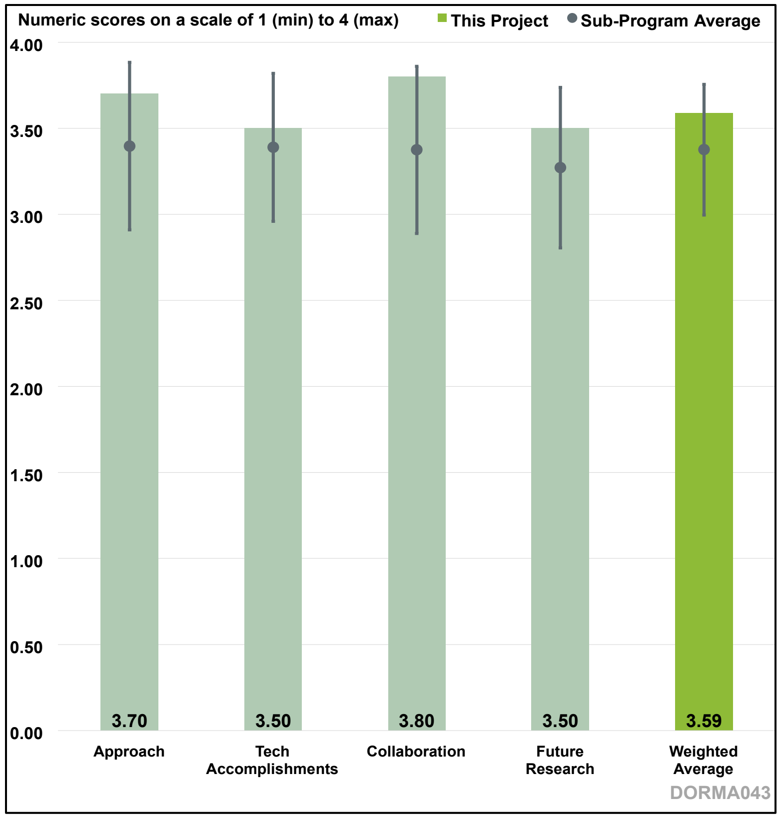

Figure 3-31. Presentation Number: DORMA043 Presentation Title: Low-load cycle emission control Principal Investigator: Yong Wang, Pacific Northwest National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer commented that the project clearly addresses fundamental science issues related to technology barriers involved in development of next generation, emissions exhaust systems. The goal of accessing more durable, cost effective, and still highly active at low temperature catalysts is a valuable one. The mechanistic focus seems like a reasonable approach to understand general design parameters for next generation catalyst formulation.

Reviewer 2

The reviewer remarked that the low efficiency of SCR in reducing NO_x at low temperature is one of the critical issues for the diesel industry to meet the new NO_x regulations. This project is well designed which is supported by the experimental research work about catalyst composition examined, the range of temperature tested and the effort in examining the reduction half cycle (RHC) kinetic modeling. The time line is well planned as the project team has completed all proposed work as planned; the data presented in this review meeting provided evidence of work completed.

Reviewer 3

The reviewer noted a very detailed fundamental experimental project that addresses low temperature SCR activity for off-road applications. Catalyst durability is an important parameter to be characterized accurately.

Reviewer 4

The reviewer stated that for the issues to address in this project, the plan was well laid out. Adding the use of operando EPR was critical in the reviewer's view.

Reviewer 5

The reviewer remarked that the project goal is to identify opportunities to improve low temperature activity, extend useful life, and/or reduce cost associated with emission control from low carbon fuels for hard-to-electrify applications that are aligned with industrial priorities The approach to performing the work was generic in description. Specific details of strategy process in defining the opportunities and challenges are missing; it was difficult to assess the end goal and timelines for meeting end goals.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer commented that the results for the NH_3 SCR catalysts certainly appear promising with the studied Cu zeolite systems. Theory has played a key role to understand conversion of a redox resistant form of the Cu sites to something more likely to undergo reduction while also helping to understand why the process favors one type of zeolite support over the other. It is good to see the direct value of the experiment-theory interplay here as well as treatment of the full reaction mechanism in the backup slides. Kinetic modeling, though very different than reaction modelling, also plays an important role in the project and highlights the need for a team with varying expertise. Use of EPR to study copper sites is well chosen and a sound technique to assist in understanding of oxidation states present in the various catalysts. The studies provided on understanding NH_3 inhibition are very important, given the field aged catalysts exhibit similar profiles. The probe of NH_3/NO ratios is also valuable to tease out the distinct impacts on RHC versus oxidation half-cycle. The six publications and three presentations are impressive productivity, with many of the reports appearing in high impact factor forums. This ensures dissemination of the fundamental knowledge gained in these studies is available for the broader catalysis community and could demonstrate impact well beyond the field of emission control catalysis. Project milestones seem on track. The team has performed the fundamental studies into SCR catalysts and the project will culminate in use of these insights to develop next generation catalysts.

Reviewer 2

The reviewer stated that this team has completed the tasks proposed. The data presented in this review meeting demonstrated the progress in this project.

Reviewer 3

The reviewer remarked that the characterization of the role of ammonia inhibition is a important finding. Are there preventive measures? Was any transient emissions tests performed?

Reviewer 4

The reviewer identified a variety of nuanced technical insights; however, how this information was used to improve the technologies or applications should be attempted with the help of industrial partners/collaborators.

Reviewer 5

The reviewer observed that the number of technical accomplishments was impressive in the time so far for the project. They were well presented and put in the order needed to make the case for what was and was not limiting the active sites. Still there is little time left to get to important remaining issues on the best way to proceed for the hard to electrify applications.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer stated that this project has collaboration with OEMs such as John Deere and Cummins and suppliers such as BASF and Zeolyst. The input from industry and aged SCR systems are critical for this project to succeed. There is no need to have other external entities.

Reviewer 2

The reviewer commented that overall, the team is comprised of a diverse set of entities that bring singular skill sets to the project. Of particular note in this project are the collaborations with theory and characterization, given these two areas were critical to studying the reaction mechanism of the systems. At the same time, it is also important to have industry partners involved that provide key knowledge of how these systems need to bridge to technology. Reliable access to field samples and aging protocols consistent with real-world aged catalysts is also important to ensure catalysts studies in the lab generally mimic field performance.

Reviewer 3

The reviewer noted that there were excellent partners in this project, familiar with the issues and in the tools needed to study them.

Reviewer 4

The reviewer affirmed excellent industry, academia and national lab collaboration.

Reviewer 5

The reviewer noted relevant partners. More partners may not be required, however, the reviewer could not tease out their active contributions from the generic statements.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer remarked that the proposed future research challenges in this project will be met by the proposed approach, especially for off-road applications.

Reviewer 2

The reviewer stated that this team has a very clear picture of the future research work. The research work proposed are typical but not new to this research community. The engine-out emissions from off-road engines should be well-known information, so it is not necessary to have it listed as a major work. The degradation factors, including thermal and chemical factors, are two well-known factors many researchers have evaluated. It may be a good idea for the research team to evaluate the changes in catalyst coated and also if there are any other chemicals that have covered the catalyst. The principal investigator may have had this included in their research in chemical factors, which should be the focus for research to aged SCR system. The testing and aging protocols simulating real world off-road challenges is important in SCR development, but it should be much easier than on-road operations, which can be completed by OEMs other than this team, so it may be a good idea to have this item removed from future work, so this team can focus on SCR catalyst and its aging research.

Reviewer 3

The reviewer stated that the proposed work description is at a high level and should attempt to provide details in backup slides. The proposed future work appear to extend and complete the identification of barriers in the context of off road applications.

Reviewer 4

The reviewer commented that the slide on future barriers and work seems to address major overarching issues, though a few statements are generic and could be further expanded on to some degree with a next level of detail (thoughts on improving durability as one example). Regardless, the key stumbling blocks, such as durability, are identified and the reviewer has no doubt the team will make progress in this and other areas. The reviewer cannot reiterate enough the key advantage of having access to field aged and “real” catalyst systems to examine in these studies. The collaboration across the National Lab group and industry makes this possible and is a strength of the effort.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer commented that this project is directly relevant to advanced engine and fuel technologies. The aging of SCR catalyst has been one issue bothering the diesel engine industry for years. The low efficiency of SCR in reducing NO_x at low temperature is the major barrier in reducing NO_x emissions as low load operation is very popular in many operation scenarios. The reviewer trusts this project is an excellent example that DOE funding can play in the future.

Reviewer 2

The reviewer commented that the project is relevant to overall VTO subprogram objectives. Projects such as this present great opportunity for enabling reduced emissions, energy security and transition to renewable energy sources and play a significant role in achieving more sustainable transportation solutions.

Reviewer 3

The reviewer remarked that the project goals and approach are well aligned with VTO interests in developing improved SCR catalysts for advanced emission control systems. The fundamental understanding of the reaction mechanism is also valuable for the broader research community and provides unique insight into Cu zeolite chemistry.

Reviewer 4

The reviewer stated that aftertreatment for NO_x will be needed for LLCF that are being studied along with other alternative fuels that make NO_x. This project is very relevant to the goals of these projects.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer stated that given the diverse skill sets of the partners and that they cover all the areas needed to probe the mechanism of the Cu catalysts, all required resources were present. In closing, the reviewer would just highlight again the key contribution of the computational and kinetic modelling effort plays in the work. The project exemplifies the potential of bringing together a team well-versed in experimental and computational catalysis and the impact these interactions can have.

Reviewer 2

The reviewer noted that performance evaluation and other advanced characterizations tools exist at PNNL and catalyst development capabilities from suppliers and research expertise from all the participating collaborators are more than sufficient to define and achieve the milestones in timely fashion. However the reviewer strongly suggests to align with industry partners on the remaining milestones.

Reviewer 3

The reviewer remarked that as stated in slides and the talk, this project makes very good use of the experimental tools available at PNNL.

Reviewer 4

The reviewer commented that national laboratories such as PNNL always have excessive resources for them to conduct the state-of-art research. The support from industry partners is also critical for the success of this project. The resources are sufficient for this team to achieve the stated milestones on time.

Presentation Number: DORMA045
Presentation Title: Biodiesel poisoning of close-coupled SCR catalysts for off-road engines
Principal Investigator: Todd Toops, Oak Ridge National Laboratory

Presenter

Todd Toops, Oak Ridge National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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

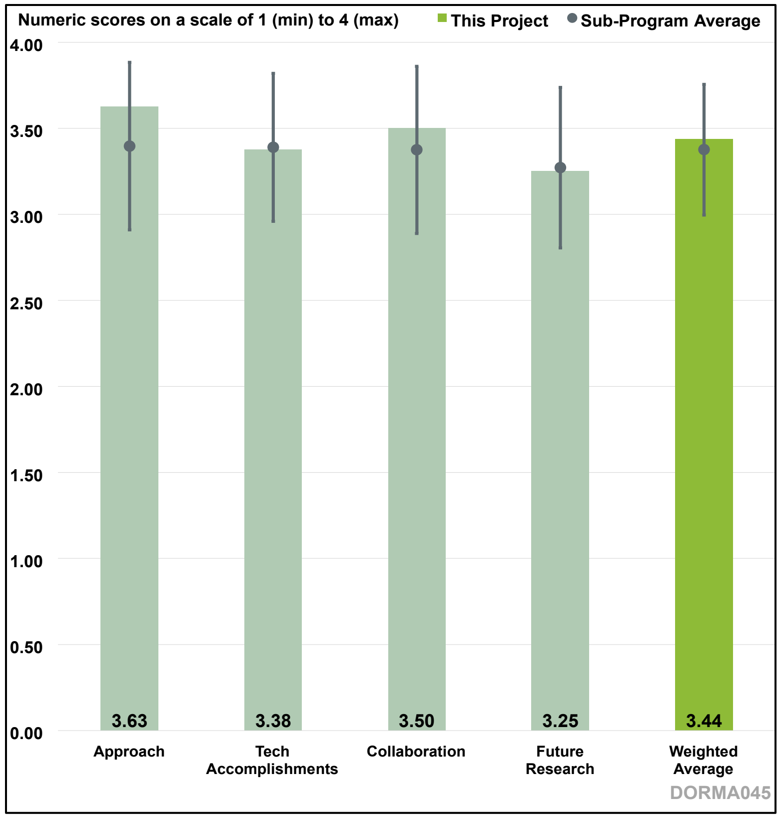

Figure 3-32. Presentation Number: DORMA045 Presentation Title: Biodiesel poisoning of close-coupled SCR catalysts for off-road engines Principal Investigator: Todd Toops, Oak Ridge National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer stated that the approach to this project is impressive, representing a very systematic approach to determine the impact of metals on SCR aging and determine methods for minimizing the acceleration factor. The investigators will identify where the metals are interacting with the catalyst and correlate the locations to changes in function in order to create better predictive models. They will achieve this by engine aging the samples with doped fuels, then use spatially resolved capillary inlet mass spectrometry (SpaciMS) to determine the local performance data. The reviewer cannot think of anything that is left out of the approach.

Reviewer 2

The reviewer remarked that the project clearly addresses technology barriers related to catalyst poisoning by contaminants in biodiesel-derived fuels within associated emission control exhaust systems. The work will also have implications for ultimately reducing carbon intensity of fuels/engine systems given the knowledge imparted about effects on catalyst from impurities in biodiesel streams. This could affect the types of purifications needed prior to engine/exhaust system exposure (as one example). There is a clear need to improve understanding of how these contaminants impact exhaust catalysts; "baselining" these effects with standard biodiesel and SCR catalysts is critical for the field as a whole.

Reviewer 3

The reviewer commented that the project appears to be on track.

Reviewer 4

The reviewer noted a great project to determine aging of vanadia-based selective catalytic reduction (V-SCR) with 100% biodiesel (B100), which is very applicable to current on-road HD engines and future Tier 5 engines. The project has a good overall design, testing methodology and measurement technique. The reviewer suggested maybe allowing some time for another iteration with higher doping levels if results are not very aged.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer noted great progress in setting up test equipment and measurement technique.

Reviewer 2

The reviewer commented that the project has just started and the progress is on target, getting things quoted and purchased.

Reviewer 3

The reviewer stated that support hardware and protocols are in place, and the project team is ready to execute the aging study. For the table on Slide 4, please verify the Tier 3 emission limits of 9.2 g/kWh instead of 4.0 g/kWh. Please also pay attention to the fine print of 0.4 g/kWh vs 0.40 g/kWh due to rounding number allowance, and for 0.040 g/kWh for CARB Tier 5. For good bookkeeping, the reviewer recommends the project team gets an estimate of engine oil consumption from an OEM and predict the sulfur exposure from both oil and B100 for the intended durability test duration. Even V-SCR is known not to be sensitive to sulfur poisoning. In addition, the project team should characterize the engine out emissions, flow and temperature of the Type D2 ramped modal cycle test with B100 and ultra-low sulfur diesel (ULSD). Finally, a DEF) sample should be analyzed for impurities as a good engineering practice.

Reviewer 4

The reviewer remarked that the presented vision for the work is clear in that moving to close-coupled SCR systems leaves a greater susceptibility to chemical poisoning. The summary of challenges with biodiesel containing higher metal content is well presented. A better fundamental understanding of metal impact on catalyst durability and effect on structure is key to maximize efficiency and longevity of the exhaust systems. In general, the conceptual plan in place seems logical and the established protocols in Slide 6 seem systematic and thorough. The reviewer was curious why phosphorus did not really seem to be a focus of doping in the B100 fuels relative to the other metals? The reviewer may have misread the slide, but it seemed like phosphorus content was not an emphasis and the reviewer did not recall this being expanded on further in the verbal presentation.

The SpaciMS seems like a unique and valuable technique to help correlate changes in activity to metal distribution. However, the presentation was a bit superficial in correlating results from the systems studied to insights on potential effects on the exhaust catalyst. Especially considering the scaled setup is not yet in place, spending some additional time on the results that have been obtained here and their potential significance for the future studies was desirable. Other products beyond milestones such as two presentations and a publication are also worth note. The publication is in a high-profile catalysis journal and provides a valuable impact of the work beyond just the specific study. The scoring here is in part due to lack of any discrete milestones in line with most of the other projects evaluated. Some idea of explicit timeline for the next series of activities would be helpful and seems like an omission to this reviewer.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer remarked that all teams seem to be working together to meet project targets. ORNL is coordinating very effectively.

Reviewer 2

The reviewer noted a good team with both formal and informal collaborators and a good plan for communication.

Reviewer 3

The reviewer recognized that cross-functional collaboration with suppliers and OEM is apparent.

Reviewer 4

The reviewer commented that the team represents a diversity of expertise one would expect for this type of project. Each member plays an important role, from the Clean Fuels Alliance America supplying the biodiesel to getting necessary catalysts samples or standard aging protocols for testing from industry partners. Clear investment from industry partners is seen with the matching funds and help with needed equipment purchase and setup. The large capital investment to set up the various system components is recognized. Lots of moving pieces still seem like they are coming together for testing in Year 2 in a reasonable fashion. However, not providing some more discrete timelines for Year 2 seems like a missed opportunity.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer stated that the future directions are to carry out the thoughtful approach.

Reviewer 2

The reviewer noted that as mentioned above, the conceptual framework is strong; it just seems like a chance to provide a better understanding for the full system setup and the stages of data analysis was missed. The project team seems poised to execute, but the fluid nature of the milestones and activities in Year 2 is a bit surprising for an applied project.

Reviewer 3

The reviewer suggested that as stated in response to Question One, maybe add some future test time for increased doping.

Reviewer 4

The reviewer requested that in a future report, please include engine out emissions of D2 cycle (B100 and ULSD) and indicate if the engine has EGR. The researchers could define what is the size of close-coupled SCR (relative space velocity), expected NO_x conversion efficiency in order to judge the severity of degradation and tolerance from impurities from B100 exposure.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer commented that the use of renewable, low carbon fuels like biodiesel is likely to be limited by the ability to meet regulatory limits for emissions. In particular, biodiesel which does not have an ASTM International standard for its neat use, can therefore have contaminants that do not bother the engine/combustion but can wreak havoc on the aftertreatment system, which has been seen for years with respect to DPFs. In order to meet the coming Tier 5 regulatory limits for NO_x, aftertreatment will become even more important, and particularly, industry will need to be certain that the SCR is compatible with higher levels of biodiesel blends to achieve both low (net) carbon fuel targets along with the regulatory targets for NO_x. Therefore this project is not only relevant, it is essential; the reviewer thinks that the industry funding that was volunteered is an excellent indication of that.

Reviewer 2

The reviewer remarked that the project goals and approach are well aligned with VTO interests in understanding contaminant effects on use of biodiesel in engines and catalyst exhaust systems. This will be critical to understand as industry moves to incorporating larger percentages of bio-derived fuels into the supply chain. In this reviewer's opinion, the connection between performance and understanding at the atomic level of composition and how the catalyst changes based on exposure to these elements is essential to moving the field forward.

Reviewer 3

The reviewer noted that this project addresses one important aspect of the B100 impact to one potential aftertreatment system (system with a close coupled V-SCR). B100 induces other changes of engine out characteristics, exhaust temperature and NO_x, etc.; the sensitivity of catalyst degradation depends on engine out NO_x, NO_x conversion efficiency target and size, etc.

Reviewer 4

The reviewer stated that the project is extremely relevant to today's U.S. Environmental Protection Agency vehicles and future Tier 5 off-road engines.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer stated that every indication is that the team has the needed resources to complete the proposed work. It is clear the partners are vested in the project moving forward. This applies to both the industry and trade association groups associated with the project.

Reviewer 2

The reviewer observed a very effective use of resources with simplified test equipment and test procedure.

Reviewer 3

The reviewer noted that the project team appears to have the right tools and knowledge base to execute the project. The project team might want to think ahead what key questions will be addressed through this study and what will not.

Reviewer 4

The reviewer commented that at this point, resources seem sufficient; however, as the project moves forward, the reviewer can see where additional experiments or diagnostics may be needed.

Presentation Number: DORMA046
Presentation Title: Ammonia for 4-stroke Marine Dual Fuel and Gas Engines (Retrofits and New)
Principal Investigator: Scott Curran, Oak Ridge National Laboratory

Presenter

Scott Curran, Oak Ridge National Laboratory

Reviewer Sample Size

A total of two reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 50% of reviewers felt that the resources were sufficient, 50% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

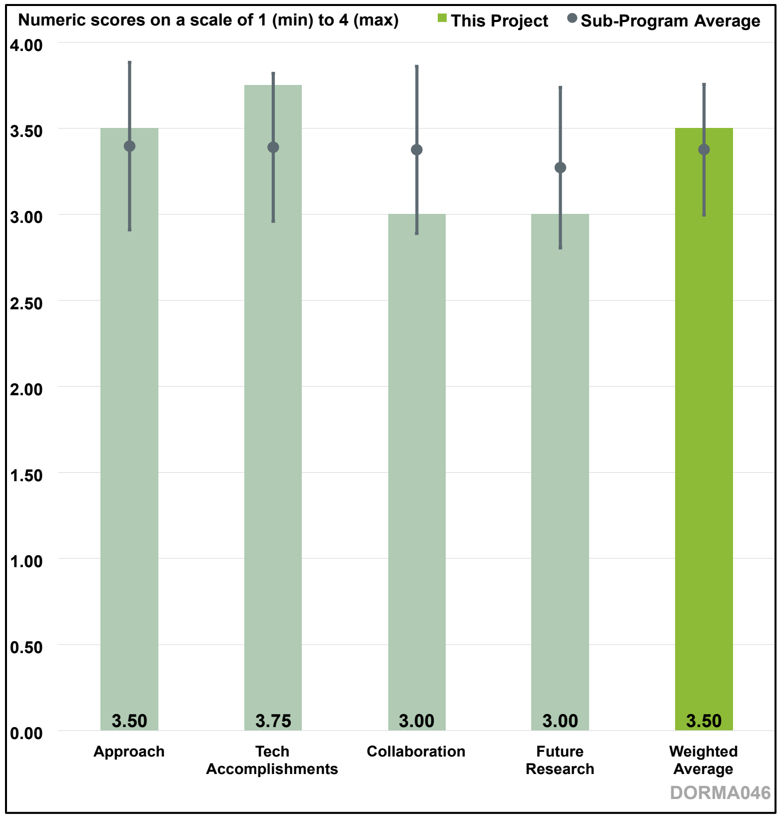

Figure 3-33. Presentation Number: DORMA046 Presentation Title: Ammonia for 4-stroke Marine Dual Fuel and Gas Engines (Retrofits and New) Principal Investigator: Scott Curran, Oak Ridge National Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer remarked the overall program is a nice mix of applied internal combustion engine development coupled with flow reactor and aftertreatment studies that address multiple facets of research on ammonia-fueled engines for marine applications. The focus on retrofit narrows the overall scope somewhat and aligns with the direction for auxiliary engines being used on large marine vessels as well as prime movers for medium-size commercial vessels. The reviewer noted the overall timeline is relatively short, but given the progress made thus far, and a clear program path, the timeline seems achievable.

Reviewer 2

The reviewer said this project is an interesting study to assess the viability of ammonia as a fuel in 4-stroke marine engines. Included are ammonia as a fuel in its own right and hydrogen-assisted combustion of ammonia. The project incorporates a team to investigate the feasibility for ammonia as a fuel in diesel 4-stroke, dual-fuel 4-stroke+hydrogen, as well as spark ignition 4-stroke and emissions control strategies. The PIs are using a single cylinder engine modified for dual fuel ammonia operation to assess performance. The reviewer noted the project also included a medium-duty multi-cylinder diesel engine. The emphasis of past work appears to be on 2 stroke engines. This project has intended to fill this gap with an emphasis on marine engines in particular. The reviewer said that here, the concern of N_2O emissions is noted with its greater impact as a GHG by a factor of 300 compared to CO_2. The dual fuel approach is quite interesting.

The reviewer said that a consideration for the use of ammonia as a fuel that was not clear from the presentation concerns its low vapor pressure. Ammonia is a gas in the standard atmosphere. This would impact its storage, transport and injection. The reviewer recommended the PIs should have a slide in their presentation which summarizes this potential concern. Also, some consideration on the production/supply of ammonia to meet the needs of the targeted transportation sector should be given. The reviewer noted that collaborations with DOE's Bioenergy Technologies Office can be useful in this matter.

The reviewer said the project incorporates reaching objectives that "…inform the next generation of ammonia-capable marine engines" by using "flow reactor experiments" and "thermodynamic analysis." The reviewer was not clear what was involved with the flow reactor and thermodynamic analysis that was related to "limitations of ammonia consumption…". The experiments and analyses noted should be clarified.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer said it is important to highlight the publication on safety considerations for using ammonia fuel in a test facility; this is an area of high interest for the industry as others look to install ammonia systems in their own facilities. Publishing this brings great value to the work conducted in the lab, which for setups usually does not deliver intrinsic value to the industry. The reviewer noted the project demonstrated a range of results using ammonia dual-fuel combustion, indicating good progress towards milestones. In addition, it is also worth highlighting that that this work appears to have leveraged learnings from prior DOE-funded research into dual-fuel combustion. Building off this prior DOE investment to accelerate this program is notable. Further, the emissions focus on not only CO_2 emissions, but relevant GHG emissions as well is recognized. The clear tradeoffs of N_2O, a GHG, emission versus the decarbonization that would be provided by low-carbon ammonia is important to understand and nicely dovetails with the combined combustion and emissions capabilities and focus of the program.

Reviewer 2

The reviewer said a lot seems to have been accomplished in the past year. However, the presentation suffered from a lack of details that would have enabled a more detailed assessment of the accomplishments. This is likely due to the limited time the PIs had to present their work. The reviewer cited as an example, it was noted that "formation pathways are under investigation through additional experiments…", but from this statement alone it was not clear how these "pathways" were to be determined and what the "additional experiments" were. Color coded figures were presented (e.g., Slides 10 and 13) showing interesting information on NH_3 and a large (93% reduction) of CO_2 though it was not evident if these figures were from simulations or processed experimental data. The reviewer said more information on these points would have been preferred. The reviewer provided as additional comments: A single cylinder diesel engine facility was modified for duel-fuel injection and made operational to carry out experiments to measure emissions including N_2O, NO_x, CO_2, and other gases with several injection approaches. Safety protocols were incorporated into the dual-fuel engine laboratory. A demonstration of an injection strategy enabling duel NH_3/hydrogen injection was shown. Formation pathways were noted to be under investigation by collaborators, which is interesting, but no details were provided. Generally large reductions of CO_2 emissions were found in the experiments, which is impressive. The flow reactor experimental configuration is intended for studying ammonia decomposition. However, the presentation did not make clear what was being measured here. Is the flow reactor intended to determine the decomposition rate of a one-step decomposition reaction?

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer said this project has clear, numerous, collaborations across different industry and university partners.

Reviewer 2

The reviewer remarked collaboration is good and seems generally effective. Monthly meetings are held with industrial partners and DOE personnel. However, the deliverables of some of the collaborators were not described so it was not evident in some cases how their contributions would contribute to the overall project objectives. For example, three university partners are incorporated into the project. It was not clear what they brought to the project. One university partner (Oakland) provides a "…deeper understanding of the chemical kinetics of NH_3 combustion." How this "deeper understanding" was developed, what metrology is involved with it, and where it fit into the project was not discussed. Similarly for the other collaborations. For the ExxonMobil collaborations, the reviewer remarked it was not clear how they are providing an "…understanding NH_3 impacts to engine oil by supplying test oil and input analysis…". What this means should be clarified.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer remarked the plan for future work seems good. In the main it will involve more testing to address various barriers that include trying to reduce N_2O emissions, assessment of commercial decomposition catalysts to produce hydrogen, more hydrogen enhanced dual-fuel experiments from the flow reactor, and others. The reviewer also recommended that the PIs address the question expressed previously regarding ammonia supply to meet national needs for marine engines, and the infrastructure to provide it to the marine sector.

Reviewer 2

The reviewer said the project has a clear scope and plan for future work, and connects. It would be useful to see a GHG comparison against a diesel baseline using low-carbon diesel fuels like renewable diesel and/or biodiesel. For larger marine applications with a dual-fuel ammonia main engine, it seems like the diesel consumption of an auxiliary engine would be small relative to the diesel use on the main engine, which may well be renewable diesel or biodiesel in future applications. Given this, it is unclear whether a dual-fuel ammonia engine would make sense for the auxiliary. The reviewer said as such, it would be useful to understand the decarbonization opportunity from ammonia relative to an engine operating on low carbon diesel rather than a petroleum diesel baseline. Additionally, understanding the effects of exhaust gas recirculation (EGR) on ammonia-fueled engines is an opportunity space that should be explored in more detail. This is acknowledged as part of the proposed work.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said this project is highly relevant to VTO program objectives of new fuels for efficient combustion, here being to the marine sector and the emissions it generates as related to global climate change. Alternative fuels that are ammonia-based have significant promise for clean combustion. This project fits well into a program constructed to provide foundational information on ammonia's potential to this end for the marine sector.

Reviewer 2

The reviewer remarked clear connection to VTO's focus on decarbonization of off-road applications, including marine.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said the project's budget is low relative to the work scope and progress, and in comparison to other projects.

Reviewer 2

The reviewer commented the resources seem adequate for this project. However, because details were not provided regarding budget breakdown for specific tasks a more thorough assessment of the financial resources for the project could not be provided.

Presentation Number: DORMA047
Presentation Title: High-Efficiency Mixing Controlled Compression Ignition Combustion of Propane Dimethyl Ether Blends
Principal Investigator: Sage Kokjohn, University of Wisconsin

Presenter

Sage Kokjohn, University of Wisconsin

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 67% of reviewers felt that the resources were sufficient, 0% of reviewers felt that the resources were insufficient, 33% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

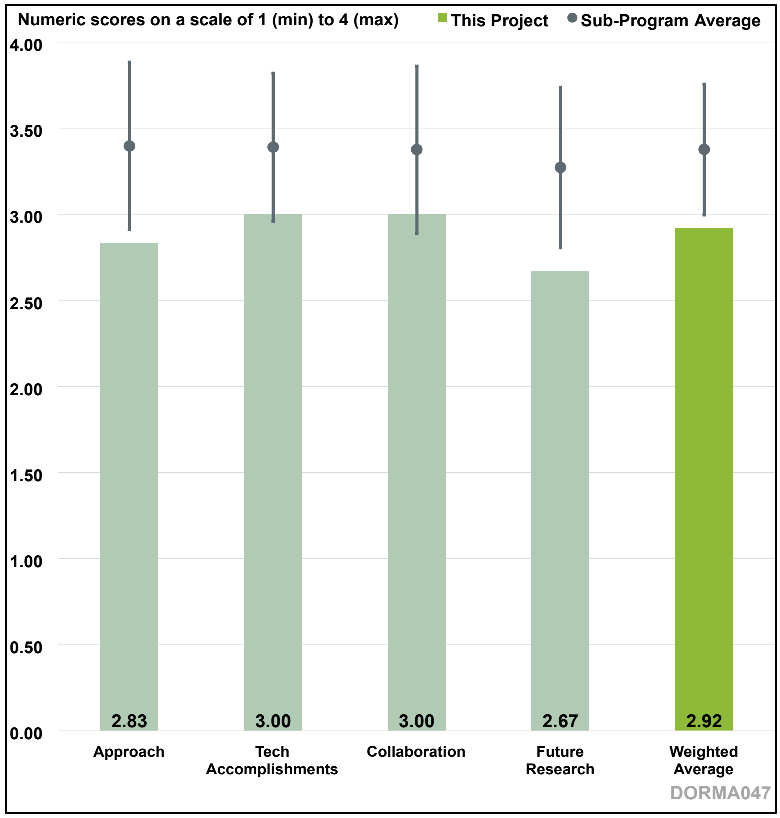

Figure 3-34. Presentation Number: DORMA047 Presentation Title: High-Efficiency Mixing Controlled Compression Ignition Combustion of Propane Dimethyl Ether Blends Principal Investigator: Sage Kokjohn, University of Wisconsin

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer said the project is well designed to address some of the key barriers for propane and DME/propane MCCI combustion. The project team is encouraged to utilize 1D system-level tools more extensively in combination with three-dimensional (3D) CFD to drive the development a full-range operating strategy.

Reviewer 2

The reviewer remarked the approach to devise a method for compression ignition (mixing controlled) for propane is rather innovative. It is a clean, low-carbon fuel that is relatively easy to produce, with lower carbon intensity than diesel. The project is investigating the necessary aspects of how to get an engine to even have a chance to CI combustion with propane, since the chemistry of propane is not easily conducive to CI. The efficiency benefits, if successful, could be significant. The reviewer said the challenge is marketplace—(MD trucks as opposed to off-road or other, where propane is more easily accepted and found. MD trucks will be offering significant competition with battery electric vehicles (BEVs), and well-to-wheels CO_2 for electrical power for BEVs is likely to continually drop over the development life of this project. However, this combustion system should have value in a variety of applications, if successful, and it is well-worth the effort to explore.

Reviewer 3

The reviewer said that for the amount of funding in this project, the approach lacks ambition. The project team is using an existing and installed single cylinder engine, and is using correlations to get to a brake efficiency number. The team is using a fuel pump/injector system that seems like it was primarily developed in a different project. The GT Power and CFD simulations, while useful, are not overly complex. The planned testing to conclude the project seems like it will only be installing a new cam shaft for the exhaust re-breathing.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer said the project team made good progress on developing the fuel injection system, generating initial engine test results, conducting 3D CFD and 1D engine cycle analysis. The gross indicated thermal efficiency/BTE results need to be compared with the base diesel engine performance to drive identification of areas for improvement. The reviewer remarked it will benefit the team to conduct a thorough assessment on a full range valve strategy along with geometric compression ratio (CR) evaluation in the 1D analysis.

Reviewer 2

The reviewer remarked the engine has been operated at high fuel pressure and has produced insightful results. The exhaust rebreathe concept looks to be effective at raising the compression temperature without raising the compression ratio of the engine. The backpressure penalty might reduce the optimum BTE a bit but it appears to provide significant leverage for consistent compression ignition of propane. The reviewer said CFD models appear to do a decent job of capturing the correct trends and comparisons, so the project can move through the test space with some confidence. The only concern the reviewer had is with the injectors and the lack of lubricity/cooling of propane and DME. The reviewer realized the injectors are part of a different project, but they have significant influence here.

Reviewer 3

The reviewer remarked the project team has identified the in-cylinder engine conditions that need to be achieved to operate on their chosen DME/propane blends and devised a method using exhaust re-breathing to achieve this. However, the solutions that are being developed seem very much like a lab-based solution and they lack direct applicability to the real world. The reviewer said it is not clear that the team will be able to operate over the full engine map with a single set of hardware (cam). And, while the team can point to existing advanced valvetrain hardware that could help them achieve these goals, the reviewer would expect more to be implemented for the amount of resources in this project.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer said collaboration is well organized with activities at each partner complement each other.

Reviewer 2

The reviewer commented that the project partners appear to have most of the bases covered—universities to perform the scoping and simulation work, a small, specialty company to work on the injectors and support from fuels organization. The project could potentially benefit from an engine OEM involvement to ensure technology transfer, if the project is successful.

Reviewer 3

The reviewer said the project team consists of two universities, an engine consultant closely linked to the project lead (Wisconsin Engine Research Consultant), a start-up company that aims to develop fuel pumping and injection equipment (WM International), and a company that produces DME. The reviewer noted there is no major OEM or Tier 1 supplier in this project team that can steer the project to more ambitious efforts and get them closer to implementation.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer said plans to conclude the project consist of running some additional single cylinder engine experiments with a modified camshaft to prove that exhaust re-breathing can achieve the in-cylinder conditions necessary to reach autoignition with high propane blends. While technically this can meet the project goals, it seems underwhelming for the amount of resources that DOE is putting into this project. The reviewer said it would be nice to see a custom solution—perhaps hardware that can achieve full-map operation. Or operation in a multi-cylinder engine that includes fuel pumping so that brake efficiency correlations do not have to be used.

Reviewer 2

The reviewer said that considering the lean burn nature, future research should involve performance comparison with the base diesel engine. The analysis should place an emphasis on how to close the performance gap including CR, piston bowl geometry, spray pattern, and valve strategy. Laser ignition may not bear strong practical significance. Diesel/DME pilot ignition may be a more feasible approach.

Reviewer 3

The reviewer commented that the future work should be able to address most of the barriers to this technology being demonstrated, if successful. Much more thorough engine testing, over a variety of conditions, is a good plan to ensure that the predicted CO_2 reductions are realized. The reviewer said it is a bit unclear how laser ignition would enable much in terms of barrier elimination, in the sense that the cost will increase, and it is not clear that the performance will increase in a similar way. It will be important to stay on top of the latest information on CO_2 well-to-wheels for BEVs, because that is the genuine competitor in this space. The reviewer said under the current regulations, the BEV also has the zero-emission vehicle advantage from a regulatory point of view, and it may be reasonable to account for that in the analysis.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said this project definitely supports DOE goals in CO_2 reduction. Propane and DME are also potentially renewable, but even in fossil form, propane has some CO_2 benefit compared to diesel. The project goal to utilize CI is quite worthwhile and should be pursued.

Reviewer 2

The reviewer said the project is well aligned with the future GHG reduction requirements. The project team is encouraged to clearly define the engine-out NO_x targets with appropriate description of drive cycles and the lean aftertreatment system to be used.

Reviewer 3

The reviewer said that while answering this question “yes”, the project goals of using mixtures of propane and DME in MD engines seem less relevant to this project then when it was initially awarded. The project has more recently shifted to heavier, hard to decarbonize applications.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer said resources are adequate to support the project milestones and the timeline.

Reviewer 2

The reviewer commented that resources available appear to be sufficient to accomplish the goals of the project.

Reviewer 3

The reviewer noted there are a lot of financial resources going into this project. For this amount of funds, the reviewer would expect a lot more work than to use an existing single-cylinder research engine with a modified fuel injection system. The effort seems underwhelming for the amount of resources being put into it.

Presentation Number: DORMA051
Presentation Title: Fuel effects on aviation engine emissions–a modeling tool for SAF screening
Principal Investigator: Dario Lopez-Pintor, Sandia National Laboratories

Presenter

Dario Lopez-Pintor, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers felt that the project was relevant to current DOE objectives, 0% of reviewers felt that the project was not relevant, and 0% of reviewers did not indicate an answer. 50% of reviewers felt that the resources were sufficient, 50% of reviewers felt that the resources were insufficient, 0% of reviewers felt that the resources were excessive, and 0% of reviewers did not indicate an answer.

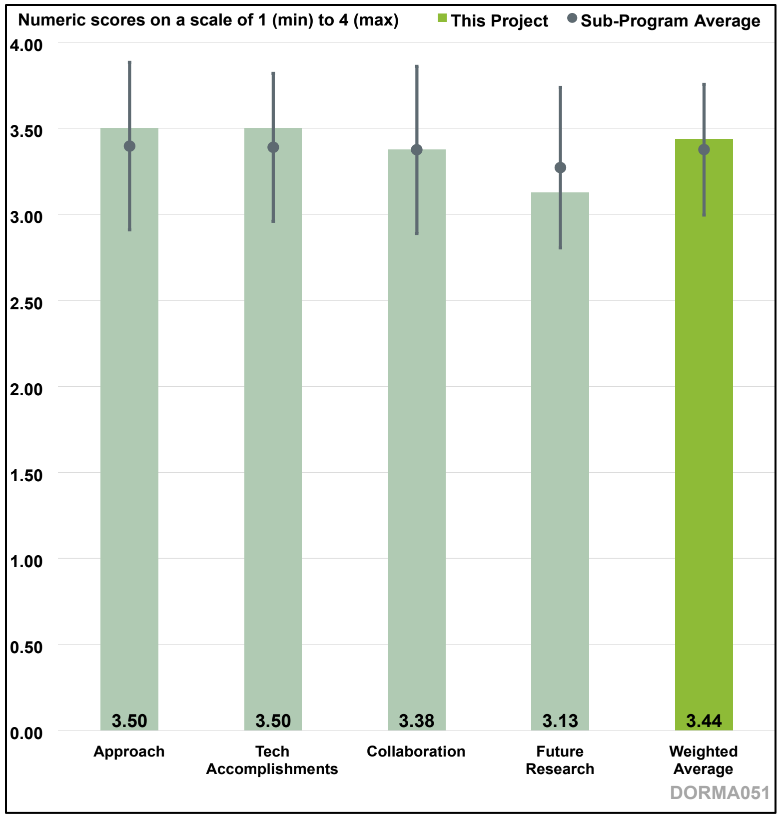

Figure 3-35. Presentation Number: DORMA051 Presentation Title: Fuel effects on aviation engine emissions–a modeling tool for SAF screening Principal Investigator: Dario Lopez-Pintor, Sandia National Laboratories

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer said the team is targeting creation of modeling tools for the simulation of particulate emissions preceding plume/contrail generation, as well as understanding the source of such emissions, specifically the impact of soot particles and sulfur oxides. The timeline is aggressive, although the project plans have been developed well to make contributions to reducing the barriers.

Reviewer 2

The reviewer remarked the project uses a combustion model to simulate soot particle mass, number, and size distributions as well as trace gas emissions for a combustor burning conventional and alternative fuels. The work allows for simulation and understanding of the fuel effects associated with different sustainable aviation fuel (SAF) formulations in a conventional, CFM56-7 engine. Future work will connect the simulated emissions to contrails, although the contrail piece of the project is not clearly described. Overall, the work is important and leverages DOE’s expertise in fuel chemistry and combustion simulation.

Reviewer 3

According to the reviewer, the approach is very well thought out and presented in the review process. The use of a rapid low-cost screening for soot is very attractive and the steps are reasonable to meet the objectives.

Reviewer 4

The reviewer said the project identifies the importance of a simplified computational tool to evaluate fuel effects on aircraft engine emissions and contrail formation. The timeline only outlines two milestones; however, the two milestones may be appropriate given the limited budget allocated for this work. The reviewer was not clear what work will be done in the interim between the second milestone completion on 6/30/2024 and the project end date of 9/30/2024.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer said progress made by the team in terms of successfully simulating particulate emissions from a gas turbine engine is significant and represent a remarkable achievement. This work represents a significant advancement to the existing state of the art. There are a lot of details embedded in this work, and they need to be shared with the community and published in the archived literature. The reviewer said based on the supporting but limited details provided, the work has been competently performed. Given that the “soot community” feels that experimental measurements (of soot mass) within a factor of two are considered good, the capturing of trends of soot mass over a range of operating conditions is remarkable. The larger uncertainties in number density are recognized, indicating that there is more work needed, but should not distract from the encouraging results. The reviewer said one minor issue needs to be addressed. The chart on Slide 5 showing the predicted and experimental soot particulate matter, is inconsistent with the similar plot on Slide 14. Also, the PAH data is missing on Slide 14.

Reviewer 2

The reviewer said the project highlights technical progress for model agreement with International Civil Aviation Organization (ICAO) data for engine emissions at varying operating conditions. This was achieved with a very low computational cost, showing significant improvement over more complex modeling approaches. The project also notes significant progress on evaluating various fuel sooting properties across multiple fuel types. The reviewer remarked the project makes valuable contributions in understanding the relationship between fuel chemical classes and sooting propensity.

Reviewer 3

The reviewer commented it seems that the results indicate that there are only large reductions in soot for Φ greater than3.5 with a change in fuel. Experimental results on the ground indicate high reductions in soot particle number across conditions with iso-paraffinic kerosene (IPK). The reviewer was unsure why the model is showing reductions with IPK at climb and take off. Discussions with NASA on past ground tests with low sooting fuels may provide data beyond the ICAO Databank.

Reviewer 4

The reviewer said the project has made considerable technical progress related to setting up the simplified simulation environment, obtaining results, and comparing these results to ground-based measurements. It is clear that the model adequately captures the trace gas and particle mass emissions, but the microphysical simulation of particle number, growth, and size yields unrealistic results. Some of this discrepancy may be due to model assumptions, while other sources of error relate to the interpretation of the measurement data (e.g., a sharp 10 nm cutoff for the measurement condensation particle counters). The reviewer remarked the project also mentions connecting the simulation results to contrails, although it is not clear how the model will be adapted to simulate engine operation at cruise conditions and what the next steps would be for the contrails piece.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer commented project collaboration is outstanding with strong external partners. The addition of Aerodyne Research (while technically not industry) as an atmospheric and engine emissions modeling subject matter expert is particularly valuable.

Reviewer 2

The reviewer remarked much of the work has been performed by the PI, but he has engaged team members well. In particular, key to the success are the CFD simulations (from Sandia) of the flow conditions in the combustor and their dependence on operating conditions as well as the detailed chemical kinetic models from LLNL, and the input from Aerodyne on the role of sulfur in water condensation. Clearly, results from other groups have contributed in addition.

Reviewer 3

The reviewer said the project clearly outlines the project team contributors and their roles. It would be helpful to more clearly see which team members contributed across the various technical accomplishments and progress. The project team includes a diverse set of collaborators: industry (Aerodyne), national laboratories (Sandia National Laboratories, LLNL, and ANL), and academia (Polytechnic Valencia, University of Illinois Urbana-Champaign, and Ecole Polytechnique Fédérale de Lausanne).

Reviewer 4

The reviewer assumed the simulations are for the design cycle points for the CFM56 engine developed and optimized under the reactor network model, but this was not explicitly mentioned. The SAF End Use Program Review Meeting is a good opportunity to engage industry and academia. The reviewer said this presentation could highlight the connections to other DORMA projects better.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

The reviewer remarked proposed future research focuses on key needs for the aviation community regarding the impact of cycloalkanes in comparison to aromatics regarding sooting and contrails. The purpose for the research is clearly stated, and the work is likely to achieve its objectives given the technical accomplishments of the team thus far.

Reviewer 2

The reviewer said there is great potential for this model for connecting changes in future SAF chemistry to emissions. The early results are very promising for bulk mass particle and trace species, although the modeled particle microphysics remains inconsistent with observations. Capturing accurate particle size and number is a very challenging problem!

The reviewer noted the initial finding that mono-aromatics strongly affect soot is an interesting conclusion that should be explored more in the future as the results of this work could serve to guide efforts to tailor the fuel aromatic and polycyclic aromatic composition. The plan for how the plume model will be refined and connected to contrail propensity is not clear and would benefit from more thought on how this will be carried out. The reviewer said the contrail modeling is particularly challenging, and may be a step too far for the present project. Last, while the reviewer understands the desire to simulate the particle microphysics from first principles and not “cheat” by imposing a prescribed particle size distribution, we do know from observations that the soot mode is considerably larger than uncovered by these simulations. Future efforts to improve the soot growth rate would be one approach to resolving this discrepancy. In the meantime, however, it would be interesting to explore how using a prescribed two-mode lognormal size distribution might improve closure between the measurements and models. Finally, it would be useful to incorporate volatile sulfate and nitrate aerosol species into the model to explore the interplay between soot particle coatings and new particle formation.

Reviewer 3

The reviewer said proposed future work is clearly presented and seems reasonable. The reviewer liked the approach to look at improvements in the current model in addition to new areas to explore. It would be interesting to compare to NREL’s reduced chemistry model when the HEFA model is complete.

Reviewer 4

The reviewer said future results are hindered by the apparent near-term termination of the project. There are only two bullets for proposed work. One is a surrogate for iso-paraffinic SAF. The creation of a single surrogate for multiple iso-paraffinic SAFs seems improbable given that the range of iso-paraffinic SAFs are yet to be defined. The second is the implementation of a 1D plume model to capture fuel effects. The reviewer said this objective may be difficult to achieve in the existing timeframe given that the characterization of soot particle emissions and how they change with fuel changes is, as yet, poorly defined. The reviewer said even specific data on (particulate) emissions from engines operating under cruise conditions are limited, for jet-A, let alone SAF fuels.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer said the embedded links appear outdated, but the work is fully consistent for the SAF Grand Challenge Roadmap.

Reviewer 2

The reviewer said the project is highly relevant to VTO and relates to future SAFs and understanding how changes in fuel chemistry impact emissions.

Reviewer 3

The reviewer remarked the project is very relevant for the aviation fuels community in answering research questions regarding fuel composition impacts on sooting and contrail formation. The work is timely and focused.

Reviewer 4

The reviewer commented soot modeling is of great interest to industry and the reviewer understands why a CFM56 was chosen to do these simulations; however, technology has advanced significantly from the CFM56. Applying the model to current state of the art technology that has emissions/soot data available would increase the relevance.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer was not sure how to respond to this question, as the resources seem to have been zeroed out in fiscal year 2023, and it is uncertain how the recent work was completed. Nevertheless, the team has proven productive, and there is plenty of (appropriate) proposed research to perform. So, the resources are not sufficient.

Reviewer 2

The reviewer said the charts indicate that this project was funded with $150,000 in fiscal year 2022 and $0 in fiscal year 2023. It seems like these simulations would cost something and $150,000 would be approximately the cost of a post-doctoral researcher. The reviewer was not sure if this is a typo or if this is accurate, but it does not seem to be reasonable if this is an accurate funding profile.

Reviewer 3

The reviewer said the project resources appear to be commensurate with the proposed research effort.

Reviewer 4

The reviewer remarked resources are sufficient and appropriate for the project to achieve the milestones on schedule.

Presentation Number: DORMA052
Presentation Title: Simulation of Jet Engine Performance using SAF Blends
Principal Investigator: Shashank Yellapantula, National Renewable Energy Laboratory

Presenter

Shashank Yellapantula, National Renewable Energy Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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

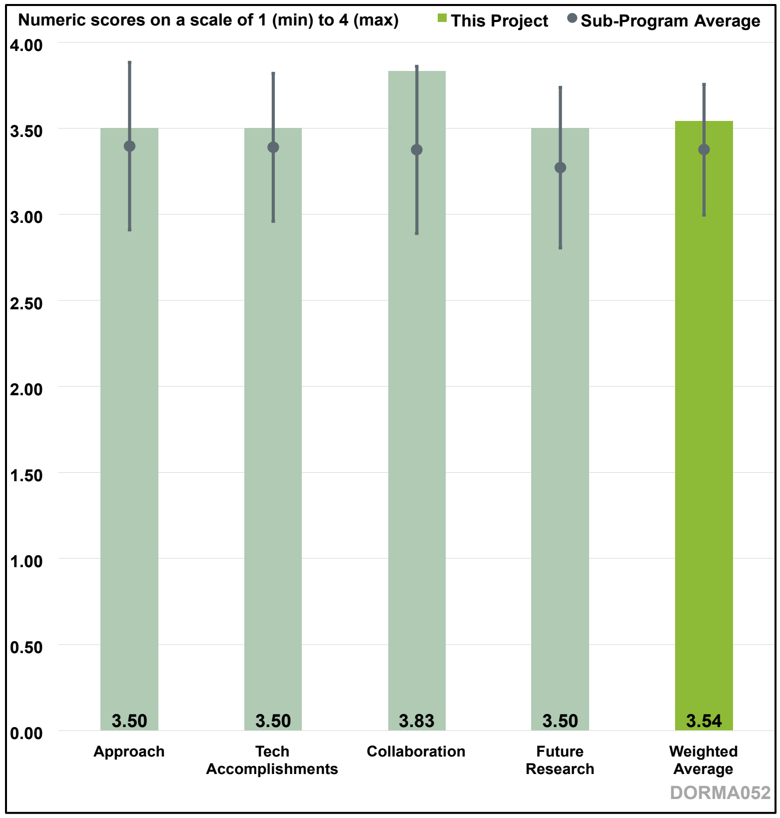

Figure 3-36. Presentation Number: DORMA052 Presentation Title: Simulation of Jet Engine Performance using SAF Blends Principal Investigator: Shashank Yellapantula, National Renewable Energy Laboratory

Question 1: Please comment on the degree to which technical barriers are addressed. Is the project well designed, and is the timeline reasonably planned?

Reviewer 1

The reviewer noted this work is focused on overcoming SAF Grand Challenge barriers, namely developing 100% SAF formulations that meet fuel property requirements, characterizing the performance benefits of those fuels, and improving methods of testing those fuels. The project aims to address these challenges by developing chemical kinetic mechanisms for the simulation of high-SAF fuels and performing numerical simulations of the combustion of these SAF blends. The reviewer said the end goal is to validate the simulation outputs using optical diagnostics data from experiments. The project is well-designed. The proposed work will enable predictive simulations that lead to quicker fuel development and certification, directly addressing the Grand Challenge barriers. The timeline is reasonable, and all milestones are complete or on target for completion.

Reviewer 2

The reviewer remarked this project tackles some very important technical barriers relating to adoption of SAF at blended and 100% replacement levels in aviation gas turbine engines. Specifically, there are many unknowns relating to approval for use of 100% SAF as well as potential performance and emissions benefits that can be gained from use of SAF at any level in existing gas turbine engines. The approach used by the PIs is that of using numerical simulations with predictive capabilities utilizing detailed chemical kinetics specifically targeting SAF (HEFA) as well as fuel thermophysical property data expressly generated for conditions relevant to aviation gas turbine engine operation. This is a very well-designed project that leverages experimental data from two combustor rigs for validation as well as pertinent simulation data from GE Aerospace.

The reviewer said the project timeline (2021-2027) is adequate for this effort and the milestones presented for this year appear to be keeping the PIs on schedule to complete the targeted project goals. The reviewer suggested clearly defining what metrics are of interest while talking about “combustor performance.” Clarifying specific metrics would help design the simulations and the conditions and manner in which they are carried out. Another comment is can this work (in combination with simulation efforts on SAF from other DOE laboratories) be used to modify ASTM certification procedures themselves? The reviewer said to the extent that predictive simulations can be a supplementary step particularly in the pre-screening process to reduce cost/time of certifying new SAF. A DOE led effort (with support of the FAA) might be able to achieve progress on this. Actually, after continuing on to the end of the presentation, it appears that such outcomes are part of the intended goals for this project and that is definitely commendable.

Reviewer 3

The reviewer said the team has excellent tools and capabilities to perform reacting spray combustion simulations with Jet-A and SAF including developing the chemistry mechanism for HEFA-SPK. And for the work planned, the project is well designed with a reasonable timeline, but the simulations are not addressing relevant combustor concepts nor the operating conditions that would impact the ASTM synthetic fuel pathway approvals and blend limits. The reviewer said the lean premixed prevaporized (LPP) injector certainly has potential for low NO_x and very low soot emissions but LPP is not a concept that is currently flying on any aircraft nor likely to fly on a next generation subsonic aircraft or first-generation supersonic aircraft (if a commercial market is established). The combustor operations of most importance to the ASTM fuel approval process are lean blowout and ignition, but simulations in this project are mostly focused on stable operating conditions. The reviewer said there may be some simulations of combustion dynamics from the Aviation Sustainability Center (ASCENT) 74 LPP experiments.

Question 2: Please comment on the technical progress that has been made compared to the project plan.

Reviewer 1

The reviewer noted that development of the chemistry mechanism for HEFA-SPK appears to be nearly complete. A 2-component surrogate model has been validated against ignition delay time (IDT) and laminar flame speed measurements and is being used for CFD simulations. For the ASCENT 74 LPP experiments, non-reacting simulations have been validated against PIV measurements of air velocity with good comparisons and the reacting spray simulations for the ASCENT 74 LPP are underway. Simulations of the NASA University Leadership Initiative (ULI) LPP injector section upstream of the combustion chamber predicting the degree of fuel vaporization and mixing have been performed ahead of testing. The reviewer said in general, there is evidence of steady progress in working towards validation of reacting spray simulations with Jet-A and HEFA-SPK against the ASCENT and NASA ULI LPP experiments.

Reviewer 2

The reviewer said these researchers have made excellent technical progress. A comprehensive set of optical diagnostic data enables these researchers to establish simulation boundary conditions and validate simulation outputs. The researchers have developed a surrogate model for fuel blends of interest that demonstrates strong fidelity to experiments. Initial nonreacting flow comparisons between simulated and experimental combustors show that their simulation approach is able to reproduce flow features observed in experiments. The reviewer remarked all of these milestones show strong work towards overcoming technical barriers.

Reviewer 3

The reviewer said the PIs have made significant progress on technical objectives. Development of predictive simulations with detailed chemical kinetics of SAF as well as well-characterized thermophysical properties at conditions relevant to GT engines is the main overarching deliverable of this work. To this extent, the PIs have shown progress on several fronts.

The reviewer noted a two-component surrogate model for HEFA has been developed (of reasonable size) showing consistency with ignition delay and flame speed measurements for HEFA-SPK. Flame speed agreement is not as good as that of ignition delay. Per this reviewer, one recommendation would be to ensure comparison of both metrics with measurements (as available) for HEFA over the range of pressures and temperatures that the simulations will be pursued for. Another comment is that the fuel property set for comparison to the surrogate should be expanded to include things like flash point, viscosity, distillation, etc., since they have been identified in previous National Jet Fuel Combustion Program work as having critical influence on various aspects of the combustion process including lean blowout (LBO). It is unclear if emissions are a target metric for this work but in that case there may be additional items to consider for the surrogate fuel. That said, the mechanism itself is a valuable contribution to the combustion community.

The reviewer said the PeLeLMeX solver appears to have the required capabilities to carry out the predictive simulations including graphics processing unit performance, multiphase capabilities in combination with the dispersed phase solver, tabulated chemistry for flamelets, and support for multi-component fuels. The reviewer provided as input direct numerical simulations from the Sandia group (Chen) appear to have shown some advanced flamelet techniques for capturing multi-modal combustion and these could be leveraged in the present work. Air-only simulations and ongoing spray simulations of the LPP rig and vaporization simulations of the ULI rig seem to demonstrate good progress towards the reacting flow simulations and will provide useful feedback to the experimental teams for fine-tuning operating conditions.

Question 3: Please comment on the collaboration within the project team. Are there specific contributions made by industry, national laboratories, or other external entities? Are there areas where more collaboration is needed?

Reviewer 1

The reviewer was very impressed by the collaboration set up by this project, and how well it was described in the presentation. Georgia Tech operates two optically accessible combustors, producing experimental data for simulation validation. One of the combustors involves a proprietary fuel nozzle from GE Aerospace; GE provides the project with boundary conditions for this nozzle from their own simulations. NREL performs chemical kinetic modeling and flow simulation, while subcontracting for combustor testing to Georgia Tech and transferring developed models to GE

Aerospace. The reviewer said this collaboration between government, industry, and academia has distinct roles for each group and seems to be producing excellent results.

Reviewer 2

The reviewer said there are strong collaboration efforts with FAA, GE, Georgia Tech, and NASA that use experimental data from LPP injectors testing under the FAA ASCENT 74 project and NASA ULI grant. Providing the NASA ULI grant additional funding to perform testing with HEFA-SPK is a notable component of the collaboration.

The reviewer said the collaborations of NREL with LLNL on chemical kinetics development for Jet-A and HEFA-SPK are not clear. The reviewer asked if they are comparing mechanism results for prediction of IDT and laminar flame speed, are the surrogate species or fundamental chemistry for lower carbon number species (such as C1 to C4) similar or the same, and what is the nature of the collaboration?

Reviewer 3

The reviewer remarked the PIs are very well aligned with several key collaborators from industry, university, and other DOE national laboratories. The collaborations, particularly with the experimental groups at Georgia Tech are key to validating simulations and providing boundary conditions/geometry/etc. The reviewer said some collaboration with the group from Sandia performing direct numerical simulation of swirl combustors could be helpful to leverage newly developed flamelet based approaches for multi-modal combustion, and the same applies to the ANL group developing tools for heat transfer and ignition relevant phenomena.

Question 4: Please comment on the proposed future research. Has the project clearly defined a purpose for future work? To what extent will future work likely achieve its targets?

Reviewer 1

According to the reviewer, proposed research tasks for the future are spot on with the overall project goals. This includes reacting flow simulations of the LPP and ULI combustors, correlating fuel properties to combustor metrics (appears that emissions are indeed part of the intended metrics as well as dynamics, this reviewer would still recommend identifying key performance metrics), studying other SAF (besides HEFA), and incorporating tools developed through this effort into the pre-screening workflow. Given the progress of the PIs so far, it appears that the future work will achieve proposed targets and address the technical barriers motivating this study.

Reviewer 2

The reviewer commented the proposed future research for this project logically builds off what has already been accomplished and contributes directly to achieving project goals. The researchers plan to move to reacting flow simulations, explore correlations between fuel properties and combustor performance, and implement neural networks to prescreen new fuel formulations. The prior accomplishments of these researchers makes it very likely that the proposed work will be successfully accomplished.

Reviewer 3

The reviewer said the project is currently focused on completing the reacting simulations for ASCENT 74 LPP and some initial configuration of the NASA ULI LPP with Jet-A and HEFA, and comparing against available test data. The project is planning further LPP simulations with SAF other than HEFA but there may not be experimental data available for comparison so the simulations would only show possible impacts of fuels on the LPP performance (presumably at the same stable operating conditions as current Jet-A and HEFA experiments). The reviewer remarked this work is clear in terms of objectives and has a high likelihood of meeting its timeline and targets. There was also a note about developing a SAF pre-screening tool. The reviewer was not sure how much of that work occurs under DORMA 052 versus 037, or perhaps it is a combination of both projects 052 and 037. It will be interesting to see how this pre-screening work compares with pre-screening low fuel volume approaches being developed under FAA ASCENT projects 25 and 65A where 25 is using a detailed FTIR spectral analysis approach and 65A is further developing the previously developed "tier α- and β-test methods" to further reduce fuel volumes and improve potential for ASTM fuel pathway approval.

Question 5: Please comment on the relevance of the project. Does the project support the overall VTO subprogram objectives?

Reviewer 1

The reviewer remarked this project is relevant and directly in support of VTO program objectives. This work contributes to new aviation fuels that will increase efficiency and decrease pollutant emissions, leading to economic and environmental benefits.

Reviewer 2

The reviewer said proposed work targeting SAF implementation in aero GT engines and developing correlations between SAF properties and combustor metrics through development of predictive simulation capabilities validated by experiments is completely in line with the objectives of the DORMA program. The project will support DOE and agency-wide efforts to achieve objectives of the SAF Grand Challenge as well as develop a solid framework of simulation approaches, kinetic mechanisms, and fuel properties which will be highly beneficial to the combustion and aviation community as a whole.

Reviewer 3

The reviewer said the project is expanding capabilities in simulating the impact of SAF and higher SAF blends on combustor performance. But to reduce the large fuel volumes and time spent in testing of synthetic fuels in the ASTM fuel pathway approval process, simulations of lean blowout and ignition for more combustor designs more representative of those currently in-service and likely to enter into service in the coming decade are needed.

Question 6: Please provide comments on the resources of the project. Are the resources sufficient for the project to achieve the stated milestones in a timely fashion?

Reviewer 1

The reviewer remarked the project has the codes and high-end computing facilities required to complete the proposed tasks. The project has made significant progress towards the reacting spray simulations with Jet-A and HEFA currently underway.

Reviewer 2

The reviewer said resources for the project are sufficient. The budget is very reasonable. The presentation established that the investigators have the necessary experimental infrastructure, computational framework, and technical expertise to carry out the plan they have established.

Reviewer 3

The reviewer said personnel and financial resources appear to be satisfactory for the level of work.

Acronyms and Abbreviations - DORMA

Abbreviation	Definition
0D/1D/2D/3D	Dimension - zero, one, two, three
L	Liter
ADT	Articulated dump truck
AE	Activation energy
AFR	Air-fuel ratio
AFRL	Air Force Research Laboratory
Al_2O_3	Aluminum oxide
AN	Ammonium nitrate
ANL	Argonne National Laboratory
APS	Advanced Photon Source
ARC	Army Research Combustor
ASCENT	Aviation Sustainability Center
ASTM	ASTM International, formerly known as American Society for Testing and Materials
AT	Aftertreatment
atm	Standard atmospheric pressure unit
B100	100% biodiesel
BEV	Battery electric vehicle
BTE	Brake thermal efficiency
CARB	California Air Resources Board
CAT	Caterpillar
CCV	Closed crankcase ventilation
CFD	Computational fluid dynamics
CH_4	Methane
CHA	Chabazite
CI	Compression ignition
CNG	Compressed natural gas
CO	Carbon monoxide

Abbreviation	Definition
CO_2	Carbon dioxide
CR	Compression ratio
CRADA	Cooperative Research and Development Agreement
CRC	Coordinating Research Council
CRF	Sandia National Laboratories' Combustion Research Facility
Cu	Copper
DC	Direct current
DEF	Diesel exhaust fluid
DFI	Ducted fuel injection
DI	Direct injection
DME	Dimethyl ether
DNN	Deep neural network
DNS	Direct numerical simulation
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DORMA	VTO Decarbonization of Off-Road, Rail, Marine, and Aviation subprogram
DPF	Diesel particulate filter
DRIFTS	Diffuse reflectance infrared Fourier transform spectroscopy
E98	98% ethanol/2% gasoline
EAS	Exhaust aftertreatment system
ECU	Engine control unit
EGR	Exhaust gas recirculation
EPR	Electron paramagnetic resonance
EtOH	Ethanol
FAA	Federal Aviation Administration
FPT	Fiat Powertrain
FTIR	Fourier transform infrared
FY	Fiscal Year

Abbreviation	Definition
g/kWh	grams per kilowatt-hour
GC	Gas chromatography
GDI	Gasoline direct injection
GE	General Electric, Inc.
GER	Global equivalence ratio
GHG	Greenhouse gas
GM	General Motors
GPU	Graphic processing units
H_2	Hydrogen
HC	Hydrocarbon
HD	Heavy-duty
HEFA	Hydroprocessed esters and fatty acids
HyREX	Optimized Low Carbon Fuel Range Extender
ICAO	International Civil Aviation Organization
ICE	Internal combustion engine
ID	Identification
IDT	Ignition delay time
IMEP	Indicated mean effective pressure
IMT	Intake manifold temperature
IPK	Iso-paraffinic kerosene
kWh	Kilowatt-hour
LBO	Lean blow-out
LCLF	Low carbon liquid fuel
LES	Large eddy simulation
LLCF	Low-lifecycle-carbon-fuels
LLNL	Lawrence Livermore National Laboratory
LPP	Lean premixed prevaporized
MCCI	Mixing-controlled compression ignition

Abbreviation	Definition
MD	Medium-duty
MeOH	Methanol
MG	Motor-generator
MIT	Main injection timing
N_2O	Nitrous oxide
NASA	National Aeronautics and Space Administration
NH_3	Ammonia
NJFCP	National Jet Fuel Combustion Program
NMC	Nickel manganese cobalt
NMOG	Non-methane organic gas
NO	Nitric oxide
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides
NREL	National Renewable Energy Laboratory
OEM	Original equipment manufacturer
ORNL	Oak Ridge National Laboratory
PAH	Polycyclic aromatic hydrocarbon
PC-MCC	Prechambered enabled mixing-controlled combustion
Pd	Palladium
PeleLMeX	PeleLMeX is the non-subcycling version of PeleLM, an adaptive-mesh low Mach number hydrodynamics code for reacting flows
PFI	Port fuel injection
PGM	Platinum group metals
PI	Principal investigator
PIV	Particle image velocimetry
PM	Particulate matter
PNNL	Pacific Northwest National Laboratory
POSF#	Fuel designation
Pt	Platinum

Abbreviation	Definition
RANS	Reynolds-averaged Navier-Stokes
RCM	Rapid compression machine
RDD&D	Research, development, demonstration, and deployment
RHC	Reduction half cycle
SAF	Sustainable aviation fuel
SCO	Selective catalytic oxidation
SCR	Selective catalytic reduction
SI	Spark ignition
SiC	Silicon carbide
SOA	State of the art
SpaciMS	Spatially resolved capillary inlet mass spectrometer
SPK	Synthetic paraffinic kerosene
SVF	Soot volume fraction
SwRI	Southwest Research Institute
TCO	Total cost of ownership
TMB	Trimethylbenzene
TRL	Technology readiness level
TWC	Three-way catalyst
U.S. DRIVE	U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability DOE partnership
UDRI	University of Dayton Research Institute
ULI	NASA University Leadership Initiative
ULSD	Ultra-low sulfur diesel
UW	University of Wisconsin
V	Volts
VoFLE	Volume of Fluid and Lagrangian Eulerian
V-SCR	Vanadia-based selective catalytic reduction
VTO	Vehicle Technologies Office
VVT	Variable valve timing

Abbreviation	Definition
WMLES	Wall-modeled LES
WRLES	Wall-resolved LES
WSU	Washington State University
WVU	West Virginia University