1. Advanced Combustion Engines

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

The Advanced Combustion Engines (ACE) subprogram supports early-stage R&D to improve our understanding and ability to manipulate combustion processes, fuel properties, and catalyst formulations, generating the knowledge and insight necessary for industry to develop the next generation of engines and fuels for light- and heavy-duty vehicles. As a result, co-optimization of higher-efficiency engines and highperformance fuels has the potential to improve light-duty fuel economy by 35% (25% from advanced engine research and 10% from co-optimization with fuels) by 2030 compared to 2015 gasoline vehicles. The subprogram supports cutting-edge research at the National Laboratories, in close collaboration with academia and industry, to strengthen the knowledge base of high-efficiency, advanced combustion engines, fuels, and emission control catalysts. The ACE subprogram will apply the unique facilities and capabilities at the National Laboratories to create knowledge, new concepts, and research tools that industry can use to develop advanced combustion engines and co-optimize with fuels that will provide further efficiency improvements and emission reductions. These unique facilities and capabilities include the Combustion Research Facility at Sandia National Laboratories (SNL), Advanced Photon Source at Argonne National Laboratory (ANL), Institute for Integrated Catalysis at Pacific Northwest National Laboratory (PNNL), detailed fuel chemistry expertise at the National Renewable Energy Laboratory (NREL), chemical kinetic modeling and mechanism development at Lawrence Livermore National Laboratory (LLNL), and the Spallation Neutron Source at Oak Ridge National Laboratory (ORNL), along with their high performance computing resources and initial work to utilize future exascale computing resources.

Project Feedback

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

Table 1-1 - Project Feedback

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Welghted Average
ace001	Heavy-Duty Diesel Combustion	Mark Musculus (SNL)	1-7	3.50	3.50	3.50	3.00	3.44
ace022	Joint Development and Coordination of Emissions Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination)	Josh Pihl (ORNL)	1-11	3.67	3.67	4.00	3.50	3.69
ace023	CLEERS: Fundamentals in Selective Catalytic Reduction (SCR), Filter, and Protocol	Yong Wang (PNNL)	1-15	3.17	2.83	3.33	3.00	3.00
ace027	Next-Generation Selective Catalytic Reduction (SCR)- Dosing System Investigation	Abhijeet Karkamkar (PNNL)	1-18	2.80	2.70	2.80	2.70	2.74
ace032	Cummins-ORNL Emissions Cooperative Research and Development Agreement (CRADA): NOx Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems	Bill Partridge (ORNL)	1-22	3.33	3.17	3.25	3.17	3.22
ace033	Emission Control for Lean Gasoline Engines	Vitaly Prikhodko (ORNL)	1-27	3.33	3.50	3.33	3.00	3.38
ace056	Low-Temperature Oxidation	Yong Wang (PNNL)	1-31	3.42	3.50	3.42	3.25	3.44

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace085	Low-Temperature Emission Control to Enable Fuel- Efficient Engine Commercialization	Todd Toops (ORNL)	1-37	3.17	3.17	3.50	3.33	3.23
ace100	Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research - SuperTruck 2	Darek Villeneuve (Daimler Trucks North America)	1-40	3.36	3.29	3.21	3.07	3.27
ace101	Volvo SuperTruck 2: Pathway to Cost-Effective Commercialized Freight Efficiency	Pascal Amar (Volvo Trucks North America)	1-46	3.14	3.43	3.29	3.14	3.30
ace102	Cummins-Peterbilt SuperTruck 2	John Dickson (Cummins- Peterbilt)	1-52	3.29	3.14	3.21	3.14	3.19
ace103	Development and Demonstration of a Fuel- Efficient Class 8 Tractor and Trailer SuperTruck	Russell Zukouski (Navistar)	1-58	2.50	2.67	2.92	2.58	2.65
ace118	CLEERS Passive NOx Adsorber (PNA)	Janos Szanyi (PNNL)	1-63	3.25	3.13	3.13	3.00	3.14
ace119	Development and Optimization of a Multi- Functional SCR-DPF (Diesel Particulate Filter) Aftertreatment System for Heavy-Duty NOx and Soot Emission Reduction	Ken Rappe (PNNL)	1-66	3.00	3.17	3.33	3.00	3.13
ace123	Temperature-Following Thermal Barrier Coatings for High-Efficiency Engines	Tobias Schaedler (HRL Laboratories)	1-69	3.25	3.13	3.00	2.88	3.11
ace124	SuperTruck 2 - PACCAR	Maarten Meijer (PACCAR)	1-72	3.17	3.17	3.33	3.08	3.18
ace128	Reduced Precious Metal Catalysts for Methane and NOx Emission Control of Natural Gas Vehicles	Michael Harold (University of Houston)	1-77	3.50	3.42	3.25	3.42	3.42

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Weighted Average
ace129	Design and Optimization of Structured Multi-Functional Trapping Catalysts for Conversion of Hydrocarbons and NOx from Diesel and Advanced Combustion Engines	Michael Harold (University of Houston)	1-82	3.38	3.25	3.63	3.25	3.33
ace130	Development of Passive Hydrocarbon/NOx Trap Catalysts for Low- Temperature Gasoline Applications	Mark Crocker (University of Kentucky)	1-86	3.25	3.13	3.38	3.13	3.19
ace135	Towards Predictive Nozzle Flow and Combustion Simulations for Compression Ignition Engines	Gina Magnotti (ANL)	1-90	3.25	2.75	3.25	3.00	2.97
ace136	Medium-Duty Diesel Combustion	Stephen Busch (SNL)	1-93	3.17	3.00	2.83	3.00	3.02
ace138	Partnership for Advanced Combustion Engines (PACE) - A Light-Duty National Laboratory Combustion Consortium	Paul Miles (SNL)	1-96	3.60	3.20	3.60	3.20	3.35
ace139	Development of an Optimized Gasoline Surrogate Formulation for PACE Experiments and Simulations	Scott Wagnon (LLNL)	1-101	3.70	3.60	3.80	3.30	3.61
ace140	Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations	Russell Whitesides (LLNL)	1-106	3.50	3.50	3.50	3.20	3.46
ace141	Advanced Ignition System Fundamentals	Isaac Ekoto (SNL)	1-110	3.40	3.40	3.60	3.30	3.41
ace142	Development and Validation of Simulation Tools for Advanced Ignition Systems	Riccardo Scarcelli (ANL)	1-114	3.63	2.88	3.63	3.25	3.20

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Welghted Average
ace143	Fuel Injection and Spray Research	Chris Powell (ANL)	1-118	3.50	3.38	3.50	3.00	3.38
ace144	Spray Wall Interactions and Soot Formation	Lyle Pickett (SNL)	1-122	3.80	3.70	3.80	3.50	3.71
ace145	More Accurate Modeling of Heat Transfer in Internal Combustion Engines	K. Dean Edwards (ORNL)	1-127	3.20	3.10	3.50	3.10	3.18
ace146	Direct Numerical Simulation (DNS) and High- Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In- Cylinder Flow and Combustion Processes	Muhsin Ameen (ANL)	1-131	3.10	3.10	2.70	3.00	3.04
ace147	Mitigation of Knock and Low-Speed Pre-Ignition (LSPI) for High-Power Density Engines	Jim Szybist (ORNL)	1-135	3.50	3.50	3.00	3.63	3.45
ace148	Overcoming Barriers for Dilute Combustion	Brian Kaul (ORNL)	1-138	3.30	3.40	3.30	3.40	3.36
ace149	Cold-Start Physics and Chemistry in Combustion Systems for Emissions Reduction	Scott Curran (ORNL)	1-142	3.20	3.20	3.20	3.30	3.21
ace150	Enabling Low-Temperature Plasma (LTP) Ignition Technologies for Multi- Mode Engines through the Development of a Validated High-Fidelity LTP Model for Predictive Simulation Tools	Nick Tsolas (Auburn University)	1-147	3.00	3.08	3.00	3.00	3.04
ace151	Hierarchically Informed Engineering Models for Predictive Modeling of Turbulent Premixed Flame Propagation in Pre- Chamber Turbulent Jet Ignition	Haifeng Wang (Purdue University)	1-152	3.20	2.80	3.00	2.80	2.93

Presentation ID	Presentation Title	Principal Investigator (Organization)	Page Number	Approach	Technical Accomplishments	Collaborations	Future Research	Welghted Average
ace152	Development of High- Fidelity and Efficient Modeling Capabilities for Enabling Co-Optimization of Fuels and Multi-Mode Engines	Matthias Ihme (Stanford University)	1-156	3.10	3.20	3.20	3.20	3.18
ace153	Chemistry of Cold-Start Emissions and Impact of Emissions Control	Melanie Moses-DeBusk (ORNL)	1-160	3.50	3.38	3.50	3.25	3.41
ace154	Heavy-Duty Hybrid Diesel Engine with Front-End Accessory Drive-Integrated Energy Storage	Chad Koci (Caterpillar)	1-163	3.20	3.20	2.70	3.00	3.11
ace155	Low-Mass and High- Efficiency Engine for Medium-Duty Truck Applications	Qigui Wang (GM)	1-167	3.17	3.08	3.25	3.25	3.15
ace156	Next-Generation, High- Efficiency Boosted Engine Development	Michael Shelby (Ford)	1-171	3.50	3.50	3.10	3.40	3.44
ace157	Low-Temperature Gasoline Combustion for High- Efficiency Medium- and Heavy-Duty Engines	John Dec (SNL)	1-175	3.13	3.38	3.63	2.88	3.28
Overall Average				3.29	3.23	3.29	3.14	3.24

Presentation Number: ace001 Presentation Title: Heavy-Duty Diesel Combustion Principal Investigator: Mark Musculus (Sandia National Laboratories)

Presenter

Mark Musculus, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 60% of reviewers indicated that the resources were sufficient, 40% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.



Figure 1-1 - Presentation Number: ace001 Presentation Title: Heavy-Duty Diesel Combustion Principal Investigator: Mark Musculus (Sandia National Laboratories)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

This is an outstanding approach from all aspects—fundamentals, experimental, and computational fluid dynamics (CFD). This is what is always expected from Sandia and people tend to forget how difficult it is to do it consistently. Bravo.

Reviewer 2:

The project is well aligned with the objective of overcoming the barriers to further understanding of combustion and simulation from conventional diesel to low-temperature combustion (LTC), to improve integration of the aftertreatment system for LTC, and to better understand the impact of future fuels on LTC. The team is comprised of great expertise in spray laser diagnostics and simulations (direct numerical simulation [DNS] and Reynolds-averaged Navier-Stokes [RANS]. Each element in the project is complementing each other well. It is not clear, however, if the work will help the LTC aftertreatment system integration directly. Also, while the barrier includes understanding the impact of future fuels on LTC, the plan does not include any alternative fuels. Perhaps it makes sense to plan at least for simulating some alternative fuels.

Reviewer 3:

The team incorporates state-of-the-art experimental and numerical tools. The project focuses a lot of attention on two-injection process. Data are presented giving the motivation, such as enabling the reduction of soot within a range of load. The study provides physical insights to the mechanism associated with the two-injection events, which come from varying approaches, experimental and numerical.

Reviewer 4:

The reviewer was initially concerned whether optical engine results were representative of production engine performance but was encouraged to see that there are plans for future partnerships with parallel metal engine experiments. That being said, the project is making progress in addressing technical barriers in our understanding of combustion and simulation from conventional diesel to LTC. However, there seems to be no plans in addressing the impact of multi-component fuels on LTC.

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

Reviewer 1:

Results are very descriptive, and the progress made since the project started is very good.

Reviewer 2:

It looks like the team has made a good progress. Leveraging the cutting-edge laser diagnosis technology is a great element in the project. Also, it is great to see the world-class DNS being used to understand the ignition characteristics and flame development. One request for the team is to prepare a slide clearly indicating the current progress relative to the goals and milestones.

Reviewer 3:

According to the reviewer, experiments and simulations have been effectively leveraged to demonstrate valuable insights in the interaction between first and second injection pulses. The establishment of the fact that ignition of the second injection is dominated by auto-ignition, not flame propagation, is very much appreciated. However, could we also extend our understanding of the impact of a third injection pulse and even more?

Reviewer 4:

The study aims at uncovering the fundamental physics of combustion and emission formation. To this end, the team's work is of high quality. It may be helpful for the PIs to make an assessment on the overall progress of this study over the course of the last 10 years. To what extent have these studies improved the capability of engines to attain a higher efficiency - low emissions target? How much wider of an operation range has been enabled by the improved understanding of the physical process?

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

There is solid collaboration between academia and industry partners.

Reviewer 2:

The reviewer was impressed by the amount of collaboration between the various parties involved in the project and how fast results can come when people are really working together toward a common goal.

Reviewer 3:

As mentioned before, the team is well organized and complementary teams are supporting each other very well.

Reviewer 4:

There are excellent members in the team. Members range from industry partners to universities. There is a concentrated effort to make the findings known. The presentation did not appear to give information regarding how the work undertaken is being assimilated by industry. One of the many engine original equipment manufacturers (OEMs) could be tasked to bridge this gap.

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

Reviewer 1:

Future work is very clear, and milestones were clearly identified.

Reviewer 2:

Research includes the overarching goal to develop conceptual models, and tools are well covered. The team could have been more specific as to test conditions, especially seeking conditions that are tied to yielding notable improvements to the engine efficiency and emissions state of the art. Barriers 2-3 from Slide 2 (after treatment integration and future fuels) received no notice in the materials presented.

Reviewer 3:

The proposed future research looks good. It is not clear if any emission or temperature tracking is planned for helping the aftertreatment system integration/application.

Reviewer 4:

The reviewer commented that extensive materials were provided for the technical accomplishments, but the proposed future work seems sketchy and was not clearly elaborated.

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

Reviewer 1:

The reviewer affirmed that, yes, this project supports the overall United States (U.S.) Department of Energy (DOE) objectives because it focuses on the development of the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional and low-temperature combustion that is needed by the industry to design and build cleaner, more efficient engines.

Reviewer 2:

The project is well aligned with the DOE objectives to come up with a way for more fuel efficiency and cleaner energy utilization.

Reviewer 3:

There is no improvement in efficiency or emissions without understanding the fundamentals of combustion. This project is doing just that.

Reviewer 4:

The project work is relevant and, as suggested previously, could gain from a closer collaboration with industry, specifically attempting to correlate the work with conditions seen in real life applications. For example, how do the models help extend the use of dual injections to further mitigate soot and improve the engine efficiency?

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

Reviewer 1:

The project is being reported as 50% complete at the mid-way point of a 3-year program.

Reviewer 2:

The reviewer commented that resources are adequate.

Reviewer 3:

It looks like the team has sufficient resources.

Reviewer 4:

The reviewer remarked that it is ridiculous how little money goes to National Laboratories and academia that do so much innovative work.

Presentation Number: ace022 Presentation Title: Joint Development and Coordination of Emissions Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination) Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

Presenter

Josh Pihl, Oak Ridge National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. 33% of reviewers indicated that the resources were sufficient, 33% of reviewers indicated that the resources were insufficient, while the remaining reviewers indicated that the resources were excessive.

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



Figure 1-2 - Presentation Number: ace022 Presentation Title: Joint Development and Coordination of Emissions Control Data and Models (Cross-cut Lean Exhaust Emissions Reduction Simulations (CLEERS) Analysis and Coordination) Principal Investigator: Josh Pihl (Oak Ridge National Laboratory)

Reviewer 1:

The reviewer affirmed a great job in coordinating the collaboration activities including the Crosscut Lean Exhaust Emissions Reduction Simulations CLEERS conference and the teleconferences. The team should be commended for responding quickly to the Industry Priorities Survey in ramping down the passive oxides of nitrogen (NO_x) adsorber (PNA) work and ramping up the hydrocarbon trap (HCT) work and selective catalytic reduction (SCR) aging work. CLEERS is a good blend of coordination activities and technical work.

Reviewer 2:

The approach is well focused and spot on. The questions address the needs of the industry. The team has been creative in its approach, resorting to surveys, modeling, and testing. The industry dialogue that the team has created allows pre-competitive exchange of ideas and findings. Years after the DOE's Directions in Engine-Efficiency and Emissions Research (DEER) conference discontinued, CLEERS has done a nice job filling its vacuum and the gap created due to the absence of DEER. If CLEERS will not do it, who will?

Reviewer 3:

CLEERS activities and research and development (R&D) involve a coordinated effort between National Laboratories, industry, and academia. This coordination provides an abundance of expertise and resources to address the critical barriers in emissions reduction technology. Development of catalysts, discerning the operational boundaries, and studying the effects of aging of low-temperature exhaust conditions is vital for

realizing low emissions profile from both clean diesel and lean spark ignition (SI) platforms. The project partners are well equipped with resources to develop the models and validate with experimental results.

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

Reviewer 1:

The reviewer has been involved with and watching CLEERS since its inception. It is rare that the reviewer rates "Outstanding," but in all fairness CLEERS checks all the boxes and has exceeded its initial charter and expectations. Not only has it shown due progress and adapting to and meeting both the DOE and the industry's needs, it is also led by an intelligent, pro-active, and dynamic team continually monitoring the latest changes in the emission control field.

Reviewer 2:

The reviewer affirmed a nice study on the adsorption of different hydrocarbons on the uncatalyzed zeolite beta (BEA) formulation. Also, there is a very nice fit of the ammonia (NH₃) storage and release data with the copper (Cu)/aluminosilicate zeolite (SSZ-13) sample as a function of the storage temperature, aging temperature, water (H₂O) concentration, and NH₃ concentration.

Reviewer 3:

The CLEERS workshops for 2019 and 2020 have been successfully organized and results related to nitric oxide (NO) adsorption model and palladium (Pd)-zeolite PNA has been disseminated. In addition, measurements for HC adsorption on a zeolite-based HC trap has been completed. The 2019 CLEERS Industry Priorities Survey is an excellent way to communicate with industry stakeholders to assess the imminent topics that need to be addressed as part of government-funded research. As expected, SCR-related topics for heavy duty (HD), medium duty (MD), and light duty (LD) vehicles ranked the highest in importance. This is in line with the industry challenges with respect to upcoming California Air Resources Board (CARB) regulations and the need for the diesel industry to further reduce NO_x emissions. Complex aftertreatment packages may not be preferred by engine manufacturers; rather, the focus should be aimed at understanding inefficiencies in current SCR and also developing close-couple catalyst technologies for these platforms. Using SCR on the filter is another upcoming technology that needs better understanding. Overall, the technical accomplishment of this project is excellent.

An additional question related to the accomplishment is—for the tasks involving the study of SCR aging and its impact on ammonia inventory—whether the project will focus on unwanted species that are formed during urea decomposition that could potentially be occupying ammonia adsorption sites on the SCR catalyst. The reviewer believed that such a mechanism was proving to be a critical barrier to realizing high NO_x conversion efficiency in real-world operation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Collaboration appears strong. Coordination seems streamlined with good feedback channels and communication with the industry.

Reviewer 2:

CLEERS does a tremendous job in promoting collaboration among industry researchers on vehicle emission controls. The CLEERS conference and monthly teleconferences provide very effective forums for sharing precompetitive emissions data with peers from other companies and institutions. The Priorities survey also highlights the emission control topics that currently need to be prioritized. CLEERS also has good collaboration with Professor Bill Epling of the University of Virginia (UVA), Johnson Matthey (JM), Pacific Northwest National Laboratory (PNNL), the Advanced Combustion and Emission Control (ACEC) tech team, and the Advanced Engine Crosscut team.

Reviewer 3:

Many of the accomplishments shown in this project were not possible without outstanding coordination between the teams. Collaboration with UVA has generated interesting results for PNA NO storage. The involvement of JM for catalyst material and PNNL for modeling is also vital.

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

Reviewer 1:

The team has done an outstanding job listening to the industry needs, summarizing them in a concise fashion, and communicating them across the greater emission control community. Some of the gathered information has been used creatively to also address some of the needs, e.g., via modeling or testing. What appears to be missing is expanding into cross-functional industry collaborations to fill some of the gaps of immense industry needs. This is indeed the vision that late Dr. Stuart Daw, one of the main CLEERS architects, had in mind.

It appeared to the reviewer that one of the clear needs at this juncture in industry is a strong, low-temperature SCR catalyst yielding 90% or higher activity at about 150°Celsius (C). This fits well with DOE's goal of advancing fuel economy, since low-temperature SCR of NO_x is a strong, fuel economy strategy. Some of the estimates, which have been seen, indicate up to 7% fuel economy, should such SCR technology become available. Despite years of industry discussions, no one seems to want to take the lead for a collaboration, perhaps due to its competitive nature. With all the activities going on in low-temperature NO_x reduction, CLEERS—and perhaps CLEERS only—is in a unique position to fill such a gap, making a long-term impact on this industry as well as enabling a novel route to fuel economy, itself significant for the DOE's charter.

Reviewer 2:

The collaboration and coordination work definitely need to continue with the CLEERS conference and teleconferences. The HCT work needs to be expanded to include catalyzed HCTs so the oxidation of the stored HC species can be studied. This will be challenging for stoichiometric applications since there is no excess oxygen with which to oxidize the hydrocarbons (HCs), so methods to introduce oxygen (e.g., oxygen storage component [OSC], air injection) will need to be studied. The effects of different aging conditions (rich, stoichiometric, lean) on the HCT would also be useful. The SCR work on NH_3 storage also needs to be expanded to include NO_x conversion.

Reviewer 3:

Future research focuses on PNA, HC traps, and urea SCR catalyst. The SCR-catalyst-related work is highly important; however, the reviewer indicated a couple of questions remain related to future research work. Is PNA still a viable solution for low-NO_x, low-fuel consumption targets? For which type of application is the work related to PNA targeting? Because PNA is less favored for future emissions standards, targeting a certain application where PNA would be favored will add value to the model outcomes.

The industry is finding it hard to understand the underperformance of SCR under real-world conditions. Many factors may contribute to this underperformance—aging, deposit formation, uncharacteristic deterioration based on duty cycle, fuel impurities, etc. In order to be responsive to industry challenges, work in this direction can be addressed along with aging-related work.

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

Reviewer 1:

The reviewer remarked that CLEERS supports the DOE charter of fuel saving strategies and close interactions with the industry, above and beyond its initial charter. It is hard to think of pre-competitive discussions in this industry without CLEERS's contributions. The reviewer encourages DOE to provide more resources and

funding for CLEERS so it can expand on the outstanding value it brings to the government, industry, society, and environment. It is a win-win across all the stakeholders.

Reviewer 2:

The CLEERS conferences and telecoms provide a great forum for sharing technical data with peers from other companies and thereby promoting pre-competitive collaboration. The study of emission control technologies that allow fuel-efficient engines to go to market while meeting the appropriate emission standards is paramount for supporting the DOE objective of reducing our dependence on foreign oil.

Reviewer 3:

The project addresses important issues related to catalyst development for future emissions standards. The project was also instrumental in receiving feedback from industry to develop current and future direction of research.

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

Reviewer 1:

The reviewer indicated that a group of 33 industry entities, 23 academic institutions, and 12 National Laboratories together had all the resources to address all the milestone set forth in this study.

Reviewer 2:

The resources appear to be adequate for now, although there might be a need for more experimental and modeling resources in order to expand the HCT work to include HC oxidation as well as the effects of aging. The expansion of the SCR work to include NO_x conversion could also require additional resources.

Reviewer 3:

The reviewer has marked the project as "Insufficient." Although CLEERS does meet its goals, it also appears to have become resource-strapped given the recent (last 2-4 years) expansions in its activities and goals. In the opinion of this reviewer, given its broad-reaching impacts, providing it with more resources is warranted and will certainly create even a far stronger "value to cost" ratio.

Presentation Number: ace023 Presentation Title: CLEERS: Fundamentals in Selective Catalytic Reduction (SCR), Filter, and Protocol Principal Investigator: Yong Wang (Pacific Northwest National Laboratory)

Presenter

Yong Wang, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

All of reviewers indicated that the project was relevant to current DOE objectives and the resources were sufficient.

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



Reviewer 1:

The approach to this work is sound.

PNNL is utilizing its high-performance

computing resources and bench-scale experimentation to answer key questions in three-way catalyst (TWC) and SCR catalyst development.

Reviewer 2:

The reviewer stated that this is good work, targeting reduced platinum group metal (PGM) loading and lowtemperature catalyst performance. There are good observations reported here, such as the impact of sulfur (S). The overall findings, however, appear minimal, given that they reflect a full year of activity blessed with sufficient funding, testing means, advanced characterization tools, and modeling resources across two National Laboratories, several OEMs, one Tier 1 supplier, and three universities (some had indirect roles). It is likely more could have been achieved.

Reviewer 3:

(PNNL makes good use of its vast capabilities in fundamental science to advance the development of emission control catalysts. Instead of focusing on one topic like other PNNL projects, this particular project is a hodgepodge of different catalyst technologies including SCR catalysts, rhodium (Rh) and Cu catalysts, particulate filter development, and catalyst testing protocol development. It might be good to break up this project into several smaller projects where each is focused on one catalyst technology.

Figure 1-3 - Presentation Number: ace023 Presentation Title: CLEERS: Fundamentals in Selective Catalytic Reduction (SCR), Filter, and Protocol Principal Investigator: Yong Wang (Pacific Northwest National Laboratory) Question 2: Technical Accomplishments and Progress toward overall project goals—the degree to which progress has been made and plan is on schedule.

Reviewer 1:

The reviewer called this a nice study on the effects of sulfur poisoning and desulfation on the single-atom Cu/cerium (Ce) catalyst. It is also very nice work on investigating the NO_x conversion of the single-atom Rh/Ce catalyst; the results highlight the importance of including H₂O on all the tests, since H₂O is always present in automotive exhaust. The Rh/Ce catalyst should be tested at stoichiometry and not the very rich conditions that were used (1,750 parts per million [ppm] CO, 460 ppm NO); this would probably reduce the NH₃ formation on the test with H₂O. Also, it is a nice job on the addition of manganese (Mn)/Ce to the SCR catalyst to increase the NO₂ formation for the SCR catalyst and thereby allow the feed gas nitrogen dioxide (NO₂) to be used for soot oxidation. The effects of sulfur poisoning on this catalyst definitely need to be investigated because Mn forms stable sulfates. The reviewer noted the outstanding job of taking the lead on developing the catalyst testing protocol.

Reviewer 2:

The SCR low-temperature activity appears to be still around 80% even in the presence of Mn-Ce oxides. Are there other approaches to push this conversion higher, or are we reaching the limits of catalyst conversion efficiencies?

Activities related to TWCs show interesting results of almost over 90% NO reduction for temperatures as low as 100°C. One question related to TWC research is how representative are these results for TWC used in natural gas vehicles? The TWCs in natural gas (NG) vehicles seem to undergo significant degradation faster than that in gasoline applications. Is there work being done to understand this aspect or translate these findings to natural gas vehicle (NGV) exhaust?

Reviewer 3:

The work quality is good; however, it is the understanding of this reviewer that the accomplishments are modest relative to the capability and resources of both the core and the broader team.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that there is good collaboration with General Motors (GM), the University of New Mexico, and Washington State University on the single-atom catalysts.

Reviewer 2:

It appeared to the reviewer that the coordination looks good. The principal investigator (PI) has done a good job cross-functionally synergizing the characterization capabilities, modeling, and testing resources across the core team, and reasonably across the broader team.

Reviewer 3:

The collaboration with Cummins, Fiat Chrysler Automotive (FCA), and Kymanetics lends value and direction to this study. It would be interesting to involve Cummins for TWC related work since Cummins is a leading NGV engine manufacturer, input on issues related to TWC for NG applications is important as well.

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

Reviewer 1:

The SCR-related future work listed in the presentation is valuable and highly important with regard to specific topics related to examining aged, on-road catalysts. The reviewer believed this will lend the most value to this

study. Aging of closed couple SCRs in heavy-duty applications also needs to be considered. The reviewer commented that there is no mention of natural gas related TWC work and a decrease in NO_x reduction with age. Additionally, the opined that work related to selective catalytic reduction filter (SCRF) is also valuable.

Reviewer 2:

The reviewer remarked that the plan for "Future Work" could possibly benefit from some modifications. Though a key focus on this project is "low temperature" performance, only one out of seven tasks appears to have a low-temperature focus. The task "Conduct fundamental filtration experiments to understand effects of porosity variation across the thickness of ceramic exhaust filter walls" has been extensively studied by honeycomb suppliers and coaters. There are also several publications on flow patterns in pores of a wall-flow device. Studying such literature would propel this work forward more speedily.

Reviewer 3:

The reviewer stated that the project team needs to look at the effects of sulfur poisoning and thermal aging on the single atom Rh/Ce catalyst. Since this is being developed as a TWC, aging temperatures of 900° to 950°C need to be assessed while using the ACEC aging protocol (neutral/rich/lean aging). The OSC of the Rh/Ce catalyst needs to be assessed, because OSC is so important for TWCs. The light off tests need to be assessed with air to fuel ratio (A/F) dithering to simulate actual vehicle operation. Also, the team needs to investigate sulfur poisoning and desulfations on the Mn-Ce-modified SCR catalyst, since sulfur inhibits the low-temperature activity of SCR catalysts.

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

Reviewer 1:

This project supports overall DOE goals by addressing critical barriers and issues related to advanced NO_x reduction catalysts. Improvements in catalyst efficiency are vital to improving engine efficiency.

Reviewer 2:

The reviewer commented that low-temperature performance is synonymous with fuel savings (either via optimized combustion or cold-flow fuel savings). Thus, the work fundamentally coincides with the DOE objectives.

Reviewer 3:

PNNL is developing catalysts for low-temperature operation, which will be needed to meet the Tier 3 Bin 3 emission standards with future fuel-efficient engines that generate lower exhaust temperatures.

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

Reviewer 1:

The team has some of the world's best characterization resources, tools, and brain power. Resources are not a concern in this project.

Reviewer 2:

The PNNL high-performance computing resources are well equipped to perform high fidelity model development. Micro-reactor test benches available with industry partners can also help achieve goals of the study.

Reviewer 3:

The resources appear to be sufficient for the current workload.

Presentation Number: ace027 Presentation Title: Next-Generation Selective Catalytic Reduction (SCR)-Dosing System Investigation Principal Investigator: Abhijeet Karkamkar (Pacific Northwest National Laboratory)

Presenter

Abhijeet Karkamkar, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. 80% of reviewers indicated that the resources were sufficient while the remaining reviewers indicated that the resources were insufficient.

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

Reviewer 1:

The approach to this project has

improved in the past year for the reviewer, as it has focused on an important issue in urea hydrolysis and on new storage materials.

Laboratory)

Reviewer 2:

The project reports on a solid-material approach of storing and releasing NH_3 to tackle emissions under 180°C, albeit this is a huge distance from real-world application for the foreseeable future.

Reviewer 3:

The approach of looking for new catalysts that can decompose urea at low temperature without forming isocyanic acid (HNCO) and then store NH_3 is good. But, quantification for the effectiveness of these material is not provided. There is no other matrix presented than NH_3 storage capacity. Further, effectiveness of few high-ranking materials from this study could be pursued further for their practical application and challenges (cost, volume needed, chemical hazard analysis, etc.).

Reviewer 4:

This work has generated some interesting and relevant data, and the investigation of NH_3 storage from urea is sensible considering the current state of the art in NO_x abatement, but the project seems to leap around in terms of focus from year to year in response to reviewer comments. The responsiveness is good, but it gives the impression of improvisation as opposed to planning. The technical milestones are also poorly defined, and do not appear to align with the technical accomplishments presented.



Figure 1-4 - Presentation Number: ace027 Presentation Title: Next-

Principal Investigator: Abhijeet Karkamkar (Pacific Northwest National

Generation Selective Catalytic Reduction (SCR)-Dosing System Investigation

Reviewer 5:

Given the growing interest in using close-coupled SCR catalysts on future heavy-duty diesel engines to meet future ultra-low NO_x emission limits (see Southwest Research Institute [SwRI]/ CARB heavy-duty low NO_x test program results), how does this project fit with the use of close-coupled SCR catalyst on a heavy-duty diesel engine? Perhaps the search for a better urea hydrolysis catalyst still has some merits, but the reviewer was not sure an ammonia storage agent is important for achieving future ultra-low NO_x emission targets.

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

Reviewer 1:

Progress has been made in identifying a urea hydrolysis catalyst that limits production of isocyanic acid. The project has also identified some interesting zeolite-based ammonia storage materials.

Reviewer 2:

The oxide catalysts for largely reducing isocyanate as a product of the urea hydrolysis are very interesting. More data on their actual use are important, because these would be put in existing commercial systems. The work on titania-silica catalysts for ammonia storage is also interesting but should be pursued further.

Reviewer 3:

The NH_3 storage and desorption behaviors have been investigated on multiple materials to enable the down selection process. It is not clear whether the team has the chemistry and materials insight to identify the most promising materials. The choice of materials seems to heavily rely on recommendations instead of theory guided choices.

Reviewer 4:

A key barrier to practical application of these NH_3 storage materials—competition with H_2O —is not addressed. Though it is mentioned as a future goal, the reviewer was not sure how effective it would be in such a short duration as the project is ending in September 2020. Additionally, this whole exercise looks like a screening process without putting more emphasis on the science of urea decomposition and storage of NH_3 so that material having minimum effect of competing species (e.g., water) can be selected.

Reviewer 5:

The reviewer does not doubt the quality of the work being done, but the presentation of the results lacks clarity. Of the barriers presented, only "New materials to address the 150°C" is addressed. The technical milestones and the technical accomplishments do not match. That being said, the reviewer was interested to see the outcome of the hydrolysis catalyst work and its impact on deposit formation.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Collaborations with groups within United States Council for Automotive Research (USCAR) have been useful. Interaction with more groups outside of USCAR would also be helpful.

Reviewer 2:

The project seems be running with constrained resources despite a good intention. It is understandable, given the funding level.

Reviewer 3:

Collaboration appears to be primarily through scheduled meetings with USCAR. Consultation with industry is also mentioned, but no substantial involvement is indicated.

Reviewer 4:

It is mentioned that the USCAR team is well aware of findings and provides its voice to the project. It would be better if the team is involved in discovering the science and then applying it.

Reviewer 5:

More feedback from industry is needed on whether an improved urea hydrolysis catalyst or another ammonia storage material is needed to meet future heavy-duty, ultra-low NO_x targets.

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

Reviewer 1:

According to the reviewer, the proposed future research is well chosen to look at materials issues in this challenging area.

Reviewer 2:

Some of the tasks mentioned in future work should have been done upfront (e.g., mechanistic studies effect of H_2O) so better materials could have been selected. Zeolite modification is a broader topic and more insight has not been provided. Alternative development pathways are also not provided.

Reviewer 3:

The proposed future work is a logical continuation of the work presented here. It is difficult to tell if it aligns with the proposed technical milestones.

Reviewer 4:

The proposed work is a reasonable direction. However, it is overloaded with the limited amount of time and resources.

Reviewer 5:

Given the growing interest in using close-coupled SCR catalysts on future heavy-duty diesel engines to meet future ultra-low NO_x emission limits, is this project still relevant? Perhaps the search for a better urea hydrolysis catalyst still has some merits, but the reviewer was not sure the world needs another ammonia storage agent.

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

Reviewer 1:

This project is focused on developing an alternative source of NH_3 for the SCR catalyst on diesel vehicles that will allow NO_x conversion below 180°C, the temperature where the current source of NH_3 (urea) decomposes. Such an NH_3 source would be helpful for providing NO_x conversion at lower temperatures with advanced SCR catalysts and also for reducing the extra fueling currently required to maintain the exhaust temperatures above 180°C during low load operation.

Reviewer 2:

A low-temperature NH_3 supply is necessary for low-temperature NO_x abatement, which allows for fuel efficiency while meeting emission regulations.

Reviewer 3:

If the project is successful in allowing earlier low-temperature (T) light-off of ammonia SCR catalysts, this project is very relevant in meeting low energy efficiency in emissions control.

Reviewer 4:

Future emissions regulations for light-duty and heavy-duty diesel would require efficient NO_x conversion at low temperatures, and providing suitable reductant at these low temperatures is critical for NO_x conversion. There are other alternatives to low temperatures, such as hybridization or operating the engine at high temperatures to avoid these low-temperature regimes, but those come at higher cost of the product or higher greenhouse emissions. Therefore, industry is really looking for the technology of reductant delivery at low temperature without deposit formation.

Reviewer 5:

The reviewer understands the interest in this project to support low-temperature NO_x performance, but given the growing interest in using close-coupled SCR catalysts on future heavy-duty diesel engines to meet future ultra-low NO_x emission limits, is this project still relevant? Perhaps the search for a better urea hydrolysis catalyst still has some merits, but the reviewer was not sure the world needs another ammonia storage agent. The reviewer indicated that this is a repeat of comments on this project's future work.

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

Reviewer 1:

The project appears to have sufficient resources to complete the remaining milestone by the end of the project schedule later this year.

Reviewer 2:

Resources are very sufficient for this project at PNNL.

Reviewer 3:

The reviewer said that resources are sufficient.

Reviewer 4:

The funding level appears to be sufficient for the work performed.

Reviewer 5:

The project is delivering preliminary material selections under simple and ideal conditions. A significant amount of coordinated engineering effort is required to strengthen the research, and many fundamental aspects of the research remain premature.

Presentation Number: ace032 Presentation Title: Cummins-ORNL Emissions Cooperative Research and Development Agreement (CRADA): NOx Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems Principal Investigator: Bill Partridge (Oak Ridge National Laboratory)

Presenter

Bill Partridge, Oak Ridge National Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives and the resources were sufficient.

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

Reviewer 1:

The group has focused on understanding the aging mechanisms of Cu/SSZ SCR



Figure 1-5 - Presentation Number: ace032 Presentation Title: Cummins-ORNL Emissions Cooperative Research and Development Agreement (CRADA): NOx Control and Measurement Technology for Heavy-Duty Diesel Engines, Self-Diagnosing SmartCatalyst Systems Principal Investigator: Bill Partridge (Oak Ridge National Laboratory)

catalysts. The project team found specific features in the activity profiles as a function of temperature that change with aging and describe the kinetic half cycles of the reaction. The project team hopes to use these to determine specifics of the aging and how to incorporate such findings into models and better designed systems. With this unique approach, the project team is addressing the technical barrier–understanding field-aged samples that have yet to be mimicked with lab-aging protocols. The reviewer asserted that the project team has a well-designed plan.

Reviewer 2:

The presentation and project did a nice job of making the case for the context of the work and how field aging is distinct from hydrothermal lab aging and must be studied and modeled. The introductory material also showed well how the current project is distinct and fits into the larger collective of low-T emissions projects.

The approach taken seems very reasonable by building a transient response apparatus, collecting data, and modeling and then moving to systems of commercial relevance. While the combination of the components of this approach do not strike this reviewer as very "outside the box", nonetheless it seems effective and appropriate for a goal-oriented project.

Reviewer 3:

This project has a goal of determining the kinetics of the entire cycle of the NH_3 SCR reaction with a focus on low-temperature kinetics to improve its use in HD NO_x remediation. This relatively unique approach gains data

from a transient response reactor to use in a global-kinetic model. One useful addition to the approach was data taken on a field-aged versus a lab-aged catalyst.

Reviewer 4:

The project thus far has focused on developing a half-cycle-based kinetic model for SCR catalyst performance. In the subsequent work, the team will use field-aged catalysts to look at how the kinetic parameters have changed. The reviewer asserted that this should lead to further understanding the key SCR catalyst deactivation mechanisms found in the field.

Reviewer 5:

The project, which is focused on understanding field-aging of SCR catalyst, is well planned and targets several key aspects of aging. It includes modeling, kinetics considerations, and testing. The team is capable and includes a major engine OEM and catalyst supplier. If integrated in engine operation (to synchronize engine-catalyst operations as a model-based control) and successful, it could result in better SCR operations, system efficiency, and overall fuel economy as well as improved durability and full useful life.

The reason this evaluation is rated "Good" (not higher) is that there was no strong evidence shown that any major attempt has been invested in the project thus far. There is no strong evidence (except lightly pointing to it) seen in the project displaying what that may look like—when, how, plan, timeline, specific objectives, etc.—while the project has progressed more than 50% thus far.

Reviewer 6:

More stringent durability requirements for HD aftertreatment are expected from regulatory agencies in the coming year. Therefore, the development of viable approaches for diagnosing the state of a SCR catalyst for HD diesel applications is highly desirable from an OEM perspective. The method proposed here to monitor the state of the catalyst through a conversion inflection (CI) phenomenon is unique and offers the potential to predict the catalyst performance. However, in order to quantify the state of the catalyst, the method relies heavily on its ability to differentiate the cause of degradation and whether or not the entire SCR is affected. This requires known, in-field aging processes, which have not been demonstrated over the multiple years of this project. Being able to separate and quantify the contributions from each of the aging mechanisms on the CI phenomenon will be very challenging.

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

Reviewer 1:

Milestones seem to be on track for a project about halfway through its cycle. Overall, the team seems to address the majority of comments from prior reviews sufficiently. No aspect of the project seems to be lagging, the reactor is working, data are being collected, and the fitting seems to be moving to the point of applying the overall methodology to "real" systems. The reviewer noted that, in the slides and presentations, it would be helpful to better delineate data that are experimental versus fitted. The backup slides did this well, but it was not always clear to the reviewer in the presentation itself.

Reviewer 2:

The reviewer commented so far, so good, in developing the half-cycle model. Now comes fitting the model to field-aged hardware and linking those results to real world degradation mechanisms.

Reviewer 3:

The progress is good, noticeable, and tangible compared to its state last year. Kinetics considerations and testing (hydrothermally aged, HTA) and sulfur poisoning) have been accomplished and are further in progress. New Cummins team members, especially for modeling, have been integrated into the project.

Thus far, this project has largely focused on sulfur and temperature impacts, but not that of lube oil. The presentation only lightly mentions lube oil impact. Some studies have shown that some SCR field aging/poisoning impacts could be attributed to lube oil species (iron (Fe), potassium (K), phosphorus (P), etc.), though they have been typically reported not to be as serious as the impact of sulfur and vary depending on the catalyst type. With more than half of the project now completed, it is worthwhile for the project to investigate such impacts as well, especially since kinetics considerations are a major part of this study.

Reviewer 4:

Model development and parameter fittings are key accomplishments. The fitting of the data provides confidence in the model and approach the team is using. The new reactor should accelerate results gathering. The reviewer posed a question about whether the degradation mode will actually correlate to the data as this could be elusive. However, the project team has shown that it can obtain the needed data for the half cycles that describe the SCR reaction, and the upcoming annual cycle will provide the team with the aged catalyst data and allow testing the working hypothesis.

Reviewer 5:

A portion of what was presented in this update has been discussed in prior updates. Although the kinetic development is important, it will be difficult to differentiate the catalyst behavior resulting from different aging mechanisms. While the approach is novel, the level of progress in the past year is less than expected. It appeared to the reviewer that significant effort would be applied to building a reactor system, when one should already be available either within Oak Ridge National Laboratory (ORNL) or at Cummins to perform that work. More effort should be spent evaluating the field-aged sample in terms of correlating the performance of the SCR substrate along its length to the actual state (physical and chemical) of the sample along its length. That will help link the state of each portion of the catalyst to the overall performance and allow better modeling. The effects of oil poisons, PGM poisons, and thermal aging will have to be taken into consideration.

Reviewer 6:

A wide range of kinetic parameters was determined and used in the model. A major and interesting finding is that the field-aged catalyst data do not appear to be reflected well in the data from lab-aged catalysts. Some major efforts remain to reach the project goals.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

According to the reviewer, an excellent set of partners is on the project.

Reviewer 2:

There is obvious collaboration between ORNL and Cummins. The participation of (JM in the project was not made obvious by the presentation, unless it was the catalyst supplier.

Reviewer 3:

Cummins will need to do more in the coming year to help link modeling results with field-aging degradation mechanisms.

Reviewer 4:

Collaboration includes ORNL, Cummins, and JM. This is a strong team, but the reviewer had a feeling that some of the deep, fundamental insight is missing. Integration of a catalyst chemist from academia well versed in catalyst aging is something to think about.

Reviewer 5:

The slides and presentation could have done a better job delineating who did what, i.e., what were the specific contributions spread across the various partners. A separate slide showing a discrete example of how the team

worked together on each component of the work (reactor, data collection, and data modeling) would have been powerful in convincing reviewers the project team provides a sum greater than the parts.

Reviewer 6:

The collaboration on this project appears appropriate but appears to lack timely results. Also, the inclusion of a sensor supplier would help provide greater insight on how to accurately measure the NO_x and NH_3 in a vehicle application.

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

Reviewer 1:

The upcoming work plan begins the processes of understanding dominant, real-world degradation mechanisms and how to better simulate real world aging in the lab to assist in designing better SCR catalysts.

Reviewer 2:

Finishing the transient reactor and measurements on the field-aged catalysts are major items in the future research. The spatially resolved capillary input mass spectrometer (Spaci-MS) database measurements should be very useful. Bringing results to improving the durability of SCR catalysts would be a highlight for next year, if achieved.

Reviewer 3:

In general, the path for the project is clear. Now that the team and strategy are in place, moving to field aging and varying the catalyst formulation are needed. The presentation mentioned the catalyst formulation will vary in FY 2021. Some general comments on how it will be different (metal content, support, etc.) would have enhanced the picture of the proposed work significantly.

Reviewer 4:

The move to obtaining enough results from field-aged samples to develop and tune the kinetic parameters is the right next step. Will all samples have to be rerun in the new reactor? The reviewer hoped that is not the case. Then the challenge will be determining if those newly measured kinetics help define the real-world aging mechanisms and how to incorporate these into a model. The proposed future work is appropriate.

Reviewer 5:

The reviewer said that future steps are determining the impact of field aging on kinetics of commercial Cu-SSZ-13 SCR catalyst; and determining the kinetic origins of performance for low-temperature formulations. The reviewer asked about the impacts of lube oil and NO_2/NO_x . Both impact the pre-exponentials of the kinetics, and the impact of NO_2 was barely mentioned.

Reviewer 6:

Less effort should be placed on building a new reactor system when that resource should already be available at one of the partner organizations. More timely effort should be placed on dissecting a reference catalyst in terms of linking its performance along its length to the actual condition of the catalyst to predict an overall performance measurement.

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

Reviewer 1:

The project absolutely supports the overall DOE objectives. From the introductory slides and the focus of the research, it is clear the team has carefully considered how the work fits into the greater context of the VTO and DOE goals. The project does an excellent job of fitting into a space between a focus on primarily fundamental topics not applicable to an applied program and being so applied in nature it appears the work is a subcontract

to another specialty company. Construction of the reactor and knowledge gained from the experimental/modeling studies will do the following: certainly benefit the systems of interest with real world potential; simultaneously develop a methodology and approach that might find use in other contexts. As such, the work resides in an excellent niche very suitable for VTO projects.

Reviewer 2:

Reliable and accurate diagnostic methods are highly sought after by OEMs, especially given the future mandates for full useful life of these aftertreatment systems.

Reviewer 3:

With new regulations forthcoming and demanding a significant increase in catalyst lifetime, this work is highly relevant to ensuring the continued use of high efficiency engines.

Reviewer 4:

This work is uniquely relevant to improving our understanding the mechanism of the very important ammonia SCR reaction in HD diesel NO_x aftertreatment.

Reviewer 5:

The development of lab- or engine-based SCR catalyst aging protocols that better simulate real world performance is an important enabler to designing more durable SCR catalysts.

Reviewer 6:

The reviewer affirmed that-SCR means fuel economy, and low-temperature operation means more fuel economy. Both fit DOE's energy policy.

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

Reviewer 1:

All resources seem appropriate. As the reviewer mentioned in prior comment, all needed components to finish the project (reactor working, experimental data collection in place, and modeling moving toward the level needed to complete the project goals) are in place.

Reviewer 2:

The resources seem appropriate for the milestones over the project term.

Reviewer 3:

Between Cummins and ORNL there are sufficient resources to characterize these catalysts.

Reviewer 4:

Cummins and ORNL have sufficient resources for this project.

Reviewer 5:

Resources are adequate and modeling resources are strong. Characterization resources are good as well.

Presentation Number: ace033 Presentation Title: Emission Control for Lean Gasoline Engines Principal Investigator: Vitaly Prikhodko (Oak Ridge National Laboratory)

Presenter

Vitaly Prikhodko, Oak Ridge National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. Two reviewers indicated that the resources were sufficient while the third reviewer indicated that the resources were insufficient.

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



Figure 1-6 - Presentation Number: ace033 Presentation Title: Emission Control for Lean Gasoline Engines Principal Investigator: Vitaly Prikhodko (Oak Ridge National Laboratory)

Reviewer 1:

The passive SCR strategy is promising

to develop lean burn spark ignited (SI) engines with no external reductant tank (urea tank). The use of TWC as an ammonia generator is novel. For this strategy to be efficient it is very important for both engine and catalyst be optimized to work together. The team approach used in this study—focusing on optimizing different parts of the system, mainly engine lean operation, engine rich operation, NO_x -to-ammonia conversion etc.—is an excellent approach to realize the true benefits of this approach. Furthermore, change in the engine platform to a current/future technology engine is a very good change.

Reviewer 2:

This project is a good blend of reactor testing and engine testing. It is commendable that the project team is optimizing the engine and catalyst together as a system. The reviewer especially appreciated the aging studies on the SCR catalyst where the A/F ratio of the exhaust was varied (lean, stoichiometry, or rich). The reviewer is hopeful that the new MAHLE engine will be more amenable to the lean-burn work.

Reviewer 3:

The project is well designed and on track. However, despite its potential benefits, its overall cost to benefit ratio is unclear. Control and on-board diagnostic (OBD) aspects of this architecture are unknown, not studied and probably outside the range of the current study.

Though, from an exploration point of view, this concept is interesting, this technology will have a weak chance in the commercial space as its challenges include:

- "Efficiency, durability," are said to be the targets. However, the system's inherent fuel penalty signals lack of fuel efficiency. The hope is however that this fuel penalty (to form ammonia) is well below lean engine offering 5%–15% increased efficiency (over stoichiometric-operated gasoline engines).
- Increase in carbon dioxide (CO₂), due to excess fuel used, is another challenge of this approach.
- High-temperature NH₃ storage is degraded at 700°C aging and eliminated at 800°C.
- The upstream TWC typically exposes the SCR to higher temperatures, resulting in faster aging of the SCR catalyst, as observed.
- CO control during rich conditions is a challenge.
- Cost (\$0.5 million per year), though appearing on the high end, may not even be sufficient to overcome several of these challenges.

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

Reviewer 1:

The reviewer noted that the work is great in terms of investigating the effects of lean, stoichiometric, and rich aging on the SCR catalyst, which are important for lean-burn gasoline applications that can operate lean at low loads but operate at stoichiometric or rich conditions at high loads. Also, there is a very nice comparison of the lean SCR approach (with NH_3 supplied during lean operation) and the passive SCR approach (with NH_3 supplied during rich operation) as a function of the aging temperature and the aging A/F ratio (lean or rich). It clearly showed that rich aging is detrimental for both high-temperature performance and low- temperature performance with the passive SCR approach, while rich aging was detrimental only for the high- temperature performance with the traditional lean SCR approach.

Reviewer 2:

Installing a new MAHLE jet ignition (MJI) engine with full controls, procuring a new dynamometer and evaluating SCR performance on aged production SCR units are notable accomplishments. The reviewer had questions and/or comments on the temperature in a stoichiometric engine during the ammonia generation phase being high. This would reduce the capability of the SCR to adsorb the ammonia. Furthermore, the thermal inertia of the catalyst may also negatively affect ammonia storage during rich to lean operation change and possibly contributing to NO_x slip from passive SCR. Did the team face the issue of high exhaust temperatures? Air injection could help, but ammonia oxidation to NO_x has to be controlled. Is there CFD related work being planned to cool the exhaust before entering the SCR?

Reviewer 3:

Progress is obvious and sensible. However, there are various challenges that this project needs to overcome to make a convincing case, overall. The reviewer referenced earlier comments and stated that the project will need a stronger, broader push across the budget; novel SCR technology; and solutions to its CO emission, cold-start, and fuel penalty concerns for it to be successful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The involvement of Umicore LLC and GM is an excellent collaboration for accomplishing project goals. It is imperative to have an active catalyst and engine partner to successfully complete work with objectives such as this project. The team has shown good collaborative approach.

Reviewer 2:

There are good collaborations with GM and Umicore.

Reviewer 3:

The broader team includes one major OEM and a Tier 1 catalyst supplier. The PI has also reached across a broader team, integrating them into the project (though at lower level relative to Umicore and GM); the list is too long to name here (Slide 10).

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

Reviewer 1:

Although this is an interesting and promising approach for lean burn SI engine platforms, care should be taken so that the exhaust aftertreatment system does not become overly complex. The passenger car industry is different from HD, and complex aftertreatment system and associated diagnostic development could be a major hurdle. In order to bring strategies such as this to the forefront of production, it is imperative that future research be aimed at simplifying the packaging and the control strategy and addressing durability.

Reviewer 2:

There are several tasks planned for the "future" phase. Future work however will not be sufficient to bring this project to any conclusive end, as it will need a larger plan, more resources, and a multi-pronged approach to addressing its underlying challenges.

Reviewer 3:

The combination of higher HC emissions and lower exhaust temperatures during lean operation on the MAHLE engine will be challenging and will require attention. The project needs to explore ways to minimize the CO without resorting to the clean-up catalyst and air injection. Slide 37 showed that the clean-up catalyst (CUC) alone increased the NO_x emissions by oxidizing NH₃, and air injection would make it even worse. It is much better to produce less CO at the engine. The best way to produce less CO during the rich periods is to run less rich. It is possible to run less rich and still make NH₃ over the TWC if there is less O₂ during the rich periods. That can be verified on the project team's laboratory reactor. Perhaps the project team can work with MAHLE to minimize the amount of O₂ during rich operation. If the team had both a direct injection (DI) injector and a port fuel injection (PFI) injector, it could run lean with the DI injector and run rich with the PFI. The PFI injector results in better mixing and therefore less O₂ during rich operation.

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

Reviewer 1:

Passive SCR strategy is an excellent approach to realize lean burn SI engines with no urea tank. This will directly contribute to SI engines with significantly lower fuel consumption.

Reviewer 2:

The use of lean burn engines can reduce the fuel consumption of gasoline engines by up to 15%, helping satisfy DOE's goal of reducing our dependence on foreign oil. This project is important because it is exploring ways for lean burn engines to satisfy the Tier 3 Bin 3 emission standards.

Reviewer 3:

From a powertrain exploration point of view, the project aligns with the DOE goals. From the point of view of fuel economy and commercial potentials, this project has many challenges that would need to be overcome.

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

Reviewer 1:

ORNL, Umicore, and GM have sufficient resources to address any challenges of this study. Newly added dynamometer capability expands their resources for engine testing.

Reviewer 2:

The resources seem sufficient for the time being, as a lot of good data has been generated in this project over the last year.

Reviewer 3:

The project has many challenges. In order for this project to reach a conclusive end, it needs more resources and a more aggressive project plan to address its many challenges, such as faster SCR aging, stronger cold-start investigation, bag-1 impact, fuel penalty, and CO_2 concerns (due to excess fuel use).

Presentation Number: ace056 Presentation Title: Low-Temperature Oxidation Principal Investigator: Yong Wang (Pacific Northwest National Laboratory)

Presenter

Yong Wang, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives and the resources were sufficient.

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

Reviewer 1:

The approach to obtaining new knowledge for reducing PGM usage in catalysts and enhancing methane oxidation performance has been excellent.



Figure 1-7 - Presentation Number: ace056 Presentation Title: Low-Temperature Oxidation Principal Investigator: Yong Wang (Pacific Northwest National Laboratory)

Reviewer 2:

The work is interesting and incorporates novel approaches. Interim success metrics are met. Project is well designed, and the team is strong. The goals include increasing catalyst activity by atom trapping to create thermally durable Pd single atom catalysts with reduced PGM usage; and demonstrating activity and durability of leading candidate catalyst formulations using U.S. Driving Research and Innovation for Vehicle efficiency and Energy Sustainability (U.S. DRIVE) Low-Temperature Catalyst Test Protocols.

The reviewer commented that successful project demonstration thus far could demonstrate 70% methane conversion at less than 350°C. The next target is achieving 90% or higher methane (CH₄) conversion at less than 350°C. The approach will encompass developing a bimetallic approach using single atom catalysts by atom trapping for methane combustion; and demonstrating a greater than 95% methane conversion at less than 350°C without detrimental effects by sulfur and steam. The reviewer observed a solid project approach to problem solving.

Reviewer 3:

The project intent is to find a CH_4 oxidation active catalyst that will withstand the normal degradation modes. The team studied Pd/SSZ and ceria-based samples. The former was studied in depth, and the team showed problems with atomic (ion exchanged) versus particles as active site, the particles being much more active. These data show single atoms are not appropriate for this reaction in the SSZ material. The identification of particles being active, over the single atoms or ion exchanged species, is noteworthy because so many researchers have focused on single atoms as an answer to thrifting. Pd/ceria and Pd/aluminum oxide (Al₂O₃) are well known for CH_4 oxidation, and the characterization tools are proving useful in understanding the fundamental catalyst chemistry and the loss in performance over time for these sample types. The team is focused on the right barriers and has demonstrated why those exist.

Reviewer 4:

PNNL is continuing to focus on novel catalyst technologies that offer the potential for greatly improving emissions performance. The development of technologies that significantly increase the dispersion of the precious metal content to achieve greater light-off and sustained catalyst activity is highly desirable to meet super ultra-low emissions vehicle (SULEV) and Tier 3 emissions standards. Although this approach of employing stabilized PGM nano clusters and single atom catalysts is promising, using this technology for CNG catalysts is not of high value to LD vehicle OEMs. There is an overwhelming need for this type of catalyst technology for stoichiometric vehicle use TWCs. Much more benefit would be derived from this work if applied to gasoline stoichiometric applications.

Reviewer 5:

The work contains a published catalyst preparation technique, and the PI used this technique to evaluate CH_4 oxidation reaction. Several catalysts are screened after treating at different pre-treatment conditions. However, narrowing it down to one or two formulations and comprehensively studying those catalysts—rather than screening all pre-treatment conditions and adding more Pd, etc., for all catalysts—would have been a better approach to gain through fundamental as well as potential technical viability of the catalysts.

The project team indicated the performance target, but no cost target (or Pd amount decrease target compared to a selected baseline) was estimated or provided. Having such estimated targets would provide quantitative technical barriers and make it easy to track the progress of the project by analyzing to what degree such barriers were addressed. Therefore, the reviewer requested that the project team coordinate with the catalyst manufacturer JM, who is also a partner, to come up with such estimates and project measures.

Reviewer 6:

The presentation and project identify key technical barriers and provide strategies which attempt to mitigate the majority of issues in the area of low-T methane oxidation. The majority of the project is complete but seems to have made significant contributions to understanding of these catalysts, experimentally characterizing the materials, and getting close to milestone targets of methane conversion.

A few points for longer term consideration: while the Pd focus on the short term seems appropriate, insights into use of other more abundant metals as parts of formulations (as catalysts, supports, co-additives, etc.) appear critical. The lack of modeling, given the relative size of these systems, seems like a missed opportunity, especially with the PI's connection to the PNNL complex.

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

Reviewer 1:

As the reviewer previously noted, the successful demonstration thus far shows a greater than 70% methane conversion at less than 350°C (Go/No Go, Slide 7). The next targets are achieving 90+% CH₄ conversion at less than 350°C. The measured accomplishments are noteworthy.

Reviewer 2:

The project seems on track to reach target milestones, which is impressive regarding methane conversion levels. The project team has well characterized systems and has utilized multi-modal techniques well suited to detail location and oxidation state of the metals. The team seemed to address most concerns from a prior review adequately.

The team has published a nice number of papers in high impact journals. Differentiation of the intellectual merit of these more applied projects from those funded by fundamental science programs is key and should continue to be monitored.

Reviewer 3:

The demonstration that nano-palladiums (NPs) of Pd is superior to the performance of single-atom catalysts (SACs) is very important. The excellent stoichiometric activity of Pd added to SACs of rhodium (Rh) is very interesting. Unfortunately, recent price increases for these two metals make them PGM choices one may want to improve upon. The understanding of the deactivation of Pd NPs by alumina is a very well-done piece of work.

Reviewer 4:

The novel catalysts proposed in this work offer twin benefits of reduced cost and greater performance. However, ensuring that catalysts are compared on an equal basis in terms of thermal and chemical aging is important for determining their true benefits. Aging conditions and results should be made clearer. Also, increased conversion efficiency resulting from the addition of more PGM is not unexpected. Quantifying that effect better to optimize the use of Pd and Rh would provide greater insight into whether or not the additional PGM is simply additive or if there is a synergistic benefit between Pd and Rh. In either case, it should be noted that this is a very novel area of development that appears viable for OEMs.

Reviewer 5:

The goal of achieving lower temperature activity in unaged materials was met. The question is whether those samples (i.e., Rh/Pd/ceric oxide [CeO₂]) can withstand degradation modes. The characterization tools show interesting results that helped guide their conclusions. The thrifting aspect remains elusive; with the addition of Pd to a Rh catalyst, this goal seems challenging. The active site identification is an important result, but what will be done with it does not seem obvious. The continued use of ceria as a support seems to be problematic, but the next steps (degradation studies) will prove or disprove this intuition.

Reviewer 6:

Even though it seems the technical targets can be potentially approachable from the test done so far, a couple of comparisons were lacking, and such comparisons should not take significant resources and time to generate. It is not obvious how the base line technology performs. As a well-known supplier is part of this project, the reviewer suggested comparing (minimal work) one or two baseline technologies relevant to the ACE056 project. From such baselines it is also possible to compare PGM reduction targets; it is not expected to take significant resources to expose the catalyst to, for example sulfur, and carry out the tests. Such tests are expected to be very limited and that would give insights into the gaps in achieving the technical targets.

There are several remaining challenges and barriers proposed by the PI. In fact, these barriers are most critical for generating fundamental understanding of potentially viable technology that will be evaluated in the rest of this year. It appears that, in order to comprehensively evaluate all the suggested workflows, it will take significant resources and time. It is suggested that the critical challenges must be prioritized and comprehensively evaluated rather than evaluating all the factors superficially. Such an approach will be useful in developing deep technical insights and the potential for successfully developing a viable technology.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It appeared to the reviewer that the collaborative groups are excellent.

Reviewer 2:

The team includes PNNL scientists and labs, one major OEM, and a key Tier 1 supplier. Collaboration appears established and strong.

Reviewer 3:

There is obvious collaboration with ORNL via the synthesis and protocol discussions and exchange. JM's role in baseline catalyst supply is met. GM's role in guiding relevance is appreciable.

Reviewer 4:

The inclusion of an OEM and catalyst supplier in this work to help develop the technology and guide the direction of the work is highly desirable. However, GM is not a major user of compressed natural gas (CNG) technology for its vehicle fleet.

Reviewer 5:

The contributions, other than consulting, from GM and JM are not obvious. The questions raised in approach and technical accomplishments need their significant contributions, and the reviewer requested that the PI include them if possible and also make specific contributions more visible in the presentation.

Reviewer 6:

The slides and presentation could have done a better job delineating who did what, i.e. what were the specific contributions spread across the various partners. The reviewer is familiar with many of the involved participants, but this would not be clear to someone less versed in the science of these researchers. A separate slide showing a discrete example of how the team worked together on each component of the work would have been powerful in convincing reviewers the project team provides a sum greater than the parts.

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

Reviewer 1:

Success for the end goal (CH₄ oxidation in low temperature) has been divided into achieving it at approximately 70% first and 90+% next. This is a rational approach and appears to be a successful strategy.

Reviewer 2:

The proposed challenges to overcome are reasonable and very appropriate for ensuring that this catalyst technology will be viable for the intended application. Thermal and chemical durability is even more important now to the OEMs due to the onset of Tier 3 and SULEV emissions standards.

Reviewer 3:

The proposed embedding of Pd in a hydrophobic zeolite in the last year of the project seems ambitious, given that it will then need to be characterized, tested, and exposed to the degradation criteria. It will replace the ceria as the support, which should be helpful for degradation. But, t this seems rather ambitious in a last year, especially since the degradation aspects have to be addressed for the other materials also.

The reviewer commented that the thrifting seems to be going the wrong direction over the last year – the addition of 3% Pd to an Rh-containing catalyst seems costly.

Reviewer 4:

The presentation could provide more information regarding the state-of-the-art in Pd embedded in hydrophobic zeolites and the silica materials. Is the hydrophobicity tuned enough as a parameter to justify exploring these materials? Could the coating lead to deactivation of the catalyst? No results were shown to demonstrate otherwise.

Silica porosity (or lack thereof) may create significant issues that were unaccounted for in the presented materials. It seems a bit dubious to this reviewer that all these material types could be screened for activity in the reminder of the project.

Reviewer 5:

Technical challenges still remain for these catalysts. The reviewer indicated that it is very challenging to deal with the deactivation in water and with sulfur. The support change looks promising.

Reviewer 6:

There are several remaining challenges and barriers proposed by the PI. The reviewer assumed they will be evaluated in the rest of this year. It also appears that comprehensively evaluating the suggested workflows will take significant resources and time. It is suggested that the critical challenges must be prioritized and comprehensively evaluated rather than evaluating all the factors superficially. Such an approach will be useful in developing deep technical insights and the potential for successfully developing a viable technology.

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

Reviewer 1:

The reviewer's response was absolutely. From the introductory slides and the focus of the research, it is clear the team has carefully considered how the work fits into the greater context of VTO/DOE goals. In addition, the applications of the PIs developed catalysts could clearly extend to a range of reactions of VTO interest.

Reviewer 2:

Enabling low-temperature CH₄ oxidation, an enabler of natural gas engine technologies, appears aligned with DOE objectives.

Reviewer 3:

Improved catalysts in this area at low temperatures will lead to more efficient emissions control.

Reviewer 4:

This project supports the valorization of CH_4 for transportation applications. Low cost, but highly active aftertreatment catalysts would enable natural gas vehicle use. The standout issue is the choice of catalysts, with ceria as the support and the addition of Rh as a metal. Admittedly, the project team did learn about SSZ supported oxidation catalysts—which people have been proposing–and the team's work provides better focus for those.

Reviewer 5:

Tier 3 and SULEV20/30 enabling catalyst technologies that are cost effective and durable are very appropriate going forward.

Reviewer 6:

Methane oxidation, under both lean and stoichiometry conditions, is difficult, and the existing technologies are expensive and only work at high temperatures. This could limit, for example, applications of some engine and fuel options, such as dual fuel. Similarly, the cost of Pd might prohibit the widespread usage of NG engines that can decrease CO_2 emissions as well as make United States less dependent on oil.

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

Reviewer 1:

The project resources appear to be sufficient for ensuring a positive outcome for the development work.

Reviewer 2:

This project is an undertaking at the fundamental catalysis stage. Its execution at and with the PNNL catalysis lab/team reflects its state-of-the-art resource access.

Reviewer 3:

All resources seem appropriate. All needed components to finish the project are in place.

Reviewer 4:

The resources seem appropriate for the milestones over the project term.

Reviewer 5:

It appeared to the reviewer that there are sufficient testing capabilities available at PNNL and ORNL.

Reviewer 6:

The PI and partners have all the right reactor and advanced characterization resources as well as catalyst supplier resources to address the milestones in timely fashion.
Presentation Number: ace085 Presentation Title: Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization Principal Investigator: Todd Toops (Oak Ridge National Laboratory)

Presenter

Todd Toops, Oak Ridge National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives the resources were sufficient.

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

Numeric scores on a scale of 1 (min) to 4 (max) This Project Sub-Program Average 4.00 3.50 3 00 2.50 2.00 1.50 1.00 0.50 3.17 3.50 3.33 3.23 3 17 0.00 Approach Tech Collaboration Future Weighted Accomplishments Research Average ace085

Theis, Joseph

The ACEC testing protocols have been used in evaluating low-temperature catalysts. For the PNA work, multiple sequential tests have been performed to investigate the deactivation of the PNA Figure 1-8 - Presentation Number: ace085 Presentation Title: Low-Temperature Emission Control to Enable Fuel-Efficient Engine Commercialization Principal Investigator: Todd Toops (Oak Ridge National Laboratory)

with different reductants. This is very important, as the gradual deactivation of low-temperature NOx adsorbers (LTNAs) during repeated cold-start tests is currently the biggest issue for the technology. This must be solved before PNAs can ever be considered for vehicle applications.

Reviewer 1:

The project had adequately addressed its two main goals of low-temperature conversion and reduced PGM loading (Metalmark, etc.).

Reviewer 2:

A variety of catalytic systems has been researched for various engine platforms. This study is the culmination of different research projects carried out by ORNL. However, as a study that compiles the results of many research works, it should also critically assess the needs of the industry and the technical viability of the solution. For example, the lean spark ignition (SI) and conventional diesel combustion (CDC) solutions seem to be overly complex.

Multiple aftertreatment systems are probably required but does the work address innovative approaches of packaging five different catalytic systems under a vehicle body? It is very important to be cognizant of the packaging challenges of multiple catalysts in a vehicle. While conducting controlled studies on separate units help provide clarity, approaches—zone coating two different catalysts, a catalyzed gasoline particulate filter (GPF), etc.—should be considered, if they have not been already.

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

Reviewer 1:

There is good work in assessing the deactivation of the Pd/SSZ-13 PNA with and without reductants. The results are very consistent with the work reported by Ford, in that CO causes the deactivation while HC, hydrogen (H₂), and NO_x do not. Impressive amounts of data have been reported on the core-shell catalysts with Pd and/or platinum (Pt).

Reviewer 2:

One task has been complete during this period and two tasks are on track. FY 2020 and FY 2021 milestones are critical.

Reviewer 3:

The reviewer stated that it is fair to rank the accomplishments as "work in progress" since the project just finished its first year, is in mid-stage, and hence has one more full year of investigation to complete. In all, the project appears on track. It is ranked overall as "Good" because no major, "internal" pathway for lowering PGM appears to have been taken. Given the capabilities, resources, and close collaboration with PNNL, one wonders why such a path was not considered. After several years (more than a decade) of coaters talking about PGM reduction, it is fair to say this (lowering PGM) is something that most likely the coaters will not invest a major effort on, and that ultimately the National Laboratories (the government) and/or the smaller, private labs would need to make that happen.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The team involved in this project is extensive, and the progress shows excellent contribution from different team members.

Reviewer 2:

Good collaborations with the University of Buffalo, Harvard University, Chalmers University, the University of Virginia, and PNNL.

Reviewer 3:

Collaboration with the University of Buffalo team and a broader, internal team at ORNL is integrated into the project.

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

Reviewer 1:

Future stages are planned well and clearly defined across materials, PGM reduction, and low-temperature performance.

Reviewer 2:

It was good to see that the project team is exploring other zeolites (LTA) for the PNA work as well as cocations that could potentially re-oxidize the Pd that is reduced during testing and thereby decreases the degradation observed during repeated NO_x storage and release testing. The reviewer would encourage the project team to continue exploring catalyst formulation changes (zeolites and/or metals) as well as systems modifications (e.g., catalyst zoning, layering) that might decrease the degradation. The team might consider reducing the maximum temperature of the temperature ramps from 600°C to 400°C, or even 300°C, as these are more realistic maximum temperatures on diesel engines during normal operation. For the core-shell work, the team needs to assess the OSC of the catalysts and implement A/F dithering during the light-off testing to simulate actual vehicle operation. It would be interesting to poison the core-shell and non-core-shell samples with S and P to see if the core-shell catalysts are more robust to the poisons. Lower PGM loadings are also important to explore. While the protocols call for aging at 800°C, the team might also age some samples at 900°C if the catalyst is intended to function as a TWC.

Reviewer 3:

Future research should be more aimed at addressing the simplification of the proposed aftertreatment solutions. For the industry to accept the outcomes of this research it is imperative that it is production viable and cost-effective in manufacturing, installation, and durability.

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

Reviewer 1:

The development of low-temperature catalysts is critical for meeting stringent emission standards on fuelefficient engines that generate lower exhaust temperatures. These engines can reduce the fuel consumption of vehicles and thereby satisfy the DOE objective of reducing our dependence on foreign oil.

Reviewer 2:

Yes, the project does support DOE objects on several grounds, which include lower temperature activity (enables fuel savings) and PGM reduction (economic impact on the mobility industry).

Reviewer 3:

Overall, this project is aimed at supporting the emissions control system of future high-efficiency engines. This supports the overall objectives of DOE

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

Reviewer 1:

All the team members are highly experienced and well equipped with resources to address all project milestones.

Reviewer 2:

The reviewer affirmed resources appear sufficient.

Reviewer 3:

The reviewer stated that the resources seem sufficient for now, although additional testing resources could be needed to explore different PNA formulations with different zeolites and/or active metals. Additional testing resources might also be needed to test TWCs and core-shell catalysts with A/F dithering. Extra resources might also be required to explore reduced PGM loadings.

Presentation Number: ace100 Presentation Title: Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research - SuperTruck 2 Principal Investigator: Darek Villeneuve (Daimler Trucks North America)

Presenter

Darek Villeneuve, Daimler Trucks North America; Jeffrey Girbach, Daimler Trucks North America

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-9 - Presentation Number: ace100 Presentation Title: Improving Transportation Efficiency through Integrated Vehicle, Engine, and Powertrain Research - SuperTruck 2 Principal Investigator: Darek Villeneuve (Daimler Trucks North America)

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

Reviewer 1:

The project team's use of strategies that can carry over into production such as the friction reducing coatings are spot-on targets for the industry.

Reviewer 2:

There is a good, multi-pronged approach to find every possible source of energy savings. The honesty expressing the commercial viability being about 2% of the aerodynamic savings is very much appreciated.

Reviewer 3:

The approaches taken for both engine and vehicle are technically sound and supported by aggressive technologies developed for this program. Taking the engine as an example, it includes phase-change cooling (PCC)-type of waste-heat recovery (WHR) and two-stage turbochargers; advanced air system with two-stage exhaust gas recirculation (EGR) cooling; and friction and parasitics, etc., which would make the program likely to achieve the program goals.

Reviewer 4:

The project is on path to making decisions to meet the goals. The reviewer appreciated that this team has a "commercialization committee" that is helping direct the team on technologies that fleets really want to buy. It

shared a few examples of where technologies were taken out of their plans via this process—well done. It is actually shown as red on the waterfall chart. The project seems on track with the approach.

Reviewer 5:

The approach to achieving the SuperTruck 2 goals is solid; most of the technologies under consideration are either well developed or at least widely studied approaches in the R&D community. This gives a high degree of confidence in the potential for meeting the 115% fuel efficiency (FE) goal of the program. The reviewer was unsure, based on the results and projections shown, if the 55% brake thermal efficiency (BTE) goal will be easily achieved; the reliance on the phase change waste-heat recovery (WHR) system with all of the development required at the casting level as well as with high performance WHR equipment is risky. That said, the reviewer was not sure that there are too many other options beyond what is currently being pursued and this will be a common challenge of the SuperTruck 2 program. The other engine technologies under development are reasonable approaches, and it looks likely that a 50+% BTE will be achieved without WHR.

Reviewer 6:

The technical approach to system-level performance improvement is on track to exceeding the funding opportunity announcement (FOA) goals based on the 2009 baseline comparison vehicle. The team also established significant progress over a more relevant model year (MY) 2017 production Cascadia, but the reviewer would have liked to see a comparison to a current model year production tractor to better gauge the commercial viability of the technologies. The team identified only briefly technologies that were not viable in scope of the project objectives. Optimizing tire coefficient of rolling resistance (C_{rr}) differently between tag and pusher tires did not consider total cost of ownership (TCO) ramifications to fleet operations and replacement rates, retreading, etc. The project has significant software integration elements that were not discussed and may impact the schedule for the final, fully integrated vehicle road testing. Delay of engine delivery for the demonstrator will pressure software integration activities. There was little or no discussion of trailer and trailer partner efforts in the project, yet significant savings were identified in the FE plan. There was also no discussion of trailer tire C_{rr} improvement.

Reviewer 7:

The approach taken by Daimler covers a reasonable arrangement of technologies. The selection of 48 volt (V) for mild hybridization is seen as a good compromise. The Slide 4 figure and indicated freight efficiency numbers are a bit unclear, specifically the red marker under Tractor Aero.

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

Reviewer 1:

Accomplishments are significant against objectives, and this team did a very good job of presenting them to the reviewers and overall audience.

Reviewer 2:

There has been good progress in the past year, and it looks like all the parts of the program are on target for finishing up the work on schedule. The reviewer saw that there are some delays due to COVID-19, but that is common across all of the DOE programs, so the reviewer was not too concerned about that. In general, the measured results that were shown are consistent with what the reviewer would expect for the technologies presented, and they look promising. The reviewer would have some concerns about the additive benefits of some of the technologies since those do not always show up when the final engine is built, but the overall results look good.

Reviewer 3:

The technical accomplishments to date are significant, showing good progress toward FOA goals. The development and testing of the development truck demonstrate progress at the component and subsystem levels; however, the demonstrator build will identify integration issues that the development truck did not

explore. The integration of predictive cruise control and adaptive cruise controls was touched on briefly. There are significant operational ramifications to fuel economy in traffic conditions that may limit the benefit of these features. Data on the potential opportunity in a variety of real-world traffic conditions and variety of driver skill levels should be discussed. Very little was presented on commercial viability of the technologies within the FOA recommended time spans. The PCC WHR approach is innovative. A discussion of the cost effectiveness of this approach with respect to operational maintenance, reliability, and warranty is required with respect to FOA goals of commercial viability.

Reviewer 4:

Development procedures for aerodynamic and engine performance appear to be solid, industry-best methodologies to seek gains that are usable for validation without wild R&D risks. The test miles and other test feedback are a strong indicator of progress.

Reviewer 5:

On the engine side, achieving 52.9 % BTE is a great accomplishment at this stage. With fine tuning on all packages, it sounds like t this project has an excellent chance to meet the program goal. The technical achievements on the chassis development side are impressive, with the quantitative improvements on tires. It would be even more impressive if the similar quantitative improvements can be demonstrated in the aerodynamic and exterior development and energy management.

Reviewer 6:

The technical review covers a wide range of items in only a few pages. Some of the materials presented fail to have sufficient description to allow the reviewer to understand the impact or merit of the technology presented. This is the case for the bumper duct optimization (What are we looking at?), the delta drag coefficient (Cd) (What is x?), and cooling drag (What is the color scale? What criteria are being followed?) on slide 5. Slide 6 shows a skeleton of the air system, which appears incomplete and incorrect; the charge cooler on the engine and on the radiator pack are not linked up. What is the boost recuperation shown on Slide 7? Unfortunately, most of the material presented suffers from a similar lack of information.

Reviewer 7:

The reviewer was not sure that the same honesty seen in the aerodynamic commercialization was seen in the friction reduction attributed to the friction reducing coatings. The statement "Friction hardware shows significant improvements in brake-specific fuel consumption (BSFC) over stock hardware" implies it will be a big part of the final demonstrator package, but the data shown are a combined effect of these coatings, along with lower viscosity oil, thus a lower pumping loss. With no numbers on the graph, the reviewer had doubts that the benefit will be worth the cost and risk involved with these coatings (long-term durability and effect on oil consumption).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It looks like the work package has been split up across the team and that everyone is working well together to validate the technical paths. The vehicle work shows good technology transfer back to Daimler, and as the engine work moves toward the final build, the plans also look good for technology transfer.

Reviewer 2:

Evidence of teamwork shows on many different slides and areas. Given their fleet inputs from Schneider and the fact that Schneider heads up the North American Council for Freight Efficiency (NACFE), this would seem to be a team with fleet results in mind.

Reviewer 3:

Some of the project partners' work is provided (e.g., Michelin tires, Oak Ridge friction reduction, and NREL battery package). But details as to the other partner's work is not covered here.

Reviewer 4:

There is nice identification of the collaborators on the upper right of the Powertrain section. This really helps understand how the partners are contributing. However, this did not seem to be the case in the Vehicle section. Please consider doing this for the whole project, as it makes the review easier.

Reviewer 5:

The project team includes a cross section of expertise as desired in the FOA. Input from the fleet and trailer manufacturer team members was not significantly discussed in the presentation. The tire representative participation seems focused on the tractor tires only and there was no discussion on fleet partner tire replacement cycle ramifications. Fleet perspectives on service and operator training and maintenance and reliability of the overall systems were also largely missing from the presentation, all relevant to commercial viability as requested in the FOA.

Reviewer 6:

Project partners are significant, but the reviewer would have appreciated more recognition of their contributions in the slides and/or the presentation. Where exactly did they help in making critical decisions on the project? The reviewer suggested that a few examples would have really helped.

Reviewer 7:

Although it would be impossible to make so much progress without collaboration, the entire presentation does not give the reviewer any sense of how other team partners help the program. Without any sort of acknowledgments—even with the logo of each company or partners throughout the presentation where they are applied—it makes the project look incomplete.

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

Reviewer 1:

The plans moving forward look good; the team is entering the part of the project where all of the individual developments get put together into the final builds, and those plans all look solid and achievable.

Reviewer 2:

This team appears to be in the build-and-validate mode with minimal remaining research compared to the other teams.

Reviewer 3:

Moving to the final demonstrator truck and barring any COVID delays, the project will be on schedule.

Reviewer 4:

The project presented a competent plan for addressing COVID-19 related schedule impacts but did not discuss cost ramifications to project funding. Risk mitigation prior to COVID-19 impacts appeared to be well executed with identification and evaluation of competing approaches to technologies. The delay in engine delivery has cascading impacts to multiple systems in terms of validating operations, and this domino effect has not been quantified in any detail. For example, schedule delays could impact expediting costs for purchases, premiums for testing windows, extension of staff labor commitments for system support, etc. The reviewer would have liked to see a discussion of demonstrator testing in concert with MY 2021 production tractor and trailer to properly benchmark program potential versus the latest real-world truck technologies, a step that project management will likely be doing anyway to gauge commercialization potential. Delays in the demonstration program also may impact applicability of any of the technologies being adapted for use to aid in meeting planned future U.S. Environmental Protection Agency (EPA), Air Resources Board (ARB) and other emissions requirements.

Reviewer 5:

The team seems to know the areas of concern for the schedule to complete tasks. Virus corrections will be critical to not seeing significant delays.

Reviewer 6:

The future proposed work chart on Slide 18 focuses on the vehicle, and no mention is made on the engine activities.

Reviewer 7:

Using a very busy project timeline slide with a little or no explanation on the future research dilutes the achievement of this project. Therefore, it would be helpful if one designated slide with the detailed explanation on the proposed future research can be used.

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

Reviewer 1:

This project very well supports the overall DOE objectives because of 55% BTE goal on the engine side and 125% improvement on the vehicle side.

Reviewer 2:

This project directly meets the VTO programmatic goals for high efficiency freight technology demonstration.

Reviewer 3:

HD tractors are such a large contributor to greenhouse gas emissions that ongoing projects in this area are very important.

Reviewer 4:

The reviewer found this team to be advancing the current state of the art without being risky with technologies that do not feel like R&D-only efforts. If many of these items can be put into production in the next 5 to 10 years, the industry will gain from how these tax dollars have been invested.

Reviewer 5:

It appeared to the reviewer that work is relevant. Some indication on cost-benefit should have been given.

Reviewer 6:

Improving heavy-duty transport efficiency is a critical need both in terms of satisfying future CO₂ regulations and for addressing DOE's broader goals of energy independence, improved efficiency, and greenhouse gas (GHG) reduction. This project should develop key technical solutions to achieve these goals.

Reviewer 7:

The project relevance focuses on key technologies such as electrification of accessories through the use of 48 V systems, incorporation of waste heat recovery technologies, lightweighting, improved aerodynamics, improved tire rolling resistance, improved lubricants and coatings, improved driver assistance with predictive cruise control (PCC) and adaptive cruise control (ACC) systems, etc. What appears to be missing seemed to be significant discussion of the commercial viability of these choices and any discussion of applicability to expanding market volumes and future proofing tractor technologies such as applicability of the 48 V accessory systems to battery electric, fuel cell electric, and other alternative fuel vehicles also in work at Daimler, its subsidiaries, and partners.

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

Reviewer 1:

The project team has all it needs to accomplish the program goals.

Reviewer 2:

The budget and spend rate look good in terms of the project scope and achievements.

Reviewer 3:

It appeared to the reviewer that the resources for this project seem just right. It looks like there has been an increase in cost sharing put in by Daimler, so this project is showing very good leveraging of DOE funds.

Reviewer 4:

The reviewer said that the resources for this project seem sufficient.

Reviewer 5:

It seemed to the reviewer that the resources appear adequate.

Reviewer 6:

The reviewer is slightly concerned about the COVID-19 3-month delay, but it is understandable in these challenging times. Hopefully, the team continuity is not lost as dollars are focused elsewhere for a while.

Reviewer 7:

The project showed that the 2019 budget summary for both the engine and vehicle efforts exceeded the planned budgets by approximately \$3.1 million and reporting 70% project completion to date. The 2019 Annual Merit Review (AMR) showed underrunning budget by approximately \$2.2 million with 50% complete. The 2018 AMR showed underrunning by approximately \$0.3 million with 30% complete. The 2017 AMR showed 5% complete and program budget with no spend to date shown. For 2020, the project did not report any significant budget issues with respect to the COVID-19 schedule and manpower delays but did report there were delays. Carrying manpower longer in years 2020- 2022 than originally planned may increase budget pressure that appears to be somewhat overspent as of the 2020 AMR reporting, considering prior year reports. Any expediting of work may also pressure the budget. Insufficient information was provided in the review to determine the extent of remaining approved funding.

Presentation Number: ace101 Presentation Title: Volvo SuperTruck 2: Pathway to Cost-Effective Commercialized Freight Efficiency Principal Investigator: Pascal Amar (Volvo Trucks North America)

Presenter

Pascal Amar, Volvo Trucks North America

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-10 - Presentation Number: ace101 Presentation Title: Volvo SuperTruck 2: Pathway to Cost-Effective Commercialized Freight Efficiency

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

Reviewer 1:

The approach taken by Volvo is well coordinated and clearly indicated in this presentation. The presentation summarizes the concept-technologies grouped in vehicle and powertrain groups with what appears a comprehensive system integration. Volvo's partnership with NACFE gives a channel for the voice of the customer and assessment for adoption of the technology.

Reviewer 2:

The tractor-trailer pairing modeling adds a unique perspective on optimizing this configuration as a function of the freight route. This is an additional, and unique, way to get real-world efficiency by taking operator and fleet manager input into account.

Reviewer 3:

The reviewer liked the approach of this OEM to design specifically for a growing segment of more regional operations and having a focused specification to maximize the opportunities for technologies. This creates a focused truck for a pretty large population of trucks. Waterfall charts are helpful to communicate progress against efficiency goals.

Reviewer 4:

The project is really nice in the way it has taken a holistic view of the question of freight efficiency. Since it is widely understood that most trucks cube out rather than weigh out, allowing a 65,000 pound (lb) gross vehicle weight (GVW) limit opens up some interesting optimizations for the truck. That does beg for comparison with the other SuperTruck teams. Everyone is targeting the freight efficiency gain at 65,000 lb GVW per the project

requirements, but most of the other trucks look capable of 80,000 lb GVW (at least in principle). The reviewer thought the approach taken here is quite justifiable, but it may lead to a demonstration truck that is not particularly market attractive. Will fleet customers accept a truck that cannot achieve 80,000 lb GVW? If not, how much of what has been done here transfers over to a sellable truck?

The reviewer also had mixed thoughts on some of the technical accomplishments. The generative design work is really interesting and clearly leads to a well-optimized physical design to balance weight and structural requirements. But, how do these parts look in terms of production feasibility? That was supposed to be an important part of SuperTruck 2 so that there could be good technology transfer. Will some of these kinds of technologies be able to be brought to market at a competitive cost? The reviewer also was left with some questions on the engine walk to 55%. The individual results that were reported on showed efficiency gains in line with what the reviewer would have expected. But, in the efficiency walk, there is a path shown to 54% BTE based on the technologies developed and then a bar showing a jump to more than 55% that appears to be based on the efficiency delta between the 11-liter (L) and 13-L engines. Does this mean that the 55% engine will be a 13-L engine and the truck engine will be an 11 L? Are all of the technologies applicable to both engines if so?

Reviewer 5:

The project is well designed for addressing technical barriers and establishing technical feasibility, but details presented for commercial viability requested in the FOA were minimal. Of particular concern is optimizing the vehicle for a maximum vehicle weight of 65,000 lb when the baseline 2009 FOA vehicle is to be capable of 80,000 lb gross vehicle weight rating (GVWR). While optimizing for 65,000 lbs was explained as a project choice, and the team plans option content to make 80,000 lb GVWR feasible, the comparison to the baseline is an apples-to-oranges comparison. The target weight of 65,000 lb GVWR in the FOA was based on average loads seen in commercial vehicles; however, that can mean that a specific tractor sees weights above and below that average during the course of operations. Data were not presented as to the number of vehicles that actually operate consistently below 65,000 lb GVWR as opposed to just averaging 65,000 lb GVWR. The team presented significant progress in trailer weight reduction to assist in tractor-trailer system weight management from the addition of new technologies, such as WHR. The use of generative design optimization tools to refine weight reduction while ensuring structural integrity for engine brackets is an excellent risk reduction methodology demonstrated by the project. Evaluating alternatives sufficiently was also well demonstrated with the 710-millimeter (mm) fan selection methodology.

Reviewer 6:

It seems that the approaches taken for both engine and vehicle have all the essential and aggressive technologies to make sure that the project is able to achieve the program goal. However, the reviewer was not convinced why a $4x^2$ axle setting for this truck was chosen. Although $4x^2$ can have benefits with less weight, the issue would be the traction and the load distribution, which may make this truck unrealistic in terms of market acceptance for class 8 truck market.

Reviewer 7:

Although the project team clearly stated that 70% of truck trips are at 65,000 pounds or less, the reviewer was not comfortable that designing a vehicle with that in mind is a proper strategy. Many fleets have loads above that level and are not in a position to have a group of trucks for heavy loads and a different set of trucks for average and lighter loads. Furthermore, the secondary markets for trucks can have wildly different applications and needs from the original purchasing fleets.

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

Reviewer 1:

There has been clear progress across pretty much all the components of the program. The work rate leaves no concerns about completing the overall program on time. The path to 115% FE improvement looks clear, with

only some uncertainty in the reviewer's mind about the path to 55% BTE based on the efficiency walk and the delta between the 11-L engine with the technology package and the 55% target.

Reviewer 2:

The presentation is well organized and can be followed. This is the case for weight reduction and the cooling package. Freight efficiency building blocks are well summarized although the summary on Slide 10 does not show the WHR segment. The powertrain electrification is well documented. The advanced combustion shows Miller cam and points to reduced cylinder pressure as a gain, although the project team earlier pointed at capability to operate at 250 bar.

Reviewer 3:

The project team demonstrated significant progress toward meeting the FOA technical goals. The project showed limited progress in evaluating potential commercialization toward the FOA project objectives. Progress in employing 48 V systems was significant, as was parasitic loss reduction, including innovations with the variable oil pump. While the attention to lightweighting effectively increased the freight-ton efficiency of the system—such that a 65,000 lb GVWR vehicle effectively carried the same amount of freight as a current 72,000 lb GVWR one—the optimization of the frame and systems for 65,000 lb may not suffice for a vehicle capable of 80,000 lb GVWR, requiring additional structure and added tare weight.

Reviewer 4:

The presentation indicated light on actual numbers and facts and more marketing oriented. That said, the tractor-trailer visually is a thing of future beauty. Methodologies such as the generative design look to have huge potential to optimize future vehicles for weight and reliability. The reviewer loved the simplicity and dual purpose of an air tank designed into a cross-member for packaging and weight reduction gains.

Reviewer 5:

Accomplishments across the various systems are evident and strong for the timing of the project. The team is committed to making aggressive but realistic decisions. There is not enough evidence of commercialization decisions involved here.

Reviewer 6:

The reviewer noted really good achievements in weight reduction that is uniquely done with the generative design. It will be great to see road test validation in next year's presentation. The reviewer articulated that there are a lot of pieces to bring together.

It was clear that the 55% BTE engine demonstration had not been completed yet as it is scheduled for the last year of the project. Slide 13 says that the performance verification is complete, but the summary slide indicates that "Development work continues for the technologies selected to achieve the 55% BTE engine goal." The reviewer did not understand what development work remained. The timeline shows that the concept had been selected last year. This is confusing to understand exactly where the team is on this.

Reviewer 7:

Although the project does provide some incremental improvements of various technologies related to advanced combustion, the reviewer still has no idea what the status is in terms of the overall BTE improvement. The progress showed in Slide 15 (Progress—Validation of Powertrain Technologies) is confusing by inserting the simulated benefits into the middle of actual validated testing results, which still cannot help the reviewer understand the progress made so far. This becomes a trend of Volvo's presentation style, which is not helpful.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The work across the project team looks really good, with leveraging of abilities at many partners to achieve gains across the full vehicle and powertrain spectrum.

Reviewer 2:

The reviewer noted that work by project partners is indicated throughout the presentation.

Reviewer 3:

The project team includes a cross section of expertise as desired in the FOA. Input from the fleet member was not significantly discussed in the presentation; it is relevant to key FOA goals to establish commercial viability, such as operational cost impacts, impacts to service centers, training, warranty, reliability, resale, etc. The use of SwRI for engine testing and research for the program was a good choice for independent and objective project input. The use of ORNL in evaluating higher pressure impacts with respect to catalyst samples was an excellent choice to bring in expertise for this significant program risk area.

Reviewer 4:

There is a comprehensive list of collaboration companies and mentions of how they helped in various system and component development during the review. The reviewer appreciated having two fleets, from different market segments on the team. More evidence of their engagement would be appreciated.

Reviewer 5:

The reviewer affirmed a nice addition bringing in NACFE. It was clear where University of Michigan and ORNL contributed, but for all the suppliers listed as collaborators, it was unclear whether they were contributing research or just supplying parts.

Reviewer 6:

Although there were shared logos and a team photo at Metalsa, the presentation lacked much detail on the interactions with partners and the collaboration and coordination of the wider team. If the overall team is meeting results, it gets the benefit of the doubt that the teamwork is functioning well enough for this project.

Reviewer 7:

The team member slide should be put back into the main presentation rather than Reviewer-Only slides. Also, it would be helpful if a company logo can be added to the slides, where its contribution is made, which can help the reviewer and the reader understand how the team helped the program.

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

Reviewer 1:

The reviewer looked forward to the completion next year.

Reviewer 2:

The proposed work plan looks good and addresses the outstanding technical items. The reviewer would have liked to see some more discussion of the 55% BTE path and what can be done to deal with possible setbacks there.

Reviewer 3:

Future work is limited for the timing of this project. The team is committed to staying on course during COVID-19 challenges. The reviewer affirmed well done.

Reviewer 4:

The reviewer asserted that only a small mention is provided for the future work.

Reviewer 5:

Given how far through the program this team has ventured, it does not appear that significant future research is needed as much as completing the prototype and conducting the validation testing. It will be interesting to see

if a waste heat recovery system with loops for both coolant and exhaust recovery is a viable option to take forward to fleets for production. Adding too much complexity to diesel engines will drive fleets to battery electric and hydrogen fuel cells to avoid systems that they feel are too complex and challenging to support with their stressed-out equipment maintenance and support systems.

Reviewer 6:

Future work with respect to the program schedule is presented logically with the majority of the key project decision point now accomplished. Future work was described as optimizing the 48 V mild-hybrid and energy management system based on initial results and developing and integrating the 55% BTE engine in the demonstrator. There was, however, no mention of detailed commercialization opportunities, realities, and plans, a goal from the FOA. Comparison of the potential from the demonstrator should also be put in context of MY 2021 production vehicles, not just the 2009 baseline, especially as it relates to commercialization potential. Fleet feedback on operational potential and ramifications of the technologies, such as warranty; reliability; service center configuration; service technology and driver training; compliance with pending EPA, Air Resources Board, and other emissions standards;, etc., should be included.

Reviewer 7:

The reviewer commented that just three sentences on the proposed future research on Slide 16 of the project summary is too simplified. More detailed steps on research and future development would be helpful.

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

Reviewer 1:

This project is highly relevant to DOE goals for improving efficiency.

Reviewer 2:

The project directly supports the DOE VTO program goals.

Reviewer 3:

Class 8 HD is by far the largest contributor to national GHG emissions, and it is critical that we have ongoing research in this area.

Reviewer 4:

The reviewer commented yes, the project has high value to truck fleets that are seeking a lightweight $4x^2$ configuration and will probably light up the eyes of some within the industry. It certainly does not fit all applications within trucking, but that is acceptable as many fleets order specifically what they desire, given their duty cycles, applications, and customer needs.

Reviewer 5:

It appeared to the reviewer that the work is relevant. Some indication on cost-benefit should have been given.

Reviewer 6:

This project supports the overall DOE objectives because of 55% BTE on the engine and a stretch goal of 120% improvement on the vehicle.

Reviewer 7:

The project relevance focuses on key technologies, such as electrification of accessories through the use of 48 V systems, incorporation of waste heat recovery technologies, lightweighting, improved aerodynamics, improved tire rolling resistance, improved lubricants and coatings, improved driver assistance systems, etc. What appears to be missing seemed to be significant discussion of the commercial viability of these choices and any discussion of applicability to expanding market volumes and future proofing tractor technologies, such as applicability of the 48 V accessory systems to battery electric, fuel cell electric, and other alternative fuel vehicles also in the works with the Volvo Lights project, its subsidiaries, and partners.

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

Reviewer 1:

The reviewer said that budget and spend rate both look good for the project.

Reviewer 2:

Resources appeared adequate to the reviewer.

Reviewer 3:

The reviewer noted that the project is pretty much on schedule with the current resources.

Reviewer 4:

The reviewer remarked resources seem sufficient.

Reviewer 5:

The team appears well positioned to complete the build and testing.

Reviewer 6:

The reviewer commented that they should have all they need to complete the program.

Reviewer 7:

The 2017 and 2018 AMR reviews showed a program budget of \$40 million. The 2019 AMR review grew this number to \$50 million, maintaining the original \$20 million DOE share. The 2020 AMR review maintains the \$50 million number, with no explicit issues described with respect to COVID-19 procurement and manpower challenges. Any extension of program timelines due to COVID-19 related issues at OEM or Tier 1, 2, or 3 suppliers, may include additional, previously unplanned budget impacts for manpower and expediting costs for procurements. Insufficient information was provided in the review to determine extent of remaining project funding.

Presentation Number: ace102 Presentation Title: Cummins-Peterbilt SuperTruck 2 Principal Investigator: Jon Dickson (Cummins-Peterbilt)

Presenter

Jon Dickson, Cummins, Inc.; Ken Damon, Peterbilt Motors Company

Reviewer Sample Size

A total of seven reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 71% of reviewers indicated that the resources were sufficient, 29% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.



Figure 1-11 - Presentation Number: ace102 Presentation Title: Cummins-Peterbilt SuperTruck 2 Principal Investigator: Jon Dickson (Cummins-Peterbilt)

Question 1: Approach to performing

the work—the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The project continues to exceed expectations with a path to put the 55% BTE engine into the demonstration truck, which is well beyond what was envisioned in the proposal call. The rest of the project is equally far looking, with extensive development to build a truck that looks like it will achieve far more than what was required.

Reviewer 2:

This team continues to show its superior approach to the high efficiency demonstrations of SuperTruck, with an "all of the above" approach that is nicely illustrated on Slide 8.

Reviewer 3:

The project was very well designed, and the approach is technically sound. Use of the new engine platform by combining all the experience and technologies developed under the previous SuperTruck program allows the project a high chance of meeting the program goal.

Reviewer 4:

There were numerous examples of technologies that may carry over well into production. The bladdercontrolled cab extenders are quite logical to the challenges of ever-changing wind directions. The combination of aluminum and steel for the frame rails brings the best of both worlds into a system that does not add complexity to the fleet in operations or maintenance. The functionalities of both 6x2 and 6x4 configurations are a beautiful marriage of operational needs. Overall, the project brings many great ideas forward for better industry understanding.

Reviewer 5:

The project team's technical approach is competent. Technical barriers to meeting or exceeding FOA goals have been identified and addressed up to the spring of 2020 when the challenges from COVID-19 impacted hardware delivery and manpower. The progress on achieving 55% BTE engine has been on track with expected one-for-one schedule slip from COVID-19 work stoppages; however final integration into a complete vehicle is required to highlight any software and hardware integration issues. Aerodynamic development and analysis have been significant but need validation on the real vehicle in actual real-world conditions. Progress on the 48 V mild hybridization has been significant and positive. The team did not discuss trailer partner involvement and technical progress there. Progress made on tire Crr reduction was significant, but details were lacking in the presentation. Discussion of progress toward commercialization and applicability to future vehicles was minimal in the presentation. The lightweight chassis is innovative, combining a range of new technologies, and represents significant progress for the team. Fleet involvement in reducing risk or improving commercialization was not discussed in any detail.

Reviewer 6:

The Cummins-Peterbilt presentation technical approach is divided into engine, powertrain, and freight efficiency demonstrator (Slide 8). Subsequent slides go back and forth in and out of these groups, making it difficult to assess the technologies presented (Slide 9). The BTE gains shown should be tied into a descriptive summary to allow the reviewer to provide an adequate evaluation of the merits and feasibility of the claims. Brief and inadequate descriptions are provided for heat transfer and the heat recovery turbine. For example, no material specification is provided for the new designs; turbine outlet pressure ranges given are not discussed with respect to the system and cycle pressure ratios capability. Similarly, on the vehicle side, details should be provided to describe the drag, weight, and rolling benchmarks provided.

Reviewer 7:

It appears to the reviewer that the slides are poorly arranged. The approach and technical slides are frequently interchanged.

Reviewer 8:

The reviewer was disappointed with this review as there was very little detail for an appropriate evaluation, particularly on vehicle side.

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

Reviewer 1:

The technical accomplishment on the engine side with 53.5% BTE demonstration on the test bench is impressive. The project also made striking progress on vehicle related technologies, including aerodynamic drag with 63% reduction achieved, substantial weight reduction with 4,700 lb achieved, and rolling resistance reduction with 33% achieved. It seems that all of technical achievements demonstrated so far point to a clear path to achieve both engine and vehicle program goals.

Reviewer 2:

The project demonstrated significant progress toward exceeding FOA goals projected at 170% improvement in freight efficiency, including exceeding program targets for aerodynamic drag reduction, weight reduction, and rolling resistance improvement. Progress at a vehicle system level has been evaluated for a variety of technology implementations evaluated through analysis, bench testing, creation of functioning electrical mock-ups, and build and testing of a complete on-road mule tractor. Lightweighting of the chassis is a significant accomplishment with a hybrid dual material approach and integration of functions such as the chassis frame member acting also as an air tank. The incorporation of active ride-height control on both tractor and trailer permits significant aerodynamic drag reduction in a near-term feasible commercial product. The progress on WHR system components has been measurable through analysis and bench testing. Development of the new, dual entry turbine progressed to functioning hardware packaged at the engine level. The attention to

demonstrator vehicle, on-road safety through durability, floor stiffness, global static stiffness, jack knife impact, and roof crush-rollover analysis is a significant project positive, as well as a contributor to evaluating commercial viability.

Reviewer 3:

The presentation contained more than adequate technical results and implementation information that were lacking from some of the other teams.

Reviewer 4:

The efficiency demonstrated to date on the engine is outstanding and already best-in-class. The truck engineering looks to be equally well developed; the reviewer particularly appreciated the call-out on safety. The reviewer had no doubt that all the teams are taking that seriously, but putting in a slide discussing the efforts in that direction is a good addition to merely talking about the efficiency gains.

Reviewer 5:

The slides are poorly arranged; Approach and Technical slides are frequently interchanged. Work around the chassis, specifically the air suspension and disconnect axles, is meritorious. The team, however, fail to provide meaningful technical information. Aspects that should be discussed are stability, response times, and power requirements, and impact on the freight efficiency. Notices as to cost and customer response should also be brought up.

Reviewer 6:

Completion of the mule vehicle demo is a significant accomplishment for this team. It is also good to see that the 55% demonstration engine will be used in the final demonstration vehicle too. The one area that was not clear was the intent to retain heat in the piston via material selection and component design. This was listed under "Key Technology Development" on Slide 11. Is this not the opposite of the temperature-swing thermal coatings being done by the other teams?

Reviewer 7:

The reviewer suspected that technical accomplishments and progress are in line to meet the overall goals of this project, but there was not enough evidence in the slides or presentation to ascertain. There was no waterfall chart that describes details of where the efficiency is being attained.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that the work by the project partners is indicated throughout the presentation.

Reviewer 2:

The project seems to utilize all partners, significantly strengthening the chance to meet the program goals.

Reviewer 3:

The use of team company logos throughout the presentation made it easy to see that there are a lot of participating suppliers and industry leaders supporting this project. If the results of the integration of so many ideas are as well done as this slide deck, the performance of the vehicle should be impressive. Hopefully, this is a true representation of the project and not just excellent PowerPoint engineering.

Reviewer 4:

The collaboration appears strong. It is difficult to tell how much of the work is a true collaboration and how much is a supplier-customer interaction. There is ample evidence of strong technical development across the entire project though, so the reviewer is giving the benefit of the doubt to the team.

Reviewer 5:

The system level approach of this team is evident as the only non-vertically integrated engine and vehicle OEM SuperTruck team. The project team members include all the functional members requested in the FOA. Greater discussion of active participation and contribution to progress by the fleet, trailer, and tire members is needed. Collaboration to date has been excellent, until COVID-19 impacted schedules in March 2020. The ramification of the vehicle OEM halting vehicle integration work for the remainder of 2020 means an effective 8-month gap in vehicle integration efforts and a 1-year slip in the testing schedule. This gap increases risk that the engine manufacturer and the vehicle manufacturer may not be in sync, that experience on the project teams may change from personnel reassignments or departures, that funding demands in 2021 may increase to expedite procurements and obtain facility and technical support, that troubleshooting time and complexity for the vehicle in 2021 may increase, etc. Budget limitations may further reprioritize program activities. These challenges may lead to the project not meeting critical performance objectives. Alternatives for continuing collaboration and providing necessary resources should be investigated by the team. The trailer team member was not identified in the slides but was discussed in the verbal part of the presentation.

Reviewer 6:

The reviewer commented that there is a single slide showing collaboration, but not enough evidence or discussion on how these suppliers delivered their products with "collaboration" rather than a simple supplier-customer relationship. These projects should help teach others (160 people in the audience) about how collaborations can help deliver against such significant challenges.

Reviewer 7:

The reviewer asked if the suppliers shown on Slides 19-22 are developing new technologies, or just supplying previously developed technology. Is any of that technology in the marketplace?

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

Reviewer 1:

There is a strong plan in place to achieve and exceed the SuperTruck 2 goals, and the work progress suggests no significant problems with meeting the targets.

Reviewer 2:

The reviewer affirmed the project looks good. The reviewer looked forward to the final year's demonstration progress in next year's presentation.

Reviewer 3:

The proposed future research covers all of the necessary steps to ensure that the program is on the way to achieve the program goals.

Reviewer 4:

Much of the research is now just needing to be modeled in the test vehicle and validated and optimized on the track and on the road. If the team's confidence proves out, this should be a great combination of ideas and integration from many different parties.

Reviewer 5:

Future research is pretty limited to procuring parts and completing the build for tests. The reviewer understood the decision to break up the team given the recession situation.

Reviewer 6:

The reviewer asserted that the schedules shown are too brief and vague. Entries such as 'Vehicle Design Development' should be proven down to provide a more comprehensive work overview. Statements such as 'simulate in-use truck environment' should be accompanied by a description of what this entails.

Reviewer 7:

Proposed future work is impacted by team member reprioritization of funding and personnel. The ramification of halting OEM vehicle integration work for the remainder of 2020 means an effective 8-month gap in vehicle integration efforts and a 1-year slip in testing schedule, increasing the risk that the engine manufacturer and the vehicle manufacturer may not be in sync, that experience on the project teams may change from personnel reassignments or departures, that funding demands in 2021 may increase to expedite procurements and obtain facility and technical support, that troubleshooting time and complexity for the vehicle in 2021 may increase, etc. These challenges may lead to the project not meeting critical performance objectives.

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

Reviewer 1:

The project directly supports the DOE VTO goals of developing high efficiency technology for freight movement in the United States.

Reviewer 2:

Reduced heavy duty fuel consumption is directly in line with DOE objectives.

Reviewer 3:

Class 8 HD tractors are by far the single biggest contributor to GHG emissions, and the DOE should maintain a constant stream of projects to assist in efficiency efforts.

Reviewer 4:

This project very well supports the overall DOE objectives because of 55% BTE and a minimum 125% FTE improvements that are likely to be achieved.

Reviewer 5:

The reviewer commented that the work is relevant. Some indication on cost-benefit should have been given.

Reviewer 6:

Many of the ideas that make up this concept vehicle can be applied to production tractor-trailers. It would be great to see how the wider industry will accept the concepts as part of their specifications and operations. The ideas could optimize future vehicles without being so complex that fleets refuse to adopt them into their specifications.

Reviewer 7:

Project relevance focuses on key technologies, such as electrification of accessories through the use of 48 V systems, incorporation of waste heat recovery technologies, lightweighting, improved aerodynamics, improved tire rolling resistance, improved lubricants and coatings, improved driver assistance systems, etc. What appears to be missing seemed to be significant discussion of the commercial viability of these choices and any discussion of applicability to expanding market volumes and future proofing tractor technologies such as applicability of the 48 V accessory systems to battery electric, fuel cell electric, and other alternative fuel vehicles also in work with both Cummins and Peterbilt, their subsidiaries, and partners.

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

Reviewer 1:

The project team has all it needs to achieve the program goal in a timely manner.

Reviewer 2:

The reviewer stated that the spend rate and budget look good for the work plan.

Reviewer 3:

The reviewer commented that resources appear adequate.

Reviewer 4:

There is no indication that lack of funds will prevent the final demonstration vehicle from being built and meeting the project goals.

Reviewer 5:

Although the reviewer rated the project team as sufficient, the reviewer had significant doubts given the stated delays in the project. If financial obstacles remain, given a slow recovery out of the current challenges of both COVID-19 and a financial recession, this project may be losing momentum and expertise required to produce the results promised. It would be a shame to have gone so far and yet let the trip slip away without concluding a successful journey. Please watch this one closely and bring home the delivery to the dock as promised.

Reviewer 6:

The reviewer understood disbanding the team, but did not see a plan to document and even close out aspects of the project such that it can be restarted to complete the project efficiently. The reviewer was concerned about meeting program deliverables once the project restarts.

Reviewer 7:

The project reported spend to date at \$35.8 million against net budget allocation of \$40 million. Reporting net program spend to date is important to ascertain remaining funding against discussed plans. The project also detailed a COVID-19 schedule and manpower impacts at the vehicle OEM introducing a 1-year delay in the project, and the engine manufacturer described a 3-month impact for 55% BTE confirmation. The project did not identify a need for additional funding, rather accepted schedule slips. However, realistically there may be additional manpower and procurement costs such as storage, refurbishment, expediting, and possibly contract labor to fill short-term project needs once the vehicle OEM restarts work in 2021 from a more than 8-month hiatus. Maintaining the original scoped efforts may be at risk without additional funding. Details of a recovery plan with respect to budget and deliverables should be provided.

Presentation Number: ace103 Presentation Title: Development and Demonstration of a Fuel-Efficient Class 8 Tractor and Trailer SuperTruck Principal Investigator: Russell Zukouski (Navistar)

Presenter

Russell Zukouski, Navistar

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-12 - Presentation Number: ace103 Presentation Title: Development and Demonstration of a Fuel-Efficient Class 8 Tractor and Trailer SuperTruck Principal Investigator: Russell Zukouski (Navistar)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

This project is well along toward completion and the overall approach remains solid. The integration of a higher voltage hybrid system is positive for future applications where 14 V systems have limitations on electric-only operation.

Reviewer 2:

The project demonstrated approaches to attaining or exceeding FOA program goals. However, there are a significant number of system design selections or optimizations still in process at the engine level late in the project. The extensive use of carbon fiber for cab structure and trailer was described by the presenter as far from commercial viability due to the raw cost of carbon fiber for the foreseeable future. As commercialization potential within a few years is a key element of the FOA goals, the choice of this material solution is both a project commercial risk and added complexity, cost, and schedule to the project, and perhaps the effort should have focused on nearer term alternatives. Evaluation of a gasoline compression ignition (GCI) hybrid architecture is innovative. Fleet feedback on the potential ramifications to operations, maintenance, technician training, industry fueling infrastructure, etc., should have been included in the progress discussions as part of the decision making and eventual commercialization potential. Weight reduction and optimization of the chassis systems along with high-strength steel (HSS) steel showed progress, and evaluation of multiple shapes was performed to allow confidence in selection.

Reviewer 3:

The approach seems on track to meet project deliverables, but this review was very difficult to follow. Part of the reason is due to three presenters and it seemed very similar to prior years. The reviewer was concerned with delivery in the final year given a number of open issues.

Reviewer 4:

The presentation team seemed to have spent a lot of time talking about ideas and areas that were not proving out well for the project. Some areas are great while others, like the exhaust aftertreatment system and heat damage to the composite frame structure, are obviously challenging the team.

Reviewer 5:

The approach with continuation of the gasoline engine in the project is highly questionable. Although the gasoline engine can offer some benefits to the light loads, there would be virtually no chance that this gasoline engine would be installed into a demonstration vehicle to meet the program goal. In addition, this gasoline engine has no chance to meet 55% BTE goal as well. Then why would the project continue funding this technology? A clear justification would be required.

Reviewer 6:

Little consideration was given to the approach. The project team appeared to go right into the technical accomplishment section.

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

Reviewer 1:

It was great to see that operations can include a 20-30-mile range of no internal combustion engine (ICE) combustion while on hybrid electric mode.

Reviewer 2:

The team is pursuing many approaches to achieve a difficult target of 55% peak efficiency but appears to be making progress. It is difficult to fully assess without disclosure of more data.

Reviewer 3:

There has been good progress made on the vehicle side on aerodynamics, weight reduction, cooling, and powertrain. However, 50.4% BTE at this stage is behind to its competitors. Although nice graphics have been generated to show the progress on combustion, fuel system, and air management, it is not clear how this progress can be attributed to overall BTE improvements in an incremental manner.

Reviewer 4:

There are a significant number of system design selections or optimizations that appear to be still in process at the engine level well into budget period 4. The extensive use of carbon fiber for cab structure and trailer was described by the OEM presenter as far from commercial viability due to the raw cost of carbon fiber for the foreseeable future. As commercialization potential within a few years is a key element of the FOA goals, the choice of this material solution is both a project commercial risk and added complexity, cost, and schedule to the project, and perhaps the effort should have focused on nearer term, more commercially viable alternatives. Evaluation of a GCI hybrid architecture is innovative, and progress was shown on development and testing. Fleet feedback on the potential ramifications to operations, maintenance, technician training, infrastructure, etc. should have been included in the progress discussions as part of the decision making and eventual commercialization potential. Weight reduction and optimization of the chassis systems along with HSS steel showed progress, and evaluation of multiple shapes was performed to allow confidence in selection. A traditional schedule waterfall chart was shown in 2019 AMR but was missing from 2020 AMR presentation, making assessment of progress more challenging for reviewers.

Reviewer 5:

Good progress on key decisions to move to final integration and build. The reviewer was disappointed in the lack of detail in the slides and presentation around the objectives of efficiency and in particular commercialization. The team almost ignored the requirement of assessing fleet interest in adoption. The reviewer doubted the fleet identified is too involved.

Reviewer 6:

Cylinder activation work results applied to representative city drive are an impressive 2.9% fuel consumption gain. But, this vehicle application is likely to be longer haul. Overall, it would be advisable that Navistar applies the FE criteria for all their technology portfolio on the same cycle. This is important for assessing the overall FE impact

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Collaboration across the project team seems to be good. The contribution by each key team member has been appropriately acknowledged.

Reviewer 2:

It appears to the reviewer that work by project partners is indicated throughout the presentation.

Reviewer 3:

Collaboration on the vehicle structure appears very constructive and is making good progress. Engine features such as air handling appear well coordinated with major suppliers.

Reviewer 4:

Collaboration was noted with respect to a few of the suppliers, but very little evidence was described for National Laboratories and end-user fleet. The reviewer wondered if there is some way that an advisory committee could be incorporated into these projects.

Reviewer 5:

The project team includes a cross section of expertise as desired in the FOA with the exception of a tire manufacturer. Input from the trailer or fleet team members was not significantly discussed in the presentation, which is relevant to key FOA goals to establish commercial viability such as operational cost impacts, impacts to service centers, fueling infrastructure, technician and driver training, warranty, reliability, resale, etc. The trailer team member was not identified in the slides, only the composites manufacturer. Co-development of predictive cruise control and ACC controls were attributed to University of Michigan. Is this the same group that is working on the Daimler SuperTruck 2 (ST2) PCC and ACC systems? If so, they were not identified in the slides.

Reviewer 6:

The presentation team seemed nervous and struggling to present to our reviewers. The reviewer was not sure how that reflects on the project.

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

Reviewer 1:

The team seems committed with resources to finish even given COVID-19 challenges.

Reviewer 2:

It sounds like tough decisions have been made on which technologies to drop and which to carry forward. Optimizing hybrid operations with predictive cruise control could yield some interesting results for future production hybrid vehicles.

Reviewer 3:

The project is nearing completion with the engine target not quite achieved, but the future path looks reasonable. The future research steps were defined well in some subtasks, but not addressed very completely in the vehicle area.

Reviewer 4:

The proposed future research is not clear, specifically on the vehicle site, although the next steps on the engine side have been mentioned throughout individual progress slide. A dedicated slide for the future work would be useful to help the reviewer to understand the project's future direction.

Reviewer 5:

The absence of a traditional schedule waterfall chart previously shown in the 2019 AMR review but omitted from the 2020 AMR review presentation made the assessment of future research work challenging. A significant number of engine-related decisions appeared to be still in flux well into 2020 Budget Period 4, the period focused on tractor-trailer fabrication, integration, commissioning, and demonstration. The relationship of development work and testing with the mule vehicle with respect to applicability to the hardware and software for the demonstration vehicle was not discussed; perhaps the migration of systems from the mule to the demonstrator is expected, but no declaration of migration was shown in the presentation. There are significant software and hardware integrations ahead for this team, and adequate time and resources for troubleshooting software issues are not clearly identified as a risk factor to cost, schedule, and testing.

Reviewer 6:

There appears to be a rather large gap between the engine demonstration status and target improvements (Slide 4). This year's work is indicated as a "down-selection" period, ahead of the commission and demonstration. How does Navistar expect to bridge this gap? The vehicle freight efficiency improvement roadmap (Slide 11) lacks clarification if these are projections, simulation estimates, or actual data. Little confidence is provided on the following slides of its capability to meet the stretch goal target. The continued efforts of Slide 17 are vague. Statements such as "WHR system development" should be given much greater thought and conveyed here, specifically with respect to the gaps noted in their roadmap to attain the program goals.

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

Reviewer 1:

Class 8 HD tractors GHG reductions are key to DOE goals as they are by far the largest fuel user. The DOE should maintain a constant stream of projects in this area.

Reviewer 2:

This project supports the overall DOE objectives if it can achieve 55% BTE on the engine and 140% improvement on the vehicle.

Reviewer 3:

Hybrid configurations seem highly likely (might be diesel but it also might be hydrogen), and the work being done here to operate in an engine-off mode when possible is a step in the right direction.

Reviewer 4:

The project is discovering and demonstrating technology for reducing fuel consumption and emissions from medium- and heavy-duty vehicles (MHDVs) in the freight sector.

Reviewer 5:

The project relevance to potential future production solutions to reduce emissions and improve efficiency is significant. However, the technology choices per the FOA need to address commercial viability in a short time frame of 2-3 years. The choice of carbon fiber as a major structural component for the cab and trailer are worthy of research, but as R&D activities rather than core choices for the SuperTruck II effort. The chicken-and-egg aspect of carbon fiber is that raw material price is high with only marginal decreases over time due to low volumes; the reviewer recognized that for volume to increase so that price may decrease, projects need to implement carbon fiber in production uses. Projections for market adoption modeling of carbon fiber would be beneficial to this team making the case with the assistance of ORNL researchers with expertise in the material.

Reviewer 6:

The reviewer remarked that the overall work is relevant. Some indication on cost-benefit should have been given.

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

Reviewer 1:

The reviewer affirmed the resources appear adequate.

Reviewer 2:

The project is well along and does not seem to have hit any major setbacks, which would stretch the resources.

Reviewer 3:

The project reported no significant detail on budget spend to date nor the impacts of COVID-19 related manpower and procurement issues. The project is reporting completion to the original end of 2021 schedule. The 2020 AMR report states 67% complete. Impacts to the OEM and Tier 1, 2, and 3 supply bases from COVID-19 shutdowns reasonably should be expected, so to stay on schedule with original work content would require expediting, overtime, and other schedule recovery methods that may pressure the budget. The project should provide a level of detail to permit assessment of project resources against scoped work content and schedule. Prior year AMR reports for 2017, 2018, and 2019 AMRs similarly do not report spend to date details or remaining budgets.

Reviewer 4:

Responding to the question of how sufficient resources are for the project, this reviewer indicated that there is little evidence, otherwise.

Reviewer 5:

If resources are moved from areas that have been eliminated to areas of future focus, the team should be on track.

Reviewer 6:

The reviewer was not sure if the project will have sufficient resources to achieve the engine program goal.

Presentation Number: ace118 Presentation Title: CLEERS Passive NOx Adsorber (PNA) Principal Investigator: Janos Szanyi (Pacific Northwest National Laboratory)

Presenter

Janos Szanyi, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

Three reviewers indicated that the project was relevant to current DOE objectives while the other reviewer indicated that the project was not relevant. All reviewers indicated that the resources were sufficient.

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



Figure 1-13 - Presentation Number: ace118 Presentation Title: CLEERS Passive NOx Adsorber (PNA) Principal Investigator: Janos Szanyi (Pacific Northwest National Laboratory)

Reviewer 1:

The project has met, and is on track to

meet, its annual milestones that include key technical barriers of NO_x adsorption capacity, reasonable NO_x release characteristics, improved zeolite thermal stability, and understanding important hydrothermal durability mechanisms.

Reviewer 2:

This is a solid and well-planned exploration of the fundamentals of NO_x adsorption on Pd exchanged zeolites, building off of previous work. The work trends closer to basic research than applied, but this is somewhat expected. The reviewer asserted that it would be nice to see how this work contributes to modeling, as this is one of the identified barriers.

Reviewer 3:

The project has responded to reviewer comments from last year and put adequate emphasis on cycling and high-temperature stability studies.

Reviewer 4:

The technical barriers for commercial use of the PNA technology are low storage capacity per unit cost of the material; and storage capacity decrease with the use (sulfur, hydrothermal aging, and presence of reducing components) apart from how to effectively use the component in a real-world system. There has been emphasis on selecting the Pd/zeolite by varying the zeolite in this work, but not much has been done to keep the storage level high with different aging. Also, raw data curves are shown in the presentation without much processing of the data to bring new features from these experiments, e.g., storage capacity with respect to temperature, efficiency of storage when some NO_x is already stored, etc.

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

Reviewer 1:

The project has identified a promising zeolite-based PNA with good hydrothermal stability and has developed an understanding of the impacts of CO concentration on NO_x desorption for this PNA material.

Reviewer 2:

Good progress has been made against the milestones, and the issues raised by prior work (such as high-temperature deactivation) are being addressed here.

Reviewer 3:

This project has generated abundant data that have fair connections to real-world applications, despite the delays caused by the global pandemic.

Reviewer 4:

In this work, cause of degradation of PNA material such as HTA and effect of CO/ HC are illustrated. The goal of the project was to provide molecular level understanding, but it was not clear where Pd is in the zeolite, how many types of Pd there are, and what makes Pd special that it stores NO while Pt cannot. There are some conflicting results from the literature about the impact of low concentration of CO on NO_x storage and release. For the most part, the work seems like a report on making a few varieties of PNA by changing the zeolites, but it is not much focused toward understanding the cause and providing solutions for improvement.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer stated that promising new materials have been compared and analyzed.

Reviewer 2:

The contribution of key teams is mentioned in the presentation.

Reviewer 3:

Collaboration appears to take place primarily through monthly teleconferences and sample exchanges with other laboratories. It is good to see collaboration across National Laboratories (ORNL), industry (BASF), and academia (Sofia University).

Reviewer 4:

The project would benefit from more collaboration with ORNL staff who are also working on PNAs. The topic of HC interactions on the PNA, in particular, looks like it needs to be addressed under more realistic exhaust gas conditions that are being used in another ORNL PNA project.

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

Reviewer 1:

As this project is completed later this year, work is rightly targeting measuring performance metrics using more realistic exhaust gas conditions.

Reviewer 2:

The future work is well planned, but it would be good to see more emphasis on application.

Reviewer 3:

Some of the proposed work should have been completed during the course of program.

Reviewer 4:

The team promised a large amount of work. For VTO projects, the deliverable should focus on creating better solutions. The compatibility with a diesel oxidation catalyst (DOC) would be particularly intriguing.

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

Reviewer 1:

PNA is critical for diesel emissions control.

Reviewer 2:

The reviewer commented that work on PNAs are an important enabler of cold-start NO_x performance.

Reviewer 3:

This work directly addresses several objectives put forth in the U.S. DRIVE ACEC Roadmap with a focus on NO_x abatement for low-temperature combustion.

Reviewer 4:

This project is not very relevant for various reasons, at least for heavy-duty diesel:

- The cost of Pd (active metal for PNA) increased a lot in last few years compared to Pt.
- NO_x storage is not stable and shows some irreversible degradation.
- It is difficult to control in real operation in the presence of NO_x from the engine.

However, this project is somewhat relevant for light-duty diesel. The scope of PNA in those applications is also limited.

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

Reviewer 1:

According to the reviewer, resources are sufficient for this project.

Reviewer 2:

Current funding levels appear to be sufficient.

Reviewer 3:

The reaction testing capabilities, characterization tools, and funding level are all appropriate for the proposed research.

Reviewer 4:

The reviewer suggested focusing resources on measuring PNA performance using more realistic exhaust gas conditions.

Presentation Number: ace119 Presentation Title: Development and Optimization of a Multi-Functional SCR-DPF (Diesel Particulate Filter) Aftertreatment System for Heavy-Duty NOx and Soot Emission Reduction Principal Investigator: Ken Rappe (Pacific Northwest National Laboratory)

Presenter

Ken Rappe, Pacific Northwest National Laboratory

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. Two reviewers indicated that the resources were sufficient while the third reviewer indicated that the resources were excessive.

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



Figure 1-14 - Presentation Number: ace119 Presentation Title: Development and Optimization of a Multi-Functional SCR-DPF (Diesel Particulate Filter) Aftertreatment System for Heavy-Duty NOx and Soot Emission Reduction Principal Investigator: Ken Rappe

Reviewer 1:

This project has uncovered an interesting pathway to improving the passive soot oxidation performance of an SCR coated diesel particulate filter (DPF) using a manganese (Mn)-based additive that increases internal oxidation of nitric oxide NO to NO_2 . The performance and durability of this approach under diesel engine exhaust conditions remain to be demonstrated.

Reviewer 2:

The barriers identified are cost effectiveness and durability of aftertreatment devices. While combining units (and reducing system complexity) points in the direction of cost reduction, these barriers are not addressed quantitatively (i.e., the impact on system cost and durability are not addressed directly).

The addition of a selective catalytic oxidation (SCO) phase to the SCRF is an interesting approach to increasing passive soot oxidation. It is good to see the experimental work accompanied by modeling, as the two have potential to inform the other. The reviewer was interested to see the results of the sulfur-poisoning work, as this has weight in the practical applicability of the technology.

Reviewer 3:

Overall, the project used catalyst synthesis to improve oxidation capability to generate more in-situ NO₂, tried reactor and engine tests, and used modeling. Therefore, most of the approach was satisfactory, but all of these concepts were used earlier and are available in the literature; a key bottleneck with in-situ NO₂ generation is sensitive with sulfur and nitrous oxide (N₂O) generation. It would be better if key technical barriers for

commercialization of this technology—the effect of sulfur, lower temperature regeneration, and hydrothermal stability—were explored; some of those are in the future work, but the reviewer was not sure as the project is ending in June.

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

Reviewer 1:

Good progress has been made in characterizing the performance of a Mn SCO-SCR coated DPF. A Mn dimer has been identified as the active site for NO selective oxidation. Work on sulfur poisoning is underway, a key to understanding the viability and durability of this approach. Model development is in progress.

Reviewer 2:

The reviewer recommended further data processing of the experiments to derive relevant parameters, such as what fraction of NO_2 is used in SCR versus soot oxidation. This parameter will change axially and with temperature and would be very useful.

Some of the portrayed advantages of NO₂ generation occurs at temperature higher than 300°C, which helps with soot oxidation but hurts on SCR because of slow SCR and therefore demands higher diesel exhaust fluid (DEF) consumption. It is also surprising that NO₂/NO_x in the feed from 0 to 0.3 does not have any impact on the catalyst with 30% SCO.

Reviewer 3:

The model development appears to be running behind somewhat (scheduled for completion in April but still ongoing). This is understandable given the situation with the pandemic. Some interesting technical results are presented, but it is difficult to tell how far along the path to practical application we are.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

There is good collaboration with PACCAR and its suppliers on this project.

Reviewer 2:

Both PNNL and PACCAR teams were well coordinated and shared the roles and findings regularly.

Reviewer 3:

Collaboration appears to be well coordinated but is currently limited to the two cooperative research and development agreement (CRADA) participants, PNNL and PACCAR.

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

Reviewer 1:

The proposed sulfur-tolerance and modeling work is appropriate and necessary. It would be interesting to see system level impacts, such as the interaction between the design of the SCRF and the DOC. For instance, does the addition of the SCO phase to the SCRF allow for any reduction in PGM loading in the DOC?

Reviewer 2:

Sulfur poisoning studies are underway as this project closes out to begin the assessment of the durability of this concept. If this project is renewed or continued, it seems that this SCR-coated DPF design is ready to get out of the laboratory and move to engine studies to flesh out the durability issues.

Reviewer 3:

The reviewer commented that this is month of June so project should be ended.

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

Reviewer 1:

This work addresses the barrier "Reduce cost, size, and complexity of emission control system with multifunction catalysts that combine multiple components onto one substrate," as stated in the U.S. DRIVE Roadmap.

Reviewer 2:

SCR-coated DPFs for heavy-duty engines are an important enabler for achieving faster SCR catalyst warm-up and reducing cold-start NO_x emissions.

Reviewer 3:

When the project started in 2016, the concept of combining SCR and DPF was one of the potential architectures to meet future challenges with cold-start emissions. But, this architecture has significant challenges, like hydrothermal stability of the SCR layer, soot cleaning, etc., and one of the challenges of preferential NO₂ consumption in SCR compared to soot was explored as part of this study.

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

Reviewer 1:

The resources for this project appear to be sufficient.

Reviewer 2:

The project appears to have sufficient resources to close out the remaining objectives around model development and sulfur impacts.

Reviewer 3:

The total of \$2.7 million for the amount of work done for this project seems high when key barriers, such as sulfur and hydrothermal aging, were not addressed.

Presentation Number: ace123 Presentation Title: Temperature-Following Thermal Barrier Coatings for High-Efficiency Engines Principal Investigator: Tobias Schaedler (HRL Laboratories)

Presenter

Peter Andruskiewicz, General Motors

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-15 - Presentation Number: ace123 Presentation Title: Temperature-Following Thermal Barrier Coatings for High-Efficiency Engines Principal Investigator: Tobias Schaedler (HRL Laboratories)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The concept of thermal/temperature swing coatings is worth investigating and potentially effective. The difficulty and risk have been borne out in this project. Persistence of investigators is acknowledged. Further work on exhaust components seems like a good idea.

Reviewer 2:

Temperature swing coatings are an area of great interest in the industry now. Novel approaches to achieve these are needed, and this project provides a unique approach that shows very promising results. The ultimate proof will be in the durability, which has always been the downfall of thermal barrier coatings. While the performance of these coatings is very impressive, the development of the seal coat looks like a barrier to commercialization. This project acknowledges that this is still a problem but does not address that issue.

Reviewer 3:

The PI took a practically viable approach to address the project objectives. The project objectives were clearly defined. Going forward, the reviewer requested the inclusion of a percentage target achieved against the program goals to evaluate what percentage of the goal was achieved. For example, there could be an additional bar chart to illustrate the percentage targets achieved clearly on the project objectives slide.

Reviewer 4:

Project appears to have had significant challenges regarding the development of prototype components. The test sequence seems technically sound, but some of the challenges encountered during the process could have been avoided with a better technical plan of execution.

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

Reviewer 1:

Significant progress is made, and practical viable solutions are being considered and demonstrated.

Reviewer 2:

Although not all the hoped-for targets and durability were achieved, the project has generated important new data about swing coatings. The outcomes for exhaust components should be interesting. New intellectual property (IP) has been developed.

Reviewer 3:

It is not clear for what budget period the accomplishments presented were achieved. If the reviewer assumed that the no-cost time extension period (during which everything was on pause) just ended, then it looks like the project just restarted. The reviewer was giving the benefit of the doubt that the reported results were for a 1 budget year period, and the accomplishments for this period of time with the material application and sealing are very good.

Reviewer 4:

Schedule has been significantly delayed due to challenges with piston coating and machining. Overall fuel economy improvements have been relatively low (2.7%) for the amount of funds this project has expended.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It appears to the reviewer that there were effective collaborations leading to practical solutions.

Reviewer 2:

The partnering with GM and suppliers has been okay.

Reviewer 3:

The reviewer noted that there was only one partner on the program. It is a major OEM, so it can support testing and guidance on objectives. It probably would have been good to have a partnership with Tier 1 and 2 suppliers that could have helped alleviate some of the technical challenges encountered.

Reviewer 4:

The reviewer questioned why the collaborators' names were not in the presentation. Saying "multiple industry partners" and "Tier 1 supplier" is not much to go on to make an evaluation. The reviewer also found it hard to tell what HRL did and what GM did.

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

Reviewer 1:

The project is nearly over, so completion of work on exhaust ports and final tests of pistons should be key in the plans. Documenting the entire project is important.

Reviewer 2:

The reviewer commented that the proposed future work plan is satisfactory. Benefits of the coatings have been shown (although the impact is relatively small). The reviewer would have preferred to see some effort focusing on the durability of the surface coatings, considering the challenges that were encountered with the project.

Reviewer 3:

The project is scheduled to end at the end of 2020, so the future work would need to be funded through a different mechanism. It was difficult to tell, but it appears that the final year milestones will be met.

Reviewer 4:

The PI and collaborators need to make it more obvious when and what measure to use to take go/no-go decisions to continue with the project milestones.

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

Reviewer 1:

Performance benefits of thermal swing coatings and their ability to enable fuel economy improvement as well as provide higher quality heat for exhaust aftertreatment meet the DOE VTO program objectives.

Reviewer 2:

Thermal barrier coatings improve fuel efficiency and support overall DOE objectives.

Reviewer 3:

The project supports improved energy utilization for internal combustion engines.

Reviewer 4:

Thermal swing coatings are indeed a fundamentally sound path to higher engine efficiency, yet difficult to perfect and commercialize.

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

Reviewer 1:

In reviewing this project more than once, the financial resources have appeared adequate.

Reviewer 2:

The project PI and collaborators appear to have sufficient resources that are relevant to achieve practical viable solutions.

Reviewer 3:

The reviewer commented that the project is coming to an end.

Reviewer 4:

The reviewer opined that this project was provided significantly too much funding for the relatively small improvements it has achieved.

Presentation Number: ace124 Presentation Title: SuperTruck 2 -PACCAR Principal Investigator: Maarten Meijer (PACCAR)

Presenter

Maarten Meijer, PACCAR; Ben Grover, Kenworth Truck Company

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-16 - Presentation Number: ace124 Presentation Title: SuperTruck 2 - PACCAR Principal Investigator: Maarten Meijer (PACCAR)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The technologies selected for development are solid, and the approach is sharply focused without extraneous explorations. The progress plan is very clear, and the team members have clear roles. The reviewer appreciated the study of high-risk engine features like thermal swing coatings. The reviewer wished the team good luck.

Reviewer 2:

The program is 1 year later than the other four and has a solid system to subsystem to component level approach. Fleet engagement appears relatively robust, and presenters suggested a customer council that is helping to focus the teams on designs that will be wanted by end users. Some areas of investigation are aggressive that could prove as big wins.

Reviewer 3:

Engine and Powertrain approaches look sound, although not much detail was provided to go on. The reviewer was glad to see some non-conventional technologies being considered. The aerodynamics work was not as clear to the reviewer. Slide 21 shows aerodynamic drag reduction of 20% and 5% on the trailer. So, does this mean that there will be 35% reduction in the tractor aerodynamics to equate to the 60% reduction overall target in aerodynamic improvement?

Reviewer 4:

Some areas of progress can greatly enhance existing vehicles if implemented in production sooner rather than later. Increasing the resistance to heat flow (R-value) of the sleeper cab by 100%, for example, will help reduce
heating, ventilations, and air conditioning (HVAC) system loads both while operating and while stationary. This should be a huge benefit toward reducing idle time in both hot and cold environments.

Reviewer 5:

The project demonstrated approaches to attaining or exceeding FOA program goals. The path to the target of 55% BTE clearly identified WHR as required in 2020 AMR slides (also in 2019), but discussion in later (AMR slides and in the question and answer (Q&A) period indicated this team did not think WHR was commercially viable and was pursuing hybrid electric solutions. Clarity is needed on the official path to target. This is a risk item in attaining the FOA goals, and alternatives were not clarified in the project schedule or budget. The progress on design elements appears otherwise sound, especially with this project starting a year after the other projects. A path to commercialization of the various technologies is not well presented, particularly an assessment by the fleet team member of ramifications of the technologies to warranty, service, technician and driver training, facility infrastructure, etc.

Reviewer 6:

The approach that uses the competitor WHR is still highly questionable because this could create an uneven playing field for other competitors. Although PACCAR claims that it is not out of off-the-shelf solutions and the architecture and component sizing are unique, it is hard to imagine that the basic structure would be different, which requires substantial funding and research to reach this basic level. It would be helpful if PACCAR can point out specific differences between PACCAR and its competitor WHR structures.

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

Reviewer 1:

The reviewer found very good progress for this stage of the project, which had a 1 year later start than the other ST2 projects.

Reviewer 2:

This project has a 1-year delay compared to other ST2 projects. The team has made considerable progress in face of a global pandemic challenge.

Reviewer 3:

The project is on track for budget and schedule, even with delays due to COVID-19 related challenges and a schedule start a year behind the other ST2 teams. Use of a functioning mule vehicle demonstrates a level of confidence for final demonstrator project integration. Investigation into ride and handling has been thought of, which is necessary for the significantly evolved configuration. The significant level of software and hardware integrations—including PCC and ACC, mild hybrid systems, and a hybrid electric powertrain—may introduce cost, schedule, and testing challenges in the demonstrator.

Reviewer 4:

The good detail in the efficiency waterfall chart that allows reviewers to understand progress. Key issues seem identified and plans in place for technical accomplishments in the future.

Reviewer 5:

It is too early for the reviewer to get a strong feeling on this question. The aerodynamic gains seem large, but the aerodynamic simulation illustration is clearly not of the SuperTruck vehicle configuration eluded to with the mule photo.

Reviewer 6:

The technical accomplishments are too vague on the engine side, giving the reviewer the impression that no quantifiable improvements have been made at this stage. For example, there is no scale on the y-axis in Slide 9 (Technology Validation) and Slide 20 (Demonstration Vehicle Progress). Furthermore, there is no definite

progress that can be seen or even indicated from all carton-style pictures on Slide 10 (Iterative Simulation and Testing).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The team overall is very strong and the roles are fairly clear. There was a good clarification that the "Cummins" WHR system is still specifically engineered and adapted by PACCAR. It is not a bolt-on part. It is great to have United Parcel Service (UPS) progressive thinking on the team.

Reviewer 2:

A good team has been put together for this project. For the suppliers shown on Slide 23, are they developing new technology for the project, or are they using technology already in production (in another product)?

Reviewer 3:

It would be more helpful if the company logo could be inserted on the slides where those partners have made the contribution to the program, allowing the reviewer to have a better picture of how the partners help the project.

Reviewer 4:

The project team includes a cross section of expertise as desired in the FOA; however, there was no indication on the charts regarding the identity of the trailer manufacturer. Q&A was required to identify the trailer manufacturer, the tire manufacturer is not listed on the first team slide, and no discussion of Crr improvement approaches was included in the review. The involvement of Cummins in WHR was addressed in comments to 2019 AMR, but it is not clear if this project will use WHR in the final demonstrator from Q&A commentary. Aerodynamics work involving 1/8- scale and ½- scale models suggests there were wind tunnel investigations with further partners and suppliers, which were not described in the presentation.

Reviewer 5:

There is a strong list of partners and great strategic areas. The reviewer was puzzled why Stoughton Trailers was given credit verbally for their development work on trailers, but they were completely left off the list of collaborators.

Reviewer 6:

The reviewer commented that some more evidence and examples of efforts that collaboration has proven successful were needed. There were 135 people in attendance that could all benefit, and the reviewer expected to learn how teamwork could increase success for projects like these. The reviewer was disappointed that none of the SuperTruck teams offered much on collaboration.

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

Reviewer 1:

The reviewer appreciated the summary slide of future work. The overall plan is very solid and explained well.

Reviewer 2:

The proposed work for the upcoming year looks good. At this stage of the project, the reviewer hoped to see significant progress toward demonstration of the proposed technologies in the mule vehicle next year.

Reviewer 3:

Plans are in place and the team is committed, but there appear to be some components that are behind in definition that might put the project at risk. The reviewer commented that a list of corrective actions even at a high level would have helped.

Reviewer 4:

The reviewer said that the proposed future research in Slide 25 covers most of the challenging issues.

Reviewer 5:

Building of the mule 2.0 with mild hybrid and battery retrofit has the opportunity of reducing schedule risk if the software and hardware integration is representative of the final demonstrator and can possibly be carried over. The WHR system is included as a FY 2021 engine future work, but the OEM also discussed that it was not commercially viable; this places budget and schedule questions with respect to attaining goals. Market evaluation of technologies for near-term commercialization is also needed but not clearly identified as a future deliverable; this is particularly needed due to a significant revision in vehicle configuration from existing baselines. While comparison to 2009 progress is inherent in ST2 FOA goals, commercial viability with respect to current model year performance and cost models is relevant and necessary and should be included in planned work.

Reviewer 6:

The reviewer was concerned about the production viability of an MX11 engine with new technologies and complexities buried deep underneath a cab and sleeper. The reviewer was willing to wait for next year's reviews to see their "secret access panels" mentioned in the Q&A. This did not strike the reviewer as being deemed production acceptable to fleet customers, but we will know in 12 months.

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

Reviewer 1:

The project is relevant to DOE objectives as described in the FOA and with respect to future freight industry needs. The system approach including a wide range of technology solutions provides a level of robustness to the potential utility of the concepts, especially where this project diverges from the four other ST2 projects, such as the radical aerodynamic shaping of the cab and investigating alternatives to WHR.

Reviewer 2:

This project directly supports the DOE VTO program goals of high freight efficiency for the U.S. marketplace.

Reviewer 3:

All aspects of the work are sharply focused on the goals and barriers and offer promise of improved economics and efficiency for freight movement.

Reviewer 4:

Class 8 HD tractors use the most fuel and create a majority of GHG emissions from commercial trucks. It is critical that DOE continue investments in HD on-road vehicle development.

Reviewer 5:

Some areas of development ideas seem questionable while others seem extremely valuable.

Reviewer 6:

This project supports the overall DOE objectives if it is able to achieve 55% BTE and greater than 100% improvement on the vehicle.

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

Reviewer 1:

The reviewer commented that the project looks good and is staying on schedule.

Reviewer 2:

It appears to the reviewer that the project team has all it needs to complete the program.

Reviewer 3:

Resources seem sufficient, but an exhibit explaining areas of concern with resources would be good.

Reviewer 4:

The reviewer gave the benefit of the doubt given a late start and COVID-19 timing challenges.

Reviewer 5:

A general suggestion is for future advanced MHDV development to shift resources more toward technology discovery and fewer resources to full on-road demonstration.

Reviewer 6:

The project started in 2017, approximately a year behind other ST2 programs. The 2020 AMR reports 53% complete and reported funding of \$13.0 million in 2019 and \$16.7 million in 2020. The 2019 AMR reported 2018 funding of \$5.7 million and 2019 funding of \$13 million. The FY 2018-2020 estimates sum to \$35.4 million out of a \$40 million budget, but the project is reported as only 53% completed in AMR 2020 with work projected to complete in 2022. The project discussed only minimal impacts from COVID-19 related manpower and procurement challenges. Inadequate detail of the program budget with respect to resources and schedule was provided to properly assess the sufficiency of the project.

Presentation Number: ace128 Presentation Title: Reduced Precious Metal Catalysts for Methane and NOx Emission Control of Natural Gas Vehicles

Principal Investigator: Michael Harold (University of Houston)

Presenter

Michael Harold, University of Houston

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives and that the resources were sufficient.

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



Reviewer 1:

The project is very well designed from a technical standpoint. The progression from density fuel theory (DFT), to mechanistic studies, to bench-scale

Figure 1-17 - Presentation Number: ace128 Presentation Title: Reduced Precious Metal Catalysts for Methane and NOx Emission Control of Natural Gas Vehicles Principal Investigator: Michael Harold (University of Houston)

testing, to model development, to prototype testing is impressive.

Reviewer 2:

The reviewer asserted that the approach is sound, and work has been distributed between collaborators to address all milestones.

Reviewer 3:

The presentation and project did a nice job of making the case for the context of the work in four-way catalysts (FWCs). The approach taken seems very reasonable and the interplay within the project of theory/experiment is clear. The group, while perhaps ambitious in its scope of work, is pursuing logical aims with no gaps readily identifiable.

Reviewer 4:

The project has a well-rounded approach to promoting three-way catalysts for reducing precious metals for natural gas vehicles. The study is fundamental in nature, focusing on laboratory-scale evaluation of catalysts.

Reviewer 5:

Although the approach here to use spinel supports for CH_4 oxidation is intriguing, CNG catalysts are not highly sought after by LD OEMs due to their focus on TWC and diesel powertrains. However, the catalyst optimization work done here and the degree of learning from the analysis is critical to arriving at a viable catalyst solution.

Reviewer 6:

The mixture of modeling and experiment is very important in guiding the direction of this project. The impact of modulation was shown last year but is explored more here. The inclusion of sulfur in the testing is important. Water—a typical poison—is included in all feeds.

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

Reviewer 1:

Milestones seem to be on track for a project a little more than halfway through its cycle, though the reviewer agreed with prior comments regarding the ambition of the work. Overall, the team seemed to address the majority of comments from a prior review sufficiently. No aspect of the project seems to be lagging appreciably. The two publications from the work are nice and seem like the appropriate venue for some of the joint theory and experimental work.

Reviewer 2:

Many catalyst formulations using spinel supports have been investigated and reported in this work. From that activity, the most promising candidates have been down-selected for further analysis and understanding. This is necessary to derive the best catalyst for an application. The modeling and formulation effort is well thought out and works well together in this project.

Reviewer 3:

A lot of progress has been made since the first year of the proposal. New spinel compounds were found that contribute to improved activity. The modulation may mediate the impact of sulfur. There are many directions of work to check out, requiring good collaboration between the laboratories on the different directions.

Reviewer 4:

The results showed good progress with promoting low-temperature CH_4 and NO_x removal. Scaled-up evaluation of parts in a real exhaust stream would provide further insight into the performance of the new technologies being evaluated.

Reviewer 5:

New spinel is identified through screening. However, it is not obvious if the desired light-off and cost targets (that are not presented) can be achieved or were achieved with the identified formulations. Such estimations will be needed for evaluating the technical accomplishments; otherwise, the judgment would be based on qualitative interpretation.

Reviewer 6:

The project looks to be progressing on schedule. The modeling results show good agreement, the experimental results are intriguing, and the reviewer looked forward to further elaboration on the mechanisms at play. Not to nitpick, but the presentation of the budget period 2 (BP2) go/no-go decision is confusing (and probably a copyand-paste error). The decision point is "Identification of a candidate material complete," and the description refers to modeling progress. It can be inferred that this was meant to refer to the modeling effort and that the Go/No-Go was answered in the affirmative.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found a good balance of fundamental to applied research among the collaborators in addressing the objectives.

Reviewer 2:

The team of collaborators on the project is excellent at University of Houston, University of Virginia, ORNL, and Clean Diesel Technologies, Inc. (CDTI). They have good contacts with OEMS but might consider a direct interaction with a company making NG engines.

Reviewer 3:

The collaboration slide, while detailing well the various work components, did not delineate who did what, i.e., what were the specific contributions spread across the various partners. A separate slide showing a discrete example of how the team worked together on each component of the work would have been powerful in convincing reviewers the project team provides a sum greater than the parts.

Reviewer 4:

The project appears to be well coordinated with cooperation across the participants. Some indication of which work was led by which party would be helpful. It looks like the heavy lifting was done primarily by the University of Houston.

Reviewer 5:

The reviewer commented that this is a good R&D collaborative effort. It would benefit from the inclusion of an LD OEM for guidance.

Reviewer 6:

Collaboration appears good with commercial catalyst partner providing materials for evaluation. Further collaboration with a clear path toward commercialization would improve the likelihood of program success.

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

Reviewer 1:

The additional work proposed will help clearly identify a best option to move forward. The modeling work will also help in the process of selecting the best catalyst.

Reviewer 2:

In general, the path forward for the project is evident and continues on the work already initiated.

Reviewer 3:

The proposed future work should provide insights into the mechanistic behaviors as well as the durability of the catalysts developed.

Reviewer 4:

Fundamental and application challenges will be addressed in the proposed future work.

Reviewer 5:

The future work is well planned and sensible. It is difficult to tell if decision points or alternative development pathways are implemented.

Reviewer 6:

The directions of the future research are quite varied, especially in the experimental area. The inclusion of another Pt/Pd ratio than 19:1 could be considered, while being wary of the potential negative interactions between Pt and Pd. The important role of partially oxidized Pt could be studied further, along with how it is affected by S. With the importance of modulation determined, the Spaci-MS work can be very useful for understanding the mechanism of the reaction through the catalyst. The project does not need new avenues to

explore. With all of the project feeds having large amounts of water, one wonders if a few experiments, with very small amounts of water or no water, would comment on the mechanism in a useful way.

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

Reviewer 1:

The reviewer commented that the project absolutely supports the overall DOE objectives. The team has carefully considered how the work fits into the greater context of VTO DOE goals and clearly contributes to reducing PGM content. The team should get particular kudos for attempting to integrate base-metal derived materials. Too often the focus is on reducing PGM loading only rather than approaching the problem from materials discovery. As such, the work resides in an excellent niche very suitable for VTO projects.

Reviewer 2:

Yes, this project focuses on reducing emissions from internal combustion engines.

Reviewer 3:

Lowering of the light-off temperature is clearly important pathway for NG aftertreatment, which the new catalysts here may do. This clearly supports DOE objectives for this system.

Reviewer 4:

This project could potentially accelerate the adoption of stoichiometric natural gas vehicles while reducing their GHG emissions. Considering the natural gas production capacity of the United States, this would help reduce U.S. dependence on foreign energy sources.

Reviewer 5:

Low-temperature methane oxidation catalysts are needed to decrease fuel economy (FE), reduce dependency on foreign oil, generate low-cost systems, and lessen dependency of rare-earth and Pd metals.

Reviewer 6:

Although the catalyst development approach is relevant for innovating new technologies in this area, the use of CNG catalysts is not at the top of the list for LD OEMs.

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

Reviewer 1:

The provided resources appear to be satisfactory to provide high probability of success for the program.

Reviewer 2:

All resources seemed appropriate to the reviewer and in place for timely completion of the work.

Reviewer 3:

The project appears to have sufficient resources to achieve project goals.

Reviewer 4:

The testing and evaluation capabilities of the University of Houston, University of Virginia, and ORNL groups on this project are sufficient.

Reviewer 5:

The collaborators have all the tools and resources needed to effectively execute the project.

Reviewer 6:

The reviewer affirmed that this project seems well funded. It looks like about half of the federal funding remains for the last year of the 3-year project. As this phase, which includes costly engine testing, this is not surprising.

Presentation Number: ace129 Presentation Title: Design and Optimization of Structured Multi-Functional Trapping Catalysts for Conversion of Hydrocarbons and NOx from Diesel and Advanced Combustion Engines Principal Investigator: Michael Harold (University of Houston)

Presenter

Michael Harold, University of Houston

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives and the resources were sufficient.

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

Reviewer 1:

This is a well-designed approach to addressing low-temperature NO_x and HC emissions. The progression from the molecular-level modeling through full-

scale prototyping is ambitious and impressive.

Reviewer 2:

The objectives and approaches were clearly defined, and work was done to address the milestones.

Reviewer 3:

With the onset of Tier 3 and low-emission vehicle (LEV) III emissions standards, many novel approaches will require investigation to help ensure that viable catalyst aftertreatment system solutions are available to OEMs for their vehicle fleets. All these solutions have the common requirement of low-temperature catalyst performance in order to make sure the catalyst system will function at a high enough level during cold portions of the drive cycle to meet SULEV 30 and Bin 30 emissions standards. The approach in this project offers this capability if executed properly. Employing the trapping technology proposed here is one way to achieve this requirement. The system approach presented in this work is an innovative way of capturing the functionality of both HC and NO_x trapping at very low temperature together with an oxidation element to achieve the desired conversion efficiency of those species for a lean, advanced combustion mode. Incorporating modeling to predict the performance is also a requirement for optimizing the solution.

Reviewer 4:

The presentation and project did a nice job of making the case for the context of the work into multifunctional trapping catalysts. The approach taken seems very reasonable, and the interplay within the project of theory



Figure 1-18 - Presentation Number: ace129 Presentation Title: Design and Optimization of Structured Multi-Functional Trapping Catalysts for Conversion of Hydrocarbons and NOx from Diesel and Advanced Combustion Engines Principal Investigator: Michael Harold (University of Houston) and experiment is clear. The group seems to have made significant progress to converge much of the work to the current point. The way forward is clear.

The work clearly demonstrates knowledge gained about the various components of the system, but the connection of a direct improvement in performance is not so evident. While the candidate materials have been identified, how close is the system to the desired metrics? A more goal driven approach could have benefited the project, since the integrated system must achieve certain performance standards.

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

Reviewer 1:

The incorporation of modeling with catalyst development is a desirable combination to down-select candidate catalyst formulations and architectures in a more time efficient manner. The methods used in this project to narrow down the catalyst field are appropriate and effective. The inclusion of multiple catalyst architectures to derive the best outcome is an essential component of this work and is well conceived. Finally, employing combinations of promising catalyst technologies to achieve the required overall functionality is appreciated. Many times, system considerations are not addressed.

Reviewer 2:

Milestones seem much closer to being on track to achieve the overall goals of the project than in the prior funding period. The team seemed to address the majority of comments from the prior review sufficiently. No aspect of the project seems to be lagging appreciably, though the HC trapping portion seems like it has less emphasis relative to some of the other parts. The project appears to be converging at the critical time to assess the system level performance.

The project is very productive based on the number of publications produced from the work.

More focus or at least clearly identifying the gap between the current system and the desired metrics would have been beneficial.

Reviewer 3:

Milestones were addressed but it was not obvious to the reviewer how far the technical and non-technical barriers were addressed and accomplished. For example, there are about four to five flavors of different formulations for PNA identified. What criteria are considered or will be considered for identifying pros and cons of these different formulations, especially if they have to be integrated with other functions and components? Also, how do these different functions, if they have to be integrated into one device, impact the performance of PNA and vice versa? Also, the empirical evaluations carried out so far did not address any practical viability of these technologies. The same applies to HC traps and oxidation catalysts (OC).

Additionally, no quantified targets (e.g., NOx, and HC storage) were proposed; so, it was difficult to evaluate progress against such potential indicators. Going forward, such targets (obviously these will be estimates the PI has to come up with industry partners) should be proposed, and the technical accomplishments should be compared against these measures. The above are examples, but the PI and collaborators have to come up with such indicators.

Reviewer 4:

Good progress has been made, and the BP2 milestones have been met. However, it seems like the project overall may be running behind, as 70% progress is reported with about 5 months remaining. Completing the project on schedule appears challenging, though this is likely attributable to the pandemic situation to some extent.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The project appears well coordinated with cooperation across academia, industry, and the labs.

Reviewer 2:

The participant level in this project brings together diverse technical strengths to address all the aspects of the project. This will help ensure a successful outcome.

Reviewer 3:

The assembled project team seems to contain all the needed parts with defined theory/synthesis/catalyst testing/industry buy in. Some additional discussion of the industrial partners' roles, and how these evolve when the group shifts to evaluating the integrated system performance, would have been beneficial.

Reviewer 4:

The reviewer commented that it would have been outstanding if the contributions from industry partners were clearly shown.

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

Reviewer 1:

The future of the project is clear and continues on the work already initiated. The next period of work is critical to assessing if the project will meet the desired goals.

Reviewer 2:

Although much work remains to be completed, focusing on integrating the different catalyst technologies to produce a viable aftertreatment system and testing its performance under "real world" conditions is appropriate and necessary.

Reviewer 3:

The future work is well planned, though it seems difficult to complete the work in the time remaining for the project. This may have to be addressed through a no-cost extension.

Reviewer 4:

The future work did not define the following: practical challenges, such as chemical poison impacts, which are critical for the viability; and other durability challenges that can be encountered in practical applications. It is not expected to evaluate under all durability conditions, but the PI and collaborators must consider critical factors when evaluating under simulated conditions. Especially, such must be considered as a part of preconditioning the catalyst.

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

Reviewer 1:

The reviewer commented absolutely. The team understands how the work fits into the greater context of VTO DOE goals, the value of an integrated catalyst design, and the thinking about improving both individual components of the system and optimization of the whole.

Reviewer 2:

This work aims to reduce cold-start HC and NO_x emissions, possibly allowing for increased fuel economy. This is directly relevant to the DOE mission.

Reviewer 3:

This activity supports USCAR advanced engine combustion initiatives that need a feasible aftertreatment system as part of the powertrain.

Reviewer 4:

Low-temperature conversion of all the proposed pollutants poses a major challenge to the cost of the systems, fuel economy and therefore more GHG, and real-life emissions control. This project is much closer to addressing practical challenges faced today and expected in the future.

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

Reviewer 1:

All resources seem appropriate and in place for timely completion of the work.

Reviewer 2:

Among the collaborators, diverse tools and capabilities are available to make this project successful.

Reviewer 3:

The resources for this project appeared to be sufficient to the reviewer.

Reviewer 4:

The reviewer had no issues.

Presentation Number: ace130 Presentation Title: Development of Passive Hydrocarbon/NOx Trap Catalysts for Low-Temperature Gasoline Applications Principal Investigator: Mark Crocker (University of Kentucky)

Presenter

Mark Crocker, University of Kentucky

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. They also indicated that the resources were sufficient.

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

Reviewer 1:

The work appears well designed, with a solid combination of characterization, experiment, modeling, and computational studies. This span from



Figure 1-19 - Presentation Number: ace130 Presentation Title: Development of Passive Hydrocarbon/NOx Trap Catalysts for Low-Temperature Gasoline Applications Principal Investigator: Mark Crocker (University of Kentucky)

fundamentals to practical application is always impressive.

Reviewer 2:

The presentation and project identify key technical barriers and provide strategies to understand structureactivity relationships as many different parameters are studied (impact of water, aluminum [Al] content, etc.). The presentation was of high quality, and the Q&A provided an honest assessment of the project's status.

Relative to other projects, this one seemed less metric driven. While the studies performed were well crafted and carefully executed and new knowledge of the systems studied is clear, it was not evident to this reviewer how the knowledge gained is directly informing catalyst design in the final stage of the project. That connection was missing.

Reviewer 3:

The project team is focused on improving low-temperature NO_x control by using passive NO_x adsorbers. Barriers listed also include low-temperature hydrocarbon control. The characterization of the passive NO_x adsorber materials and reaction chemistry are critically needed to not just better understand them, but to also address the degradation modes. These materials were growing in interest a few years ago as potential solutions to cold-start NO_x control, but since have been plagued with deactivation issues. A regeneration strategy to reactivate their ability to adsorb NO_x is critical if they are to be possible solutions. The team is addressing that challenge through careful synthesis, characterization, reaction testing, and modeling.

Reviewer 4:

Technical targets must be defined and must be quantitative: for example, 0.1 g NO_x storage-release/1 g catalyst, between 50°-200°C, etc. Such definition will help to take or change project decisions and directions as and when needed. Similarly, if possible, barriers must also be quantified. Significant work was completed but not having the above quantified/semi-quantified targets made it difficult to estimate percentage targets achieved to address the barriers and challenges.

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

Reviewer 1:

Good progress has been made, but the 2020 milestones appear to be behind schedule, and a great deal of work is planned by the end of the project even with a 3-month extension. This is understandable given the current situation with the pandemic, but the timing seems tight.

Reviewer 2:

The studies outlined in the presentation are very detailed and provide a clear knowledge gain into the factors that impact catalytic activity. The response to prior questions seemed appropriate. The milestones were not as discrete as for most applied projects. Also, given the group of researchers involved and the amount of fundamental studies presented, it was very surprising to the reviewer to see no more than a single publication submitted on this work, as it seems to align well with dissemination in journals. It also seems a missed opportunity to have only just started applying the knowledge gained in the first 2 years of the project to real automotive scenarios.

Reviewer 3:

The team has been studying both Pd/SSZ and Pd/BEA. It concluded that the latter is less interesting due to more challenging degradation issues. The team has verified CO-induced deactivation of these materials and has been evaluating these materials to determine which Pd species are important. It is also trying to identify the "right" Pd species to have in the zeolite to ensure trapping and regeneration through multiple cycles. The team showed a variety of characterization data for ion-exchanged Pd²⁺ species in the starting catalyst. CO diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) suggests a wider variety of species exist during operation, including non-ion-exchanged species. Modeling suggests a Pd+H species as the key NO_x trap site. The team has shown the ability to make zeolites with different Al pairings such that they can maximize or minimize the distribution of certain Pd species. All of these contribute to a better understanding of the reaction chemistry and therefore making a working, passive NO_x adsorber. Convergence in the results as to what species to target for synthesis, and which are lost via deactivation, is not clear, however.

Reviewer 4:

The work done was described under technical accomplishments. However, "accomplishments against the targets/milestones" were not obvious, especially how all the work done and the outcome are tied to a specific objective. Below are some additional details:

Due to the nature of the project and multi-pronged approach taken, the technical information provided is exhaustive: however, it was difficult or not possible to connect all the technical pieces to see a big picture, especially how all of these are helping to come up with a potential solution. A slide that shows the walk/approach toward achieving the goal would have been useful.

A comprehensive approach was taken (multiple characterization techniques used, model and the catalysts that appear to be fully formulated, and performance, durability and modeling techniques). However, it is not obvious how all these insights gained from the above sites are driving to develop a new formulation. It appeared that a generic statement was made indicating paired Al sites will be prepared. However, there were no insights on whether such sites improve performance or durability, etc., or how the catalyst manufacturer and application OEM would be helped with taking steps that would not have been done without this project.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The project appears to be well coordinated, with participants from industry (OEM and catalyst supplier), academia, and the National Laboratories.

Reviewer 2:

This is an unquestionably a top-notch group of scientists who are well positioned to make progress in this area. The interaction is clear, given the wealth of data regarding catalysts synthesis, performance, and characterization. Some of the skill sets of researchers is duplicated (Bell and Gounder, in particular). Having a dedicated, theory PI also seems like a missed opportunity. Some of the team (involved with vehicle modeling effort) seems to have been underutilized to this point on the project.

Reviewer 3:

There is obvious collaboration within most of the team. The only missing evidence from the presentation was the role BASF plays. All other team members had obvious contributions.

Reviewer 4:

The contribution to technical work from the industry collaborators were not obvious. Are they just consultants?

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

Reviewer 1:

The future work is well planned and progresses logically, but there seems to be a lot planned in the next 5 months. As stated by the presenter, the work on regeneration seems of particular importance, as cyclic degradation is a critical barrier to practical implementation. It may make sense to incorporate this into a decision point.

Reviewer 2:

The planned studies seem appropriate. As discussed above, reserving the more applied tests until the end of the project seems a missed opportunity. Some of the practical aspects of testing may have permitted additional fundamental studies in a feedback loop, if more time were available.

Reviewer 3:

It appeared a generic statement was made indicating paired Al sites will be prepared, but there were no insights on whether such sites improve performance or durability, etc., and how they will help the catalyst manufacturer and application OEM in taking steps which they would have not done without this project.

Reviewer 4:

The focus on synthesizing the "right" Pd species is appropriate, but the challenge remains: the degradation and how to stop it. That aspect should be the primary goal ("development of a viable regeneration strategy"). Although finding a surrogate for Pd would be nice, there is an inherent assumption that the periodic table has been tried by the catalyst manufacturers (for this zeolite system) and Pd will remain as the best candidate. Thus, the focus should still remain on a regeneration strategy. What those regeneration strategies look like was not made clear.

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

Reviewer 1:

This project aims to reduce cold start emissions, which is directly relevant to the DOE mission.

Reviewer 2:

Work is relevant to address one of the key challenges—low-temperature NO_x control—which is a major bottleneck leading to expensive systems, more CO_2 emissions, etc.

Reviewer 3:

The reviewer commented absolutely. It is clear the team has carefully considered how the work fits into the greater context of VTO DOE goals. At this stage, it is less clear how the knowledge gained to date from the project has impacted industrial catalyst design from a metric-driven perspective.

Reviewer 4:

Passive NO_x adsorbers gained wide interest several years ago and remain interesting. These would alleviate cold-start issues and enable low-temperature combustion modes. But, the degradation of these systems remains the problem to overcome. A solution would be very impactful.

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

Reviewer 1:

All resources seem appropriate. All needed components to finish the project are in place, particularly the excellent industrial collaborations.

Reviewer 2:

The resources seem appropriate for the milestones over the project term.

Reviewer 3:

Among the collaborators, the resources needed for executing this project appear sufficient.

Reviewer 4:

Resources for this project appear to be sufficient.

Presentation Number: ace135 Presentation Title: Toward Predictive Nozzle Flow and Combustion Simulations for Compression Ignition Engines Principal Investigator: Gina Magnotti

(Argonne National Laboratory)

Presenter

Gina Magnotti, Argonne National Laboratory

Reviewer Sample Size

A total of two reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-20 - Presentation Number: ace135 Presentation Title: Toward Predictive Nozzle Flow and Combustion Simulations for Compression Ignition Engines Principal Investigator: Gina Magnotti (Argonne National Laboratory)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The reviewer noted a fundamentally-sound approach to develop simulations tools. This would be done by leveraging experimental data from various real-world application sources as well as the step sequence to achieve project goals from developing physics-based models to identify bottlenecks and ways to improve scalability of solvers and CFD codes.

Reviewer 2:

The project team addresses the barriers outlined by DOE and the several areas of engine combustion research needs by developing various sub-models, which are validated against data from the collaborators. The project will be improved if it is devoted to exploring the simpler, feasible, transferrable technologies for the engine combustion community.

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

Reviewer 1:

Solid progress has been made in this project as indicated by the healthy list of accomplishments summarized in the project review.

Reviewer 2:

Technical progress and accomplishment on this project continue to move the understanding at a good pace while this project has been ongoing for a long time. Over time, the project has focused on the development of various sub-models, which requires a very high-performance computational capability. Such sub-model complexities and high-performance computation need may be difficult for engineers to use those tools effectively and to transfer good knowledge to the engine community. These issues need to be addressed.

For the multiple injection study, the flame stabilization mechanism is important for low-temperature combustion through the level of premixed since a majority of flame under LTC will impinge on the wall due to the longer ignition delay and a significant amount of combustion recession may decrease combustion efficiency substantially. The difference in the effects of the cavitation flow versus transient flow on spray structure when the flow rate is highly fluctuating is not clear. This area needs more effort for scientific understanding, modeling, and technology. The reviewer believed that the project focuses on the simple, accessible, reliable, design tool development with a fast turnaround time.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer called the collaboration work between academia, the National Laboratories, and industry partners fantastic and w. ell done!

Reviewer 2:

The collaboration level seems to be good, and the PI collaborates with a lot of groups within Argonne National Laboratory (ANL), with the National Laboratories, university, industry, and a foreign national university. However, the reviewer had concerns that most work was done with specific software, CONVERGE, which has very limited flexibility and diversity. The reviewer also expressed concerns about the lack of educational transformation of technology to industry and academia while the academic participation is not as strong as the industry participation.

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

Reviewer 1:

The PIs have listed the remaining challenges and barriers as well as proposed future work with the desire to leverage expertise and resources from the partners but no concrete plans on the development pathways. The research nature of this work is understood.

Reviewer 2:

The reviewer realized that the project is in its final year according to the ACE135 presentation (starting in 2012 and ending in 2020). The future plan seems to be the extension of the current work with the production of a large amount of data and their comparison with CFD model. No specific sub-models to bridge the gap between experiment and CFD performances are suggested. The reviewer would have liked to see how to handle the large amount of experimental data together with simulation data and the method to reduce the computational time. The detailed future plan involves further improvements to their models, including the cavitation erosion model, flamelet model, and ignition model. The team has planned model validation and also plans further extending the models to different applications. The research plan is feasible, but it needs a lot of resources.

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

Reviewer 1:

The reviewer commented yes, this project supports the overall DOE objectives because it is aimed at addressing a major industry pain point or a need for a robust simulation tool to predict engine performance and emissions.

Reviewer 2:

The project is relevant to the DOE goals of the accuracy improvement and efficiency of the simulations. The reviewer indicated that the modeling capability is needed to address short simulation turn-around time.

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

Reviewer 1:

The project team has sufficient resources.

Reviewer 2:

The funding level has been consistent over the years for the duration that this project has been active.

Presentation Number: ace136 Presentation Title: Medium-Duty Diesel Combustion Principal Investigator: Stephen Busch (Sandia National Laboratories)

Presenter

Stephen Busch, Sandia National Laboratories

Reviewer Sample Size

A total of three reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-21 - Presentation Number: ace136 Presentation Title: Medium-Duty Diesel Combustion Principal Investigator: Stephen Busch (Sandia National Laboratories)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The approach of this project—to identify and address the sources of toxic emissions along with looking at cold-start emissions—is sound. The optical engine provides an excellent tool to investigate the in-cylinder details, and the metal engine should provide proper validation to the optical engine results. There is also a good mix of simulation and experiment to accelerate progress.

Reviewer 2:

Leveraging insights from experiments to develop and evaluate novel approaches to CFD spray modeling for the catalysts heating operation, as well as leveraging experiments and in-depth analyses to develop and test hypothesis for the piston bowl geometry study, are fundamentally sound approaches.

Reviewer 3:

The project scope identifies the research priorities for mixing-controlled compression ignition (MCCI) as the reduction of engine-out NO_x and reduction of cold-start emissions. Work highlights the study of spray-wall interactions and catalyst heating as pathways. The project is setting up a MD engine to validate the concurrent work on new bowl studies and CFD models to capture the catalyst heating physics. The project could benefit from a review of common approaches on SI/CI used in modern catalyst heating. Also, similar bowls have been considered in the past; the results from this work may prove too valuable in assessing the benefits/challenges associated with the new geometry proposed, increased surface areas, and disruption on the large-scale motions.

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

Reviewer 1:

This project has made some significant progress in the relatively short period of time that it has been running. The optical examination of late-cycle injection and the presence of HC in the piston bowl is insightful. The improvement in the modeling of this process is also good. The development of the dimple step-lipped (DSL) piston should be interesting as the project moves forward. The link to catalyst heating will be important to establish, since this is a major thrust of OEMs for a variety of reasons. It will be very important to link the detailed work with the overall performance of the engine from an efficiency and emissions point of view.

It would also be beneficial for this project to be included in Co-Optima (or its successor program) going forward. The experimental setup and work here would be subject to differences in fuel properties as well, which would be of significant mutual benefit to Co-Optima and this project.

Reviewer 2:

Limited progress was demonstrated for this reporting period and slow progress in the laboratory due to the COVID-19 pandemic was established as the root cause during the project review. It will be helpful to start putting some points on the board to establish some confidence that the project objectives will be achieved. For example, no results from the catalysts heating operation have yet been demonstrated at the mid-way point of this 3-year program.

Reviewer 3:

It appears that the program has experienced delays in meeting some of their key deliverables, with respect to the complete engine shakedown and pollutant emissions and catalyst heating work. It may be useful to describe the test space of injection strategies (work from 2019) and how this has been carried forward. No indication is provided regarding the chemistry in the catalyst. The strategy on the catalyst is a bit unclear. There is discussion of unburned hydrocarbon (UHC) reduction and their use for catalyst heating. What is the direction? There has been a lot of work from 2016 to 2020 on piston and injector imaging. Has any of this work been consolidated in specific models or laws that may be used across broader applications?

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

There was reasonable collaboration between the Sandia National Laboratories, Ford, and the Wisconsin Engine Research Consultants.

Reviewer 2:

Work by project partners is indicated throughout the presentation.

Reviewer 3:

The collaboration and coordination among project partners appear to be good. However, this project appears to be operating a bit in a vacuum with respect to other Advanced Combustion Engine (ACE) projects in the DOE portfolio. It would be helpful to seek some collaboration with other MD/HD MCCI projects that may lend some insight into issues facing this project.

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

Reviewer 1:

The future work appears appropriate—the metal engine is close to commissioning and this will be very important to validate the optical engine results. The influence of the (DSL piston upon efficiency and the subsequent impact upon emissions (particularly NO_x) will be critical for this project.

Reviewer 2:

The future work may be enhanced by tying the UHC, the heat release trace (experimental and simulation), and the catalysis heating. Will there be work dedicated to the catalyst chemistry?

Reviewer 3:

The sequence of experimental and analysis tasks outlined in the roadmap for both the catalyst heating operation and piston bowl geometry are reasonable, but enough progress has not yet been demonstrated to provide the confidence that the project objectives will be achieved by the end of the 3-year program. The lack of an engine control unit (ECU) that automatically compensates for the pressure waves in the rail is a concern that should be addressed. The researchers may also want to look at multiple pilot injections and multiple post injections.

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

Reviewer 1:

This project directly supports the DOE goal of examining opportunities for MCCI engine efficiency improvement and emissions reduction.

Reviewer 2:

Yes, this project supports the overall DOE objectives because it will help to improve our understanding of fuel injection, air motion, and combustion chamber geometry effects on combustion and pollution formation, which is a critical enabler for the development of fuel-efficient diesel engines that will comply with low emissions regulations.

Reviewer 3:

The overall work is relevant. Relevance could be improved with a better visibility with respect to engine-like conditions and catalyst engine in-and-out emissions analysis. Hopefully, this will be the case as the engine comes online.

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

Reviewer 1:

It appears that the resources are sufficient for the project goals and timeline.

Reviewer 2:

The reviewer affirmed resources appear adequate.

Reviewer 3:

The reviewer was not sure how much of the budget for this 3-year program is left ,but the limited progress demonstrated at the mid-way point albeit due to extenuating circumstances with the COVID-19 pandemic left the reviewer with the impression that sufficient funds should still be left.

Presentation Number: ace138 Presentation Title: Partnership for Advanced Combustion Engines (PACE) - A Light-Duty National Laboratory Combustion Consortium Principal Investigator: Paul Miles (Sandia National Laboratories)

Presenter

Paul Miles, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-22 - Presentation Number: ace138 Presentation Title: Partnership for Advanced Combustion Engines (PACE) - A Light-Duty National Laboratory Combustion Consortium Principal Investigator: Paul Miles (Sandia National Laboratories)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

Kudos to the Partnership for Advanced Combustion Engines (PACE) Leadership Team on organizing such a broad spectrum of research and keeping it focused on barriers relevant to high- volume LD combustion. The presentation was well structured. The reviewer really liked the structure of the PACE presentations focusing on a PACE deliverable by a team leader rather than by National Laboratory. This clearly shows the collaborative nature of the new Partnership.

Reviewer 2:

The approach is well designed to meet objectives. It is organized into relevant categories and tasks that are measurable and that lend themselves to effective management. A key part of the approach is the utilization of DOE's world-class high-performance computing to reduce engine design cycle times.

Reviewer 3:

The PACE umbrella is focused on important topics that are relevant to industry. The collaboration between labs all working toward critical goals is an improvement compared to past projects where labs worked independently. The project addresses current barriers to accurate engine simulation.

Reviewer 4:

The approach to this project is excellent. The reviewer had long thought that a more coordinated effort among the various National Laboratories was needed, and this project addresses that. The project is very well focused

on three overarching goals. The project has a well thought out work plan with important milestones and success measures documented. The reviewer believed the project is feasible, but it will be very challenging to meet all of the goals and milestones laid out. This is the only reason the reviewer gave this an "Excellent" score and not an "Outstanding" score.

Reviewer 5:

On paper, the program looks good. It is an early effort, however, so the proof will be clearer once the program has progressed forward. The reviewer commented that it is good to see "open source" sub-functions as primary simulation deliverables. Delivering a usable, open-source product to OEMs is a key target. Moving forward, it will be important to show uptake by end-users, so the reviewer suggested considering implementing technology transfer metrics into the program to track adoption of the sub-models being developed.

If the high performance computing (HPC) is being used as benchmark for simulation, it will need to be very clear on how accuracy of the HPC simulations are evaluated. These will need to be validated against experiments and, if they are being used as a reference, it will be critical to evaluate whether they are delivering results that are real.

The reviewer would have liked to see greater detail on how specifically machine learning is being applied to increase speed. Machine learning can be a trendy buzzword, so specificity on how this is improving program delivery is important. In future AMRs, the reviewer would like to see clear, concrete results on how machine learning has benefited this program.

Many of the individual projects appear to be efforts that have been in-flight for multiple years now in a different guise, and these projects need to be brought together in a very cohesive form. Also, for projects that have been in-flight for a while, why have these not been picked up by OEMs already? Are the technologies still relevant? Moving forward, there will need to be a close connection to, support from, and endorsement by engine manufacturers that technologies being developed are of interest and have the potential to be commercially viable. Especially for novel combustion programs, such as Major Outcomes 5 and 7 on Slide 14, PACE should look to "dual-use" developments, which have greater crossover with conventional gasoline and diesel applications for higher utility in case OEMs do not adopt a specific concept. Also, the project team needs to include robust, actual decisions with consequences and Go/No-Go decisions to ensure efforts are moving forward.

While recognizing that the move to a single engine platform may increase the speed to deliver modeling advancements, this reviewer was concerned that limiting to one engine design will impact the ability to deliver model validation. Improved, validated, modeling tools should be engine-agnostic and validated across a range of different engine platforms. The project team needs to be clear on how the new format—grouping all labs/programs under a common umbrella—will deliver improved performance and results to the automotive companies on such a spread array of topics. Consider focusing on fewer, but higher impact, topics, which might be a better utilization of lab resources. The reviewer would like to see key identification of barriers and connection for each program, including both a clear opportunity statement and vision of success. What are the key limitations and barriers to progressing the technology to market, and how are these being addressed?

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

Reviewer 1:

The program is about 25% complete, which is on target given the start and end dates. With such a large program, it can be difficult to keep the goals in focus. This overview did a nice job laying out goals and milestones, and the reviewer hoped they are maintained (and completed) throughout the program.

Reviewer 2:

Even early on in the program, there have been notable collaborations. For example, the development of a new gasoline fuel surrogate demonstrated successful collaboration between multiple National Laboratories, and this hopefully indicates how well the PACE collaborative approach will work.

Reviewer 3:

Since PACE is quite young, the expectations for technical accomplishments are low. Focusing on the definition, formulation, and validation of a common surrogate fuel is a great first step. Also, it is good to see there is some effort to identify a common engine architecture.

Reviewer 4:

Developing a surrogate for gasoline has proceeded at a fast pace and results are already available. Prediction of knock has also made good progress.

Reviewer 5:

The reviewer recognized that this is a very early phase effort starting in in the fall of 2019. This specific presentation focuses on the high-level and administration effort, but the overall effort has not seen significant progress beyond planning. Accordingly, judgment of overall accomplishments and progress will likely need to be withheld until 2021. Most project milestones are phased toward the end of the year, either quarter (Q) 3 or Q4. These are generally "on track," but this is not particularly informative given the time remaining. Moving forward, the reviewer would like to see more project milestones that are more specific and represent significant progress. Shift away from readily achievable, but meaningless, process milestones toward those delivering answers to specific obstacles, barriers, or steps along the research pathway.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The collaboration and coordination in this project are outstanding. One of the main strengths of this program is the multi-National Laboratory leadership and execution. The strengths of the various National Laboratories and groups are leveraged, but toward a few common, focused goals. This helps avoid redundancy among the National Laboratories and significantly increases the chance of success of this program.

Reviewer 2:

There are six National Laboratories being coordinated effectively to collaborate with no duplication and instead complement and supplement each other. The input from the U.S. DRIVE ACEC Technical (tech) team, which represents the needs of the light-duty OEMs, has been received very well and the program has been designed to meet ACEC priorities.

Reviewer 3:

The fuel surrogate development shows great collaboration between National Laboratories.

Reviewer 4:

There is clear evidence of collaboration in this new Partnership. It is much better organized than past, somewhat isolated research efforts. The reviewer really liked the structure of the presentations. Being focused on the deliverables rather than by PI or National Laboratory provides assurances that goals will be achieved. The reviewer was glad to see the CFD vendors being part of the Partnership. With regards to cold-start emissions, the reviewer would have liked to see more information on how PACE will collaborate with aftertreatment research teams.

Reviewer 5:

There is a clear and significant focus on working together, but it is not clear how well the projects are truly linked behind the scenes. They appear to be a standalone set of projects, with primarily alignment in high-level purpose, platform, and fuels. The reviewer would like more detail on the program's external connections

beyond the U.S. DRIVE ACEC and Advanced Engine Combustion (AEC) Memorandum of Understanding (MOU). These are not well detailed and simply stated as "numerous." The reviewer would appreciate highlighting organizations and explain how these form a cohesive connection to the task and purpose of the program, and how the output of this program sees uptake by customer organizations. It may also be useful to the program for a method to solicit active review and directional input outside of AMR and ACEC review meetings. For example, the Co-Optima program has stakeholder engagement and oversight boards.

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

Reviewer 1:

The reviewer looked forward to results of the Partnership.

Reviewer 2:

The future plans were not discussed extensively in the presentation. Questions remain as to how some of the barriers will be addressed.

Reviewer 3:

The overall goals and targets of the program are laid out well, but there is not necessarily a coherent work plan provided in this summary. Several of the thrust areas, the major outcomes, are not overly specific as to what final success looks like: for example, Major Outcomes 3-8. More clarity is necessary in these areas to define a quantifiable result state, which could be considered success. This is especially important for projects that have been in-flight for a number of years already. Lack of a defined target and focus on "improvement" is a recipe for an evergreen program.

Reviewer 4:

The use of artificial intelligence (AI) and machine learning (ML) should be handled carefully. Lots of precious time can be wasted in perfecting a ML model with little or no understanding at the end. PACE should develop sub-models to encapsulate physical understanding. Oftentimes, these sub-models can be very expensive with high run times. Machine learning should be used to handle the turnaround time and leave the physics for the sub-models.

The partnership with the software companies should be effectively managed to put all the knowledge and understanding gained from the program into the hands of OEM engine designers in a platform that they can use and afford.

Reviewer 5:

In the oral presentation, the speaker described future models coming from this program as "user ready" and "plug 'n play." The reviewer would urge the group to spend some time scoping out this part of the program. It sounds relatively easy, but in practice this can be very difficult. Also, the reviewer realized that there are many other presentations covering PACE in the merit review; however, the reviewer still would have liked to see some additional information on the codes that will be used for the direct numerical simulations (DNS). Why are these codes needed if the ultimate goal is to get the models into commercial codes used by the OEMs?

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

Reviewer 1:

There is a clear connection to DOE Vehicle Technologies Office's objective to improve vehicle energy efficiency and emissions. Sub-programs address an array of topics supporting technology development to understand and address topic areas relevant to increased engine efficiency. Simulation tool development can aid automotive manufacturers by enhancing their tools for developing new technologies to increase engine efficiency and improve emissions.

Reviewer 2:

The reviewer commented yes, this project supports the overall DOE objectives. One of the four R&D Focus Areas of the EERE VTO is Advanced Combustion Systems and Fuels with a 35% fuel efficiency improvement target. This project very clearly supports that mission.

Reviewer 3:

This program is highly relevant to the light-duty OEMs. Light-duty internal combustion (IC) engines will be in the market for many decades to come. Achieving emissions, efficiency, and goals for engines is a key part of reducing national CO_2 and meeting clean air goals. Distributing the effort in the three areas of knock and low speed pre-ignition (LSPI), dilute gasoline combustion, and cold-start emissions is right on the mark in meeting the highest priority areas for the light-duty OEMs.

Reviewer 4:

The work is expected to lead to improved engine simulation tools that will help manufacturers improve engine efficiency and reduce energy consumption.

Reviewer 5:

Improved understanding and computer-aided engineering (CAE) tools will directly enable OEMS to produce more efficient and cleaner ICE.

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

Reviewer 1:

The tasks laid out for the PACE project are very daunting and it is likely that more resources will be required to meet the goals. In addition, sooner results would help industry, which also requires more resources.

Reviewer 2:

The reviewer believed that the resources are sufficient. It is a significant amount of funding; however, there is a substantial amount of work under this program. If the goals are met, it will have been well worth it.

Reviewer 3:

Resources are generally sufficient. It is critical that the efforts to provide a common engine platform (single, optical, and multi) to all the participating National Laboratories has prompt and sufficient funding.

Reviewer 4:

The reviewer commented sufficient.

Reviewer 5:

Overall funding of \$9 million per year covers a wide breadth of projects. Looking at specific budgets, however, there is a wide range of project funding levels and individual sub-project splits across different PIs. There is little explanation for the disparity between funding levels, and why certain efforts require more funding, in some cases significantly more, than others. Additionally, given that projects are at varied progression, with some new efforts and others appearing to be minor variations on projects that have been running for a long time, more clarity on how effort and funding are determined would be useful.

Presentation Number: ace139 Presentation Title: Development of an Optimized Gasoline Surrogate Formulation for PACE Experiments and Simulations Principal Investigator: Scott Wagnon (Lawrence Livermore National Laboratory)

Presenter

Scott Wagnon, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-23 - Presentation Number: ace139 Presentation Title: Development of an Optimized Gasoline Surrogate Formulation for PACE Experiments and Simulations Principal Investigator: Scott Wagnon (Lawrence Livermore National Laboratory)

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

Reviewer 1:

The reviewer called this a fantastic approach and really liked the quick organization of a surrogate working group to develop a common fuel for PACE. How does RD5-87 fuel compare to pump grade 10% ethanol content gasoline (E10)? The reviewer suggested maybe getting a fuel specification from one of the OEM research fuel suppliers.

Reviewer 2:

The multi-variable optimization approach provides a good means to generate fuel surrogates, especially if the model can run on massively parallel architectures. It appears that the optimizer adjusts the mass fractions of pre-selected species. Are there any plans in the future to allow the optimizer to choose both the species and mass fractions?

Reviewer 3:

It appears to the reviewer that this is a well-designed project to holistically develop gasoline surrogates that match knock metrics: research octane number (RON)/motor octane number (MON), particulate matter index (PMI), distillation curve, auto-ignition timing, heat release, etc. It covers mechanism development for fuel combustion and pollutant formation, validation, as well as model reduction. However, it is not very clear what the final outcome of the project is. In addition to better developed surrogates, will this project develop a tool

that facilities OEMs or other researchers developing a mechanism/surrogate that matches the desired fuel properties mentioned above?

Reviewer 4:

The reviewer would suggest looking at the boosted CFR engine work of ANL's Chris Kolodziej, who has done a considerable amount of work on knock in boosted conditions with respect to fuel properties. Maybe consider having him evaluate some of the surrogates since RON and MON can be difficult to model if high percentages of aromatics or olefins or both react nonlinearly (sometimes) if they are present in the surrogate in large quantities and they are in the presence of ethanol. The knocking potential also changes differently with boost and fuel composition. To confound things more, knock and ignition delay (from a rapid compression machine [RCM]) are considerably different. An RCM is designed to take out as many physical effects as possible to measure the chemical effects of ignition delay. There are physical phenomena that are affecting the end gases in an engine that are not present in an RCM, such as the pressure wave from the flame front, heat transfer, and bulk fluid motion. This can be characterized in the CFR engine (which is designed to withstand knocking events) and may help with the correlation between the RCM and the metal engine.

Reviewer 5:

This is a solid approach to a central element bridging the experimental measurements and simulations that are a key output of the program. The use of a large sub-team to gather appropriate expertise is laudable. The optimizer appears to have been a very powerful tool to enhance the speed of the effort.

With surrogates, the key questions always are how representative a reduced set of components are to mimic operation of the target fuel. Given that, this reviewer had concerns with the assumption that tetralin can be added to match PMI and account for the high boiling range components otherwise not included in the surrogate. Tetralin can have a strong impact on particular behaviors, such as PM emissions and LSPI, and may not be fully representative of the heavy-end components. It will be important moving forward to compare tetralin against potential other components for extending the boiling range and matching PMI to understand if effects found are truly representative of matched fuel properties or if tetralin is having an overwhelming impact on results. In the presentation, it is unclear what specific projects are under this effort, as opposed to merely related works.

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

Reviewer 1:

The team has a thorough approach of validating surrogates and kinetics with distillation, flame speed, and auto-ignition measurements. Furthermore, will the optimization tool be available as open source?

Reviewer 2:

The reviewer affirmed the project team is making great progress on matching the relevant fuel characteristics.

Reviewer 3:

The project made good progress, accomplished about 25% of this 4-year program, observed some delays but understandable due to the current pandemic situation. The team developed new measurements and kinetic models and delivered reduced kinetic model for cold-start simulations. An initial shared surrogate fuel was defined, verified, and tested in research engine tests.

Reviewer 4:

The reviewer indicated that the computational efforts in developing surrogates are unique and impressive. The reviewer did however, question the extent of the validation efforts. RON and MON are fairly complex and do not always match well with engine and RCM data. RCMs have a low-intake air charge motion in the combustion chamber and engines have different end-gas conditions, so using a CFR engine to validate RON and MON should be done. Also, RCMs are CI in nature (and attempting to measure chemical effects) and

knock occurs in forced combustion (SI) where conditions are not the same as an RCM. That being said, if there were a way to give this a 3.9 instead of a 3.5, the reviewer would.

Reviewer 5:

Overall, this is a strong first-year effort, delivering a recommended surrogate fuel and evaluating across a range of platforms to understand and validate performance against the target fuel.

Performance was documented across a range of platforms, with shortcomings of the proposed surrogate fuel identified. This reviewer did take issue with the idea that behaviors are "well validated," because that term usually implies very closely matched performance. Across the different platforms, different shortcomings were identified as were aspects where surrogate fuel and target fuel performance deviated, in some cases significantly. This does not square with the phrase "well validated."

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It is impressive that there is cooperation across four National Laboratories.

Reviewer 2:

PACE structure is clearly showing improved collaboration versus past efforts. The reviewer really liked the goal-oriented approach (focus on deliverables).

Reviewer 3:

The team from Lawrence Livermore National Laboratory (LLNL) is engaged across National Laboratories to validate against experiments and link with CFD simulations.

Reviewer 4:

Good collaboration across a range of National Laboratories to support this effort. The cross-laboratory subteam stood up to help develop and test a new surrogate fuel for the project. Fuel was tested across a range of different engine platforms, leveraging experimental facilities across different National Laboratories.

Reviewer 5:

The reviewer found strong collaboration with National Laboratories, along with a few universities. The PIs should strengthen collaborations with OEMs.

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

Reviewer 1:

Generally speaking, the future research is well planned. As researchers are exploring new gasoline combustion modes, the reviewer hoped a tool can be developed and publicly shared to generate surrogates at the end of this project.

Reviewer 2:

With surrogate mixture design for the PACE effort nearing completion, there should be a declining need for a similar effort moving forward. Understanding properties and developing kinetic models for use in simulations is a prudent next step. The nature of the work in this project may lead to an activity that drives on in perpetuity. Given the need for simulation efforts and experimental work to link together, there will reach a point where development needs to be frozen to allow the other efforts, central to the PACE program, to move ahead.

Reviewer 3:

The reviewer remarked that the team should continue to pursue changes to get better soot match at high catalyst heating conditions.

Reviewer 4:

Getting an agreement between the RCM and one engine does not validate the surrogate. It is promising that the surrogate agrees with the ORNL engine and RCM data, but validation in a couple of broadly different engine platforms will show how well the surrogate performs.

Reviewer 5:

It is unclear from the presentation material if there are unique experiments that are needed to validate surrogates and mechanisms specific to each of the objectives outlined in Slide 4. Do the National Laboratories have the capability to provide relevant experimental validation measurements, especially for cold start?

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

Reviewer 1:

This work is absolutely relevant to DOE objectives. Motor gasoline accounts for 45% of the crude consumed in the United States. Advancing gasoline engine technologies will continue to play a key role in reducing GHG emissions. Fuel surrogates and mechanisms are crucial to the success of future engine development.

Reviewer 2:

Common surrogate gasolines for all PACE work are critical.

Reviewer 3:

Developing validated surrogates and kinetic mechanisms that each of the National Laboratories can share is vital to the PACE program goals.

Reviewer 4:

This project fits the overall DOE objectives of the PACE group. This project will go a long way to enabling the modeling portion of PACE to interface with the fuel spray and combustion portion of PACE.

Reviewer 5:

The overall PACE effort supports the DOE objective to increase vehicle fuel economy and reduce emissions through development of modeling tools for automotive manufacturers. Surrogate fuels are an important link between experiments and CFD models.

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

Reviewer 1:

The team has sufficient resources.

Reviewer 2:

Sufficient, the PI did not indicate research is hampered by lack of resources.

Reviewer 3:

The project could use testing in a CFR engine to understand how the surrogate performs under knocking conditions, allowing for a better prediction of knock. The leap from RCM to full metal engine is pretty large, and an effort should be made to compare the surrogate in several engines. Overall, this a really well-run project.

Reviewer 4:

Overall, the team has most resources to conduct the relevant research—RCM, engine, modeling tools, etc. However, additional experiments should be conducted for model validation, such as flame speed and ignition delay (ID) at higher temperature.

Reviewer 5:

There is not great clarity within the presentation on the scale of activities being funded under this effort. Funding expands moving forward though the key deliverable, a surrogate formulation, is well on its way to completion. It is not clear why the future work for the program requires the sharp increase in funding. Presentation Number: ace140 Presentation Title: Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations Principal Investigator: Russell Whitesides (Lawrence Livermore National Laboratory)

Presenter

Russell Whitesides, Lawrence Livermore National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-24 - Presentation Number: ace140 Presentation Title: Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations Principal Investigator: Russell Whitesides (Lawrence Livermore National Laboratory)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

Using supercomputers helps provide a benchmark against which engineering-level simulation tools can be compared, so this project is very useful. In addition, the use of supercomputers to develop faster simulations helps the speed of engineering simulations. The goals of this project are well aligned to the overall goals of the PACE umbrella.

Reviewer 2:

This presentation reviewed three separate tasks. Overall, the approach to each task is sound and well planned. A minor concern is the handling of the challenges associated with the third task (mechanism reduction). Effort is needed to generate a more coherent plan to identify other possible solutions, r to establish that a suitable mechanism reduction may not be possible. The reviewer provided further comments in the Technical Accomplishments and Progress section.

Reviewer 3:

The use of a neural network to choose the integrator on the fly is a very interesting technique. Please provide information about the integrators in Slide 7. Also, please compare the approach in this project to the Hybrid model of Professor Hai Wang at Stanford University.

Reviewer 4:

The project directly addresses a major technical barrier to enhanced-fidelity engine simulations – the computational cost of reaction kinetics in CFD codes. The use of a neural network to choose the most appropriate integrator to use at each condition is a creative solution to provide another step in computational cost reduction. The challenges in applying the zero-order reaction kinetics combustion software package (Zero-RK) to new platforms are disappointing, but hopefully will lead to new understanding that enhances the ability to deploy these routines. Automated mechanism reduction routines, targeting both kinetic performance and a range of other key properties, are another way this project can directly address technical barriers.

Reviewer 5:

Chemistry calculation is always the time-consuming part of engine simulations, so its acceleration is definitely very important. Using machine learning or smartly reducing the mechanism to a much smaller size is the appropriate approach. The reviewer agreed with the approach to explore the potential of using supercomputer for such a study. One potential concern is about the detailed chemistry. Are we at the stage of truly trusting the accuracy of it due to the many uncertainties for so many reactions?

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

Reviewer 1:

It appeared to the reviewer that progress is on track. The PI has shown the progress of using a neural network (NN) to accelerate the chemistry and potentially exploring chemical states.

Reviewer 2:

Significant progress has been demonstrated in multiple areas, including the neural-network integrator selector, and the automatic reduction of mechanisms. The knowledge from this progress is already driving key insights; for instance, kinetic mechanisms for high-fidelity CFD will remain sizeable (300- 1,000 species) despite reduction, in order to maintain accuracy across a range of conditions.

Reviewer 3:

The continued speed-up of simulation time is impressive and will be needed for accurate engineering simulations to be useful.

Reviewer 4:

The progress on the neural network task is excellent. A minor suggestion would be to show additional validation results for more complex fuels and geometries. Such an effort would go a long way to convince potential users of the suitability of this approach. The graphics processing unit (GPU) supercomputer transitioning is behind schedule, but for reasons outside of the control of the project team – namely, the COVID-19 pandemic and an issue with the GPU hardware. The team is pursuing alternate solutions, and thus this effort should be expected to be back on track soon.

Most concerning are the accomplishments and progress with regards to the mechanism reduction effort. As noted by the presenter, most of the errors in the reduced mechanism with regard to ignition delay occur precisely in the region that is critical for SI engines. (Could this possibly be because reactions critical for low-temperature chemistry are being removed in the reduction?) More needs to be done to resolve this problem, especially if other efforts are to use this reduced mechanism. Finally, it would be very prudent to explore and show how other critical properties such as flame speed perform in the reduced mechanism.

Reviewer 5:

Please provide some information about the RD5-87 surrogate. The collaboration with Convergent Science is very good since it will improve a software package that is available to industry. Please explain how this project will improve the CONVERGE software that is available to industry.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Overall, these three tasks are well coordinated and collaboration among the team appears to be good. The engagement with outside entities is excellent and will ensure that industry can readily benefit from this work.

Reviewer 2:

The collaborations encompassed by the project, between LLNL, ANL, and GM, will push the boundaries of high-fidelity engine CFD through reduced computational costs, which allow the use of more accurate models. Other key applications, such as mechanism reduction, will be used widely by PACE and Co-Optima.

Reviewer 3:

It is good to see collaboration that includes Convergent Science because this is key to deploying your new techniques to industry.

Reviewer 4:

The PI is working with the right teams, Convergent Science has the most popular engine CFD software, and GM brings the industry technical inputs. The team also works with other team, to implement the methodology to other DOE-sponsored codes.

Reviewer 5:

Please provide information about the role of each collaborator (e.g., ANL, Goldsborough, and rapid compression machine experiment).

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

Reviewer 1:

The future work was not discussed in significant detail, but overall the planned work is in the appropriate direction. It would be helpful to have had a coherent plan, including backup and risk mitigation plans for each task. This is especially relevant for the mechanism reduction effort. Some minor suggestions with regards to this are to evaluate the potential of reducing the optimization region, or to show how alternate approaches perform to establish that the proposed method is the "best possible" one.

Reviewer 2:

Thank you for focusing future work on finding solutions to Summit problems. Please state decision points. The Reinforcement learning based mechanism reduction is very interesting.

Reviewer 3:

All the future planned work is relevant and interesting. If resources allow, the team might also consider soot (polycyclic aromatic hydrocarbon [PAH]) related species into their kinetic model. Emission modeling is more demanding than ever.

Reviewer 4:

Slide 18 shows that accelerated solvers have eliminated the chemistry bottleneck in combustion CFD calculations. Can any of the project team's acceleration techniques be applied to other areas of the simulation to speed those up as well?

Reviewer 5:

Enabling additional computational cost reductions through improved handling of species transport will further address technical barriers. It would be nice to see greater plans to share and put to use the automated mechanism reduction routines, so that researchers with less experience in numerics could put this work to use.
Question 5: Relevance—Does this project support the overall DOE objectives? Why or why not?

Reviewer 1:

This project supports DOE's overall objectives. Most notably, it will result in a rapid deployment of improved simulation techniques to industry to help improve the efficiency and reduce the emissions of future engines.

Reviewer 2:

The reviewer remarked that it is a very important topic. The project can answer what the best chemistry methodology is in engine simulations.

Reviewer 3:

Knock prediction is relevant to industry and the DOE. Collaboration with an industrial partner (GM in this case) supports the DOE objectives.

Reviewer 4:

Improved chemistry calculation speed makes robust simulations available to engine designers working on the next generation of IC engines and should contribute to DOE's goal of reduced energy consumption.

Reviewer 5:

Fast and accurate kinetics are an enabler for high-fidelity CFD - a primary objective of the PACE project. Computational cost is high for accurate kinetics – efforts to lower this cost will enhance the regimes to which CFD can be practically applied.

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

Reviewer 1:

This project significantly contributes to overall PACE goals of improving engine CFD fidelity and should not see a reduction in budget.

Reviewer 2:

The resources are sufficient for the various tasks to succeed.

Reviewer 3:

The resources appear to be sufficient in the sense that the scope of the future work addresses the issues.

Reviewer 4:

The reviewer stated that resources are sufficient.

Reviewer 5:

The pandemic might delay the progress, but overall resources seem reasonable.

Presentation Number: ace141 Presentation Title: Advanced Ignition System Fundamentals Principal Investigator: Isaac Ekoto (Sandia National Laboratories)

Presenter

Isaac Ekoto, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-25 - Presentation Number: ace141 Presentation Title: Advanced Ignition System Fundamentals Principal Investigator: Isaac Ekoto (Sandia National Laboratories)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The PI and collaborators are using a good approach to overcome the barriers in understanding and predicting ignition phenomena in engines.

Reviewer 2:

The approach to the project is well designed: performing detailed measurements of the phenomena occurring during ignition for different ignition systems under different conditions, then coupling this with advanced simulation approaches to maximize the progress and learning.

Reviewer 3:

The modeling effort to replicate spark and corona ignition is excellent. There are different theories on how jet ignition works. If the nozzle quenches the combustion, radicals will ignite the fuel air mixture. This is significantly different than spark or corona ignition. This effort is needed to understand the mechanisms this ignition process uses.

Reviewer 4:

The reviewer suggested continuing to pursue stoichiometric dilute combustion versus lean. Is there a point in the research where you can narrow the options to one ignitor path? Can you focus more resources on that single path (i.e., go deep on one idea or try to touch on multiple different methods but do not go so deep)?

The project tends to go very deep into the physics. While this work is very impressive, more basic measurements of the ignition energy, both primary and secondary, should be made and reported.

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

Reviewer 1:

The reviewer affirmed the technical accomplishments are excellent.

Reviewer 2:

The modeling of the spark and corona ignition was excellent, and the design and development of the crossflow ignition test facility that reproduces relevant in-cylinder densities (30 gram [g]/L) and velocities (30 meters/second [m/s]) are impressive.

Reviewer 3:

The reviewer was impressed by project outcomes when considering the limited funding it relies on.

Reviewer 4:

The reviewer found great progress, considering that the project started in Q3 of 2019.

Reviewer 5:

So far, results that can be used by industry in extending the EGR tolerance of stoichiometric gasoline combustion have not been met.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Collaboration is excellent. The reviewer was pleased that USCAR was engaged in accessing research priorities.

Reviewer 2:

There was excellent collaboration between experimentalists and modelers.

Reviewer 3:

The extent of collaboration and coordination across the team is very good and supported by results despite the current (difficult) environment.

Reviewer 4:

The new PACE structure clearly improves collaboration and allows focus on barriers.

Reviewer 5:

The reviewer commented that perhaps more collaboration with conventional ignition system suppliers is required to keep the project at a practical level.

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

Reviewer 1:

The proposed future work is in line with project goals and milestones.

The question raised regarding comparing the results between these new ignition systems and current ignition systems with equal energy input raised an important point. In the reviewer's opinion, this should be integrated into future plans.

Also, the reviewer thought that an emphasis on EGR tolerance at stoichiometric conditions should also take a more prominent role in future work. Pursuing ultra-lean combustion has the potential for yielding higher efficiency so it is important. However, the reviewer's impression is that industry is not eager to pursue lean burn systems because of the increased cost of the aftertreatment systems, especially in light of the investments they are making relative to electrification. In the near term, the reviewer guessed that industry will be more interested in extending EGR tolerance at stoichiometric conditions than pushing lean limits.

Reviewer 3:

The reviewer was looking forward to active pre-chamber research. Are catalyst heating conditions sufficiently represented in the future plans?

Reviewer 4:

Predictive ignition modeling serves multiple purposes in PACE by allowing for prioritization needed, depending on the current state of the art and the available test time. Pre-chamber (PC) or low-temperature plasma (LTP) igniters are likely to remain at the engineering level in the next several years. High turbulence, pressures/temperatures, and convective flows are challenging to mimic in combustion vessels and should be explored. How do we leverage current understanding for electrode wear?

Reviewer 5:

The focus should be significantly more on extending EGR tolerance than on lean limit extension. Also, investigations on advanced compression ignition (ACI) combustion modes should be included in Co-Optima reports and not on PACE reviews. More work on pre-chamber ignition and high-load ignition should be conducted as these are important to the OEMs.

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

Reviewer 1:

The high-energy ignition systems look to be an enabling technology for advanced SI and mixed-mode engines. This will be important to DOE's mission as ICEs will be part of the vehicle mix for decades to come.

Reviewer 2:

Advanced igniters and understanding the ignition source contribution to cyclic variability will improve both dilute combustion and catalyst heating mode operation.

Reviewer 3:

Understanding and controlling ignition is a prerequisite for better efficiency and emissions in advanced combustion strategies.

Reviewer 4:

The close coordination between PACE and U.S. DRIVE and USCAR makes DOE relevance essentially by default.

Reviewer 5:

While the project is highly relevant to DOE and OEM objectives, the approach and focus can be modified to have more impact.

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

Reviewer 1:

The resources look to be sufficient for the research being conducted.

Reviewer 2:

Funding should support post-doctoral staff to help accelerate and possibly improve the project outcomes.

Reviewer 3:

The reviewer commented sufficient. The PI did not indicate additional resources would improve the outcome.

Reviewer 4:

There was no indication that funding was insufficient.

Reviewer 5:

Resources are sufficient but need to be channeled to higher probability of impact areas as mentioned above.

Presentation Number: ace142 Presentation Title: Development and Validation of Simulation Tools for Advanced Ignition Systems Principal Investigator: Riccardo Scarcelli (Argonne National Laboratory)

Presenter

Riccardo Scarcelli, Argonne National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-26 - Presentation Number: ace142 Presentation Title: Development and Validation of Simulation Tools for Advanced Ignition Systems Principal Investigator: Riccardo Scarcelli (Argonne National Laboratory)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The presentation nicely outlines current challenges with the predictive ignition model. It presents how the current project is working toward overcoming the barriers.

Reviewer 2:

The hybrid experimental-numerical approach to providing insight into ignition system processes, which can be leveraged to create sub-models for CFD, is well founded and addresses a notable technical barrier to CFD applications for SI engines.

Reviewer 3:

This work is developing and adapting models for advanced ignition systems, addressing key technical barriers that could result in improved ignition systems for internal combustion engines. Overall, it is very well designed and planned. The investigators clearly have a very good understanding of all processes involved in advanced ignition.

A minor concern from this reviewer is that cyclic variability and its potential impact on the modeling and assessment of these advanced ignition systems is not at all included in the work plan. Given the extent to which cyclic variability and stochastic processes can impact early flame kernel growth, in the opinion of this reviewer it would be prudent to include variability in the initial and boundary conditions somehow in the work plan, or somehow otherwise look at cyclic variability.

Is there an effort to quantify stochastic inputs for the models (e.g., voltage, current)?

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

Reviewer 1:

The progress is slightly delayed, and the exact reasons for the delay were not made clear. Nonetheless, the accomplishments to date are impressive.

Reviewer 2:

The team showed several validation examples with fundamental measurements. For the machine learning analysis, how many DNS simulations were run to generate the results? How are these results going to improve the discrepancy in lean burn, flame kernel development shown in Slide 11? Does the team believe the ignition models already have enough fidelity to cover high load and cold start? It would be clearer if the team links the validation work shown in Slides 8-16 back to the specific PACE outcomes on Slide 4.

Reviewer 3:

The accomplishments are nicely summarized, although it is unclear if the project relies on existing software tools—VizGlow and VizSpark—or if the focus is rather on model implementation using currently available commercial CFD software like CONVERGE.

Reviewer 4:

The demonstrated progress in advancing spark ignition models (C.02.04) highlights the important work being done under this program and would receive a rank of "Excellent" if ranked alone. Why are the Sandia DNS simulations (C.02.01) performed using Jet A rather than a gasoline surrogate? Further, why are the accomplishments shown here based on aircraft-engine applications, rather than automotive engine applications? The Sandia DNS results do not seem aligned with the rest of the PACE program, its automotive focus, and its standardized use of RD5-87 gasoline. This task would receive a ranking of "Fair" if ranked alone.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The ANL collaboration with the University of Perugia and Tenneco is a great example of working with partners to make advances in areas of new technologies such as plasma ignitors. Collaborations between the Sandia National Laboratories (SNL) DNS work and the NREL ML work represent an effective transfer of knowledge between National Laboratory partners. Collaborations between Ekoto's experimental work and Scarcelli's modeling work have consistently yielded insights into the fundamental processes underlying advanced ignition systems, as well as practical constraints of these systems and influences of key parameters, such as system geometry, gas composition, and electro-dynamics.

Reviewer 2:

The team has shown collaboration with industry, academia, and other National Laboratories. The team is also leveraging other DOE programs to advance results.

Reviewer 3:

This work is well connected and coordinated with other experimental and modeling efforts within PACE, as well as with external collaborators.

Reviewer 4:

It looks like the project is well organized to leverage experimental data and simulation capabilities (DNS and large eddy simulation [LES]).

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

Reviewer 1:

The focus of C.02.04 on modeling of sparks rather than LTP is a prudent choice. The initial lean/dilute focus is also a good choice that will have the most immediate impact.

Reviewer 2:

While the proposed future work is appropriate and well planned, it would be beneficial to outline a plan for how this work can ultimately get to the point that industry could use or benefit from it and communicate this clearly.

Reviewer 3:

Why are cold-start and high-load targeted as later priorities over lean/dilute combustion? Adjusting these priorities would lead to more benefit to industry in the near term.

Reviewer 4:

While the proposed future work looks reasonable, it is not very clear how the "engineering level" CFD models are planned to be developed with any enhancement from the current.

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

Reviewer 1:

This work is fully aligned with DOE's objectives and is addressing key challenges and barriers.

Reviewer 2:

The project certainly supports the DOE objectives to develop technologies for high-efficiency engines. It is true that the community lacks advanced ignition models to capture and predict those advanced ignition systems.

Reviewer 3:

Advanced ignition systems represent a key area of uncertainty in the design and simulation of advanced lean/dilute combustion systems, and therefore tasks supporting development of engineering-level predictive models advance DOE goals of improving energy efficiency in transportation.

Reviewer 4:

What is the plan to disseminate the sub-models to industry?

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

Reviewer 1:

The reviewer commented the team is sufficiently funded.

Reviewer 2:

This reviewer noted that the scope of the effort appears to have been trimmed to match the available resources.

Reviewer 3:

It appears like the resource are sufficient. The PI stated that the future work is subject to change, based on funding levels. It would be the best for the PI to lay out options to convince the reviewers for additional funding.

C.02.04 is under-resourced relative to its foundational role in accurately modeling spark-ignition engines (in which the ignition process plays a huge role in determining operability, performance, and cycle-to-cycle variations).

Presentation Number: ace143 Presentation Title: Fuel Injection and Spray Research Principal Investigator: Chris Powell (Argonne National Laboratory)

Presenter

Chris Powell, Argonne National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-27 - Presentation Number: ace143 Presentation Title: Fuel Injection and Spray Research Principal Investigator: Chris Powell (Argonne National Laboratory)

Question 1: Approach to performing

the work—the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The proposed approach is solid and will contribute in addressing some of the key technical barriers. Even though success is not guaranteed due to technical challenges, the approach maximizes the probability of overcoming technical barriers by leveraging the expertise and strengths of the different National Laboratories in the PACE consortium.

Reviewer 2:

The approach is in line with project objectives.

Reviewer 3:

This multi-pronged project approaches issues surrounding sprays in a systematic and thorough way. In particular, the experimental work complements the simulation work. The experimental work uses a range of useful diagnostics to probe different physical processes during a spray at a range of relevant conditions.

Reviewer 4:

The experimental and computational coordination between SNL, ANL, ORNL, and Los Alamos National Laboratory (LANL) seems very good and appears to have a well-established foundation from the Engine Combustion Network (ECN). Using all of the labs' unique capabilities seems to be a robust approach to tackle the technical barriers, and it also seems to help upgrade or improve the existing capabilities. The project being broken into six or so tasks will clearly make project progress clearer and more manageable. It is a bit uncertain or unclear how strongly all of these separate tasks are being integrated toward the PACE goals, but maybe this

is being done at a higher PACE level. The PACE program origin/structure/purpose is not fully clear to those who may not be a light-duty OEM or those who did not see ACE138.

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

Reviewer 1:

According to the reviewer, there are very nice results on so many topics of interest for the DOE program.

Reviewer 2:

The project is largely on track and many key milestones have already been met. There is obvious connectivity between the different partners in the task and a significant amount of comparison between different types of data, which is important. The PIs have identified important future work and remaining questions and seem on track to meet their goals.

Reviewer 3:

Even though some required housekeeping activities like the baselining of current diesel and gasoline injection models have to be completed first, the developed spray-wall interaction model is the main progress that has been reported so far. This is good progress. However, the operating conditions that have been selected to demonstrate the spray-wall interaction model fidelity for gasoline direct injection (GDI) applications are limited.

Reviewer 4:

The broad range of technical accomplishments looks to be quite good, both experimentally and computationally, as indicated by the publications and presentations. The transfer of physics understanding into computational codes and simulation methodologies looks to be starting or moving on well. The comparison of spray parameters between National Laboratories and codes and experiments was a good indicator of this movement. There is clearly a lot of work yet to be done. It is clear that CONVERGE CFD code is relevant toward the application of the knowledge learned in this project. It is not clear that the LANL simulation effort will be useful, due to the lack of commercial adoption by engine and fuel systems OEMs.

It is interesting that much of the technical discussion surrounded spray behavior with the ECN Spray G injector, but there is a clear lack of fuel system design and manufacturing expertise in the project. If the goal of this spray effort is to understand the fundamentals of sprays, fuel injection, and the predictive modeling of such, there should be a strong link to the fuel injector design. The reality may be that new spray physics understanding is generated, but there is nothing that can be changed or modified in the technology design to make improvements based on this new physics understanding. The reviewer would propose that the team try to clearly articulate how the spray physics understanding being pursued could be mapped back to the technology and design requirements. This may help focus where to really apply the R&D effort.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The collaboration between the National Laboratories, Engine Combustion Network, and industry partners is fantastic. Please keep up this good collaborative posture!

Reviewer 2:

There are excellent collaborations between the various National Laboratories.

Reviewer 3:

There is significant coordination between the different members of the project team. Each experimental measurement is complemented by others, and the presentation made clear that the physical understanding on the project is coming from the combined knowledge gained from these measurements. Further, there is a lot of

simulation that complements the experimental work, which is very helpful, and comparisons are done thoroughly.

The only area where the PIs should consider a more nuanced comparison is the issue of cycle-to-cycle variation (an overall goal of the PACE initiative), which manifests in this project as shot-to-shot variation. Capturing this well (and without enormous computational cost) in simulation is difficult but can be done—methods have been proposed to look at variance and rare events in simulation and should be incorporated into this work for better comparison to experiment. It cannot just be about comparing root mean square (RMS) levels but really getting to the root of the variance.

Reviewer 4:

It was very clear that there is a concerted effort to communicate broad National Laboratory coordination on this spray effort by the documentation in Slides 6 and 7. Maybe it would be useful to show how other collaboration is being brought into these spray efforts through the ECN, AEC, and other related collaborations. Again, there is no direct input from fuel system entities.

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

Reviewer 1:

There was not a large amount of future research project planning or critical decision points outlined in the presentation. However, this is more fundamental research work, and the collection of experts working on the tasks give the reviewer confidence regarding the proposed future research direction. This seems to be all in context of alignment with the overall PACE goals.

Reviewer 2:

The future work plan looks robust and covers topics of great interest to the community. There are two things that should be considered in moving forward. First, several of the future tasks have to do with multi-component fuels (measurements, preferential vaporization, etc.), and these should be done in close collaboration with the efforts in PACE that are working to develop surrogates. Additionally, these efforts should effect careful thought about how to compare these results to simulations and how the chemistry and physical properties are being modeled in the surrogates. This is an extremely important topic but one that is very hard to capture fully. Second and referencing prior comments, the reviewer commented that the issue of cycle-to-cycle variation should also be addressed in simulation as it is being researched in experiments.

Reviewer 3:

The reviewer was concerned that the experiments are testing relatively old hardware. The reviewer understood there is a task to re-evaluate this next year, but it will be helpful to have a solid plan for upgrading the experimental hardware.

Reviewer 4:

It was not very clear to the reviewer how the differences between results obtained at different labs are implemented in future work.

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

Reviewer 1:

The work aligns very closely with the overall objectives of the PACE program and direct links between the overarching goals of the program and the subtasks here can be easily drawn. Coordination between this task and other similar tasks looks good as well.

Yes, this foundational project on fuel injection and spray research supports the overall DOE objectives because it is a critical enabler for fuel-efficient, clean, and cost-effective internal combustion engines.

Reviewer 3:

Yes, this clearly supports energy efficiency improvements and energy security with the linkage and alignment to the PACE program. All of this work obviously focuses on automotive gasoline, which is clearly a large portion of the energy consumption in the United States.

Reviewer 4:

It is impossible to improve IC engines without better research on fuel injections and sprays.

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

Reviewer 1:

The resources, both personnel and financial, seem sufficient. In particular, unique experimental capabilities are being used very well in this project.

Reviewer 2:

About half of the milestones in the project have been completed and most of the others are on track. This indicates that the milestones have been appropriately set to the level of resources assigned to the project. In addition, the physical resources and experts are working and already in place to effectively and timely complete the stated milestones.

Reviewer 3:

The funding should support more post-doctoral staff and collaborations with academia to help accelerate and possibly improve the project outcomes.

Reviewer 4:

The resources for this project should be looked at if that is the reason for the testing with relatively old hardware.

Presentation Number: ace144 Presentation Title: Spray Wall Interactions and Soot Formation Principal Investigator: Lyle Pickett (Sandia National Laboratories)

Presenter

Lyle Pickett, Sandia National Laboratories

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-28 - Presentation Number: ace144 Presentation Title: Spray Wall Interactions and Soot Formation Principal Investigator: Lyle Picket (Sandia National Laboratories)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The approach has covered the scope of the work needed to understand spray-wall interactions extremely well. The key aspects of spray impingement on the walls and subsequent soot formation and the key variables that affect them are all being addressed very well.

Reviewer 2:

The approach appears to be comprehensive, involving both experimental and simulation efforts at multiple National Laboratories. Each of the barriers from the roadmap appear to be addressed by this project: studying the mechanisms of fuel films and the physics of how they are deposited and removed. The link to knock/pre-ignition appears to be a little less clear. But, the other barriers are all directly addressed.

Reviewer 3:

The approach is excellent as indicated by the content in Slides 6, 7, and 8. It is clear this is very thought out and each major task has an approach that seems to be reasonable for its experimental or computational focus. It would be helpful to articulate how the approach will feed back and iterate with the PACE goals as knowledge and milestones are completed or missed. If there is something learned that changes the PACE assumptions and goals, how does that impact the approach?

Reviewer 4:

Many experimental techniques (X-ray, neutron) are used, which is outstanding. How does this compare with the work done by Professor Lee at Michigan Technological University?

The approach utilizes a mixture of experimental and simulation spray diagnostics. The utilization of vertical and horizontal impinging walls provides excellent insight for model development.

The disparity in fuel rebound between experiments and simulation is large. The initialized approach where the Lagrangian switches to a volume of fluid during impingement must have vaporization added for accuracy. This was mentioned by the project team. However, the surface-temperature question during the live discussion comes into play with this first principle model development as well. The vaporization model should be developed for both cold and hot walls.

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

Reviewer 1:

The progress on the experimental and simulation side is quite good! The project shows progress in multiple aspects of both measurement and simulation. There are fired and unfired engine conditions, benchtop and pressure vessel type experiments, and different types of simulations to attempt a predictive approach to understanding these conditions. The work was very comprehensive in using multiple tools to understand fuel/wall interactions. The link to knock/pre-ignition and the link to dilute combustion were not explicitly made in this report, and no accomplishments were shown toward these tasks.

Reviewer 2:

Excellent progress is being made in understanding a very complex phenomenon. The physics has been broken down into relevant categories to probe more deeply into the physical phenomena to make more measurements to better understand them. The shortcomings of the CFD models, like the over-prediction of the rebound, are being identified and provide areas where the models have to be improved. The effect of engine speed showing the stronger in-cylinder flows on spray collapse is very interesting.

Reviewer 3:

The project is very multifaceted and is making acceptable progress. Experiments that can distinguish between soot development modes as the flame progresses over the surface would be extremely helpful.

Reviewer 4:

Slides 7 and 8 show that the many tasks are complete. The reviewer also commented that the others are on track.

Reviewer 5:

There is a tremendous amount of technical progress and accomplishments as indicated by the eight completed milestones. The volume of presentations and publications is also high and as many as the completed milestones. The reviewer understood the fundamental nature of supplying gasoline spray wall film and soot physics knowledge and validation data, which these technical accomplishments make progress toward. There was some good discussion in the presentation on how to use the gained technical information in the predictive simulation tools. Is the goal here to help make simulation tools be as accurate as possible, or give representative key physics behavior for engineering decision making? It is not clear why there is an effort with the FEARCE code, as this is likely not a tool/code that will be adopted by industry.

Is the pursuit of wall film and gasoline soot minimization purely a cost effort? It may be helpful to clearly detail the link to the more expensive technologies required to deal with gasoline engine soot and/or cold start (e.g., particulate filters and electrically heated catalysts).

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The team and the collaboration among team members was truly impressive. This team integrates very diverse experimental and simulation work across several different National Laboratories. The coordination effort was quite noticeable.

Reviewer 2:

Collaboration with the other free spray experiments at Sandia as well as experiments and modeling at Argonne are excellent. This area of work is being coordinated very well, and the leader of this subset of work is to be congratulated.

Reviewer 3:

This would be one of the benchmarks for complex project collaboration as evidenced by the strong ECN and National Laboratory coordination.

Reviewer 4:

Slides 4 and 5 show how well the teams work together.

Reviewer 5:

The multiple investigators are working on complementary experiments and models. Results appear to be well communicated between the investigators.

It has reached the point where reviewing the large collaborative efforts is nearly impossible. Teams are spending much of their time overviewing the various responsibilities and collaboration between members. There are usually only a couple minutes discussing the technical content and singular slides representing the congruous contributions from all other portions of the project. It almost seems that the reviewer would need to review all the presentations from all the collaborators to fully understand how well the projects are addressing the full scope. It is very difficult to ask questions on the technical attributes with a menagerie of content from all the collaborators.

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

Reviewer 1:

The listing of the detailed future work is really excellent on Slides 27 and 28. The reviewer saw no issues with the future work as there has been significant milestone accomplishment and presentation and publication history.

Reviewer 2:

The critical influence of wall temperature on soot formation has been incorporated into future research. Going forward, the multi-component nature of gasoline on soot formation will be critical and this is planned. The influence of ambient air temperature and wall temperature should be studied independently as well as in unison.

Reviewer 3:

Proposed future work certainly addresses the challenges and issues that were encountered during the conducting of this work by the various team members. However, no explicitly listed future work outlines how this fundamental study of wall films will link to engine measurements of knock or dilute combustion. Those two barriers are important to include in this project, sooner versus later.

It is a worthwhile endeavor to upgrade the experimental facilities for conditions that are closer to that of an engine.

Reviewer 5:

Evaluating spray impingement and soot formation with both high- and low-temperature walls will provide a better identification and validation if data sets for the first principle evaporation models being constructed. Careful manipulation of the wall temperature may also aid separation of the multiple soot formation pathways.

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

Reviewer 1:

This project is extremely relevant and addresses probably the number one priority for OEMs, i.e., cold-start emissions and particulate matter emissions.

Reviewer 2:

The comparisons between simulated and experimental data are shown very clearly (example: Slide 19).

Reviewer 3:

GDI SI engines will be part of the light-duty automotive fleet for several years to come. To reach the efficiency and emissions compliance potential of this technology, understanding cold-start emissions and the effect of wall-wetting on knock and dilute combustion will be very important toward helping OEMs enhance GDI technologies.

Reviewer 4:

Developing fundamental insights on fuel impingement and soot formation can eventually lead to lower vehicle emissions, which is well aligned with DOE objectives.

Reviewer 5:

Yes, this project is relevant to the DOE objectives of clean and secure energy in the transportation sector. This is only aligned to automotive applications or light commercial applications.

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

Reviewer 1:

The provided resources are being extremely well utilized in focusing on the critical and high impact issues.

Reviewer 2:

The resources appear to be sufficient to achieve the future work.

Reviewer 3:

The resources appear to be well suited to studying a problem of this size and importance. There are several National Laboratories that utilize different tools and equipment to mesh together important results. Current resources need to continue to be applied to this important work.

Reviewer 4:

The teams appear to have the support they need to modify and design the experimental devices and models required for this investigation.

Reviewer 5:

Generally, the budget seems sufficient for the tasks outlined. The tasks are rather fundamental and open ended, so it is not clear which tasks may need more resources than the others. The reviewer assumed that PACE has the ability to move budget and resource effort on a semi-regular basis to help with this. The only outlier task

looks to be the FEARCE D.02.04 effort as it seems high for the value and the lack of understanding of the use and application of the code.

Presentation Number: ace145 Presentation Title: More Accurate Modeling of Heat Transfer in Internal Combustion Engines Principal Investigator: K. Dean Edwards (Oak Ridge National Laboratory)

Presenter

K. Dean Edwards, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-29 - Presentation Number: ace145 Presentation Title: More Accurate Modeling of Heat Transfer in Internal Combustion Engines Principal Investigator: K. Dean Edwards (Oak Ridge National Laboratory)

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

Reviewer 1:

It looks like this project will leverage outcomes of other projects and come up with an incorporated simulation tool (or approach). It is understood that this is rather a demonstration project.

Reviewer 2:

The team has used and leveraged the possible resources; the challenging part will be the integration of all the pieces.

Reviewer 3:

The approach to performing this work is reasonable. Predicting cold-start using CFD simulations is a tremendous challenge since it depends on a lot of uncertainty factors including heat transfer, low-temperature chemistry, spray model predictions of liquid length penetration and vapor length penetration. The work on conjugate heat transfer (CHT) and comparisons with experimental neutron diffraction data are pretty impressive. Additionally, the spray wall impingement work is also critical.

Reviewer 4:

There is a good combination of simulation and experimental work. Linking to the spray work is critical, and the reviewer was glad to see it. The neutronic engine approach is wild. Capturing a dynamometer and engine in a framework for the measurements is certainly novel. The reviewer did have questions about how the data are acquired. How much can be acquired? Is it an ensemble averaging process in both x, y, z, and time? How many unique conditions can be measured considering the complexity?

The project goals are well aligned with PACE, but it is unclear how the project approach will deliver results in a challenging topic area.

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

Reviewer 1:

Overall, good progress has been achieved in all three areas: i.e., computational modeling, spray imaging, and neutron diffraction in situ measurements.

Reviewer 2:

The reviewer was looking forward to the experimental neutron imaging data to calibrate and validate the CHT modeling. The collaborative link to the fuel spray work is also critical. There are interesting data showing the sensitivity of wall temperature to soot formation.

Reviewer 3:

The reviewer found the experimental setup to characterize the thermal barrier coating (BC) for modeling evaluation to be very unique. The wall-film measurement will be key for an appropriate sub -development.

Reviewer 4:

The modeling accomplishments (B.02.01) shown here have illustrated a number of stumbling blocks faced by common CFD approaches but have not demonstrated progress in overcoming these challenges. The neutronic engine work (B.01.01) potentially offers new, sought-after measurements of temperature distribution throughout the engine structure. However, it may be challenging to reach the potential of the diagnostic techniques during the PACE project duration. The choice to subcontract the engine to SwRI will likely support the rapid timeline desired for this task. The presented fuel wall-film measurement results (D.01.04/5) have a clear link to understanding soot formation processes but have not yet shed light on heat-transfer phenomena.

Reviewer 5:

The accomplishment presented is okay. However, it looks like rather a typical engineering-level exercise. The PI needs to better specify the original breakthrough.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

This is an excellent example of collaboration between various different National Laboratories, GM, and Convergent Science.

Reviewer 2:

The project incorporates neutron diffraction measurements for the engine and leverages spray measurements in a constant volume chamber. Essentially, coordination and keeping collaboration and communication would be the key to the success to the project. It looks like the project is keeping it at the right level.

Reviewer 3:

The PACE structure appears to be promoting good collaboration across National Laboratories. The reviewer was glad to see involvement with software vendors.

Reviewer 4:

The reviewer said that the team has very good collaboration with various expertise included. Again, the challenge will be integration of all the pieces to work together.

A large number of external collaborations are highlighted across the tasks and PIs. The tasks seem well linked, although only a small number of examples of inter-project coordination are given.

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

Reviewer 1:

The proposed future work falls in line with existing task direction and is a logical extension of the results presented here.

Reviewer 2:

In the soot formation work, the reviewer suggested also considering higher speed and load conditions typical of the 20-30 second period of the Federal Test Procedure 75 (FTP-75) cycle. Fueling increases and metal temperatures can still be cold.

Reviewer 3:

The future work is comprehensive. In the reviewer's opinion, one important element is missing, i.e., kinetic model or combustion model. When approaching cold conditions (less reactive), challenges on combustion and kinetics become critical and might affect the evaluation.

Reviewer 4:

Proposed research looks reasonable. It is not clear what sub-models are to be integrated into CONVERGE for model improvement.

Reviewer 5:

The reviewer asked the team to take a step back to understand where the discrepancies in modeling are arising from. Is it from spray/vapor penetration and spreading, chemistry, heat transfer models (e.g., Woschni type model)? To understand this, every aspect of the model should be introspected and compared with fundamental experiments with cold walls. The reviewer believed that low-temperature chemistry may play a big role, and the chemistry mechanism needs to be tuned for it. In addition, how many engine cycles are needed to be simulated is a question.

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

Reviewer 1:

This project is well aligned with the DOE objectives to develop a way for more fuel efficient and cleaner engines.

Reviewer 2:

PACE goals are aligned with LD ICE needs.

Reviewer 3:

Cold-start related investigation is of high interest to the community.

Reviewer 4:

Yes, the project supports overall DOE VTO objectives. These are the kind of fundamental understanding experiments and simulations that National Laboratories should pursue.

Improved modeling of near-wall phenomena is critical for improving engine simulations targeted at limiting cases, such as cold-start or high-load. The tasks here are foundational to improving understanding of near-wall phenomena.

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

Reviewer 1:

It looks like the project has sufficient funding.

Reviewer 2:

The reviewer commented sufficient; the PI did not indicate additional resources would improve the outcome.

Reviewer 3:

The reviewer commented the project is on track.

Reviewer 4:

If additional neutronic engine experiments need to be performed, then the budget may be a little insufficient. Otherwise, the budget seems to be reasonable.

Reviewer 5:

The ORNL modeling task (B.02.01) and SNL experimental tasks (D.01.04/5) are resourced appropriately, but the ORNL neutronic engine task (B.01.01) is under-resourced if this task is expected to deliver results under the PACE timeline.

Presentation Number: ace146 Presentation Title: Direct Numerical Simulation (DNS) and High-Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In-Cylinder Flow and Combustion Processes Principal Investigator: Muhsin Ameen (Argonne National Laboratory)

Presenter

Muhsin Ameen, Argonne National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

100% of reviewers indicated that the project was relevant to current DOE objectives, 0% of reviewers indicated that the project was not relevant, and 0% of reviewers did not indicate an answer. 60% of reviewers indicated that the resources were sufficient, 40% of reviewers indicated that the resources were insufficient, 0% of reviewers indicated that the resources were excessive, and 0% of reviewers did not indicate an answer.



Figure 1-30 - Presentation Number: ace146 Presentation Title: Direct Numerical Simulation (DNS) and High-Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In-Cylinder Flow and Combustion Processes Principal Investigator: Muhsin Ameen (Argonne National Laboratory)

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

Reviewer 1:

Overall, the work is well designed and planned. The approach to cross-correlate results (shown on Slide 7) is particularly excellent, and the plan to make sure the project results can be usable by industry is excellent. A minor concern is that while the work plans to identify the root causes of cyclic variability, the approach to doing so should be laid out more clearly. The presenter mentioned that the project hopes to use machine learning to do so, but a clearer and more explicit plan would be helpful.

Reviewer 2:

The project addresses the barrier of understanding and mitigating cycle-to-cycle variations and cold-start emissions, and using cutting edge simulation approaches. Leveraging DNS and large-eddy simulation (LES) would certainly be value added in understanding current limitations as well as planning to further it.

Reviewer 3:

While the reviewer appreciated the importance of super high-fidelity simulations to provide benchmarks against which to compare more affordable simulations, it is still not clear how results from this work will be used to develop sub -to improve engineering level simulations.

Reviewer 4:

Has the team considered validating the high-fidelity model against port flow simulations spanning a range of valve lifts to verify bulk flow parameters, such as discharge coefficients, mass flow rates, etc.? These types of

validations are important to industry and help build confidence in the tool. Also, it would be interesting to use the tool to simulate the breakdown process of tumble flow to turbulence and compare with RANS and largeeddy simulation (LES) models. Additionally, will the team consider simulating sprays using a full Eulerian approach?

Reviewer 5:

Some key technical barriers of incomplete understanding of fuel-air mixing, stochastic combustion, and coldstart emissions are briefly mentioned. This project is to develop methodologies of accurate ICE flow analysis and combustion and emissions modeling through multi-fidelity turbulent combustion flow analyses. However, the reviewer did not understand why multiple in-house codes have to be used. These codes do not look suitable for solving realistic engine geometries within a reasonable time frame throughout the project. It seems unreasonable to invest heavily in a research-oriented code like Nek5000 just to provide some DNS data for a wall heat transfer model. There are a couple of commercial codes available now for LES analysis in real engine situations and the vendors usually open for co-development on sub-models, and this would provide engine OEMs with one of the valuable tools to improve engine efficiencies.

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

Reviewer 1:

The team is demonstrating the capability for next level, state-of-the-art simulations.

Reviewer 2:

Both ANL and SNL made meaningful progress on ICE relevant flow/spray/extended coherent flamelet model (ECFM) combustion modeling and soot onset/flame propagation, respectively.

Reviewer 3:

The identification of shortcomings in soot models will hopefully lead to improvements because this is the most difficult thing to simulate. In order to achieve accurate soot modeling results, all elements of the simulation must be correct: airflow, fuel injection, vaporization, mixing, wall films, combustion chemistry, and then finally soot formation.

Reviewer 4:

The reasons for project delays were not discussed. The progress to date is nonetheless encouraging and promising.

Reviewer 5:

The project has made a nice progress in LES of the reference engine as well as DNS. ECFM implementation is not very impressive, as the model has been around for decades and it has limitations. It is worthwhile for the PI to justify such an effort.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It looks like the project is in good collaborations within PACE and with external collaborators.

Reviewer 2:

Overall, it looks like the collaboration was done well with PACE teams and external collaborators, mostly using the Nek5000 code.

Reviewer 3:

The team would benefit by engaging an OEM partner.

The approach of developing sub-models that can be provided to engineering level simulation developers may not work out if there are incompatibilities in the approach. What if commercial software developers were included as collaborators to ensure that sub-models are developed to work with commercial codes?

Reviewer 5:

This appears to be a collection of unconnected efforts with no coherent plan for integrating them or collaborating among them. The three efforts are aligned with the overall PACE effort, but they are not clearly coordinated with each other.

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

Reviewer 1:

The proposed future work is appropriate and logical.

Reviewer 2:

The team is responding to past reviewer comments by working on coupling to engine CFD codes.

Reviewer 3:

What is the timeframe for development of sub-models that will be useful for commercial CFD codes?

Reviewer 4:

It is good for the project team to complete implementing spray-ignition-combustion models in FY 2020 and try to execute multi-cycle LES on the Sandia optical direct injection spark ignition (DISI) engine in FY 2021. It is not very clear what the project team plans to do for the development of an open-source platform for sub-model development, but it seems like a right direction.

Reviewer 5:

It is not very clear what the CONVERGE simulations will add a value to. The major goal of the project is to develop and leverage Nek5000. Please specify the connection between the efforts.

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

Reviewer 1:

Full DNS in engines with moving valves and piston is groundbreaking.

Reviewer 2:

This work is fully aligned with DOE's objectives and will provide tools for industry to improve the efficiency and emissions of internal combustion engines.

Reviewer 3:

This project supports overall DOE objectives in attaining higher engine efficiency for diluted SI combustion through the development of sub-models for combustion, emissions, etc.

Reviewer 4:

This project is very much relevant to the DOE objectives to further understanding cycle-to-cycle variations and cold-start emissions and to mitigating them for more efficient and cleaner engine development.

Reviewer 5:

Improved simulations will contribute to better engine design tools that will help improve engine efficiency.

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

Reviewer 1:

The resources for the project are sufficient for timely execution of the project milestones.

Reviewer 2:

Progress is being made, and the project has access to adequate computer cores.

Reviewer 3:

The project looks to have sufficient funding.

Reviewer 4:

Slide 6 suggests the project is linked to the Exascale Computing Project (ECP). Is there computer time reserved for ECP solvers? A project of this nature should not be thwarted due to lack of computer resources.

Reviewer 5:

The DNS analysis for a realistic engine geometry at relevant operating conditions is prohibitively costly with Nek5000. The reviewer did not mean more support on this code development for this project is necessary but had a concern about the overall approach and efficiency in using the code.

Presentation Number: ace147 Presentation Title: Mitigation of Knock and Low-Speed Pre-Ignition (LSPI) for High-Power Density Engines Principal Investigator: Jim Szybist (Oak Ridge National Laboratory)

Presenter

Jim Szybist, Oak Ridge National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-31 - Presentation Number: ace147 Presentation Title: Mitigation of Knock and Low-Speed Pre-Ignition (LSPI) for High-Power Density Engines Principal Investigator: Jim Szybist (Oak Ridge National Laboratory)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The two projects presented are each individually very well designed and planned and are addressing key technical barriers that inhibit further improvement in spark-ignition engine efficiency. This reviewer noted that the two efforts are not really connected to or integrated with one another.

Reviewer 2:

The approach appears well suited to addressing the technical barriers for knock mitigation and fuel-oil influences on LSPI.

Reviewer 3:

The approach to this work is outstanding. The PIs have recognized that there is a measurable difference in knock mitigation between catalyzed and uncatalyzed EGR. It may be beneficial if the PIs had access to a CFR engine capable of running catalyzed and uncatalyzed EGR. This would allow them to vary the pressure-temperature (P-T) trace in both the beyond-MON and beyond-RON regions into the knocking regime without damaging the engine.

Reviewer 4:

The methodologies used here to investigate knock and LSPI are sound, following good scientific practice to isolate variables of interest and separately interrogate various factors influencing the system.

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

Reviewer 1:

A good sweep of pre-TWC versus post-TWC EGR influence on knock limited combustion phasing was presented. Initial results from LSPI fuel-oil interaction study were also presented.

Reviewer 2:

Even with the COVID-19 shutdown, the researchers have made significant progress in their research.

Reviewer 3:

The assessment of EGR effectiveness as a function of engine load and speed is highly relevant and a strong technical result. The LSPI task is conceptually interesting but does not have substantive results yet.

Reviewer 4:

Both projects appear to be on track and progressing well. With regards to the EGR project, the reviewer had two minor suggestions. First, the team should consider an EGR mixing approach that more closely approximates what would occur in a real implementation, e.g., cooling the EGR to a specific temperature and mixing it with fresh air that is also at a specific temperature so that as EGR rate increased charge temperature would also increase. While the current approach is cleaner and easier to interpret, the effect of increased charge temperature in a real application could outweigh the benefit of the EGR.

Second, while this reviewer applauds the ability of the PI to find creative ways to create plots, such as those on Slide 11, a concern is that some information that is important is lost with this current approach. Specifically, the extent to which combustion variability (and other engine limits, if applicable) change with EGR rate also need to be communicated along with the knock benefit. The LSPI project is not as far along but has made promising progress.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The team is well coordinated and complementary. The presentation was very well structured, with just enough focus on the collaboration for it to be understandable without detracting from technical content time.

Reviewer 2:

The project team has good coordination (work in the same lab), but it may be beneficial for the team to have some outside research or evaluation from groups such as USDRIVE, USCAR, and/or the Coordinating Research Council (CRC).

Reviewer 3:

Although PACE is a coordinated effort and the tasks here fall in scope, the demonstrated collaborations with other National Laboratories are seemingly less substantial than is seen with other projects. In particular, the LSPI task does not identify specific collaborations contributing to its outcomes.

Reviewer 4:

The two projects that were reviewed are not integrated with one another but do appear to be well aligned with the overall PACE effort and well coordinated with external collaborators. This reviewer noted that exactly how the machine learning work is or will be integrated was not really discussed.

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

Reviewer 1:

The scheduled future work is both appropriate and very well planned.

Reviewer 2:

The future research plan is logical to elucidate the impacts of the exhaust constituents on knock.

Reviewer 3:

Future work plans lack specificity but appear to generally be in line with the tasks and their current state of progress.

Reviewer 4:

Causes of increased EGR effectiveness with aftertreatment with a TWC are unclear. It is not clear what individual compound or combination of compounds cause knock mitigation. The researchers should investigate the effect of CO and NO on knock.

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

Reviewer 1:

This project is fully aligned with DOE objectives and is addressing key barriers that prevent further improvement in spark-ignition engine efficiency.

Reviewer 2:

Both the knock mitigation work and the LSPI work directly contribute to DOE's PACE project goals of developing models that can accurately predict knock in modern SI engines and developing phenomenological models for LSPI.

Reviewer 3:

Minimizing SI knock will reduce the amount of fuel enrichment (saving fuel) and possibly enable further engine downsizing and boosting.

Reviewer 4:

It is important to understand how to mitigate knock to increase the fuel economy of ICE vehicles. ICEs will be around for at least two or three decades so it is important that we understand EGRs effect on knock.

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

Reviewer 1:

The project resources are sufficient for timely completion of the planned work.

Reviewer 2:

The researchers appear to have sufficient resources to complete their work. They have made excellent progress with the resources they have.

Reviewer 3:

The resources for these tasks are commensurate with their planned work and contributions to the PACE effort.

Reviewer 4:

The team resources appear to be well matched for the investigation.

Presentation Number: ace148 Presentation Title: Overcoming Barriers for Dilute Combustion Principal Investigator: Brian Kaul (Oak Ridge National Laboratory)

Presenter

Brian Kaul, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-32 - Presentation Number: ace148 Presentation Title: Overcoming Barriers for Dilute Combustion Principal Investigator: Brian Kaul (Oak Ridge National Laboratory)

Question 1: Approach to performing

the work-the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The collaboration is focused on addressing the multitude of challenges associated with the barriers of extending dilute combustion. Using ML to explore for insight into predictive capabilities for cyclic variability is full of challenges and complexity, but interesting, and, if successful, will be a tremendous advancement.

Reviewer 2:

All the topics in this project are highly relevant to industry. Please provide more information about the geometry of the igniters to see if they could be fitted in an automotive engine.

Reviewer 3:

Ignition system development for flame propagation combustion systems is an important pathway toward improving engine efficiency in the marketplace. The work needs to go beyond lean limit dilution tolerance tests to answer critical questions necessary for commercialization: how does the igniter behave under cold-start and catalyst heating conditions, what is the tolerance to combustion phasing retard for torque reduction during shifting, does the igniter function during a cold start at -40°C, and others? It is not clear how each of the three projects presented relate to one another.

Reviewer 4:

This is a solid method exploring different advanced plasma ignition systems and using ML to investigate the possibilities of control closed crankcase ventilation (CCV) to push the dilution limit. The PACE surrogate development seems more challenging than expected. Should the team rethink the methodology? Why not simply use a real fuel and use a surrogate or a real fuel chemistry in modeling?

The approach on the three distinct tasks seems to be okay. They are all three fairly different tasks, however. It seems like the approach of using a single-cylinder engine, which is typically very much a steady-state device, for the next cycle ACI control is flawed. A real-world, multi-cylinder engine approach would likely be preferred if continued ACI research is warranted or desired by PACE.

How is the focus on ACI and lean gasoline combustion relevant for automotive applications today? As electrification increases for ICE powertrains and the displacement of ICE powertrains, it is clear that the ICE operating range and ACI/LTC/homogeneous charge compression ignition (HCCI) opportunity/region is becoming irrelevant. Efficiency improvements in three-way-catalyst capable gasoline combustion systems seem to be more of a relevant focus.

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

Reviewer 1:

The reviewer commented that the project is on track according to Slide 4.

Reviewer 2:

There is very good progress on various fronts. The reviewer understood the challenge between different topics, but still encouraged more interactions between PIs on the team.

Reviewer 3:

The work of trying to identify an appropriate surrogate fuel is very important and their efforts toward this end are quite positive, even though they are not completely there. The work on ML is showing some encouraging results but still has a long way to go. Even if bringing the full power of supercomputing fails to resolve cyclic variability into predictable behavior, the knowledge will have been important.

Reviewer 4:

The ignition system accomplishments are excellent and clearly benchmark the state-of-the-art lean-limit extension. Why is there not a pre-chamber type ignition system in this work? Is it elsewhere in PACE? Pre-chambers are a well-known (more than 50 years), robust, lean combustion ignition system used throughout the reciprocating natural gas industry.

The machine learning and Bayesian cyclic variation control algorithm development looks to be making good progress as evidenced by the application and analysis of multiple engine operation data sets. How are the physical sources of variation being linked to the observed SI cyclic variability? Or rather, how is the team linking the observed sources of variation to control variables or design variables? Can the team actually effect a change based on the team's ML predictions with the physical engine technology?

The Crank angle at 50% mass fraction burned (CA50) control and next cycle control accomplishments seem like very good technical work; the reviewer just questioned the value of this low load ACI focus and the value of controls work on a single-cylinder engine. The RD5-87 fuels work looks to be achieving the milestones and producing very good data for the PACE program.

Reviewer 5:

The Transient Plasma Systems nanosecond repetitively pulse discharge (NRPD) ignition system is stuck in a perpetual research phase. Additional studies showing combustion benefits are not required; these have been done for 5 years. What is needed is progress toward commercialization, and there is no evidence of this.

Regarding double direct injection–partial fuel stratification (DDI-PFS), it is convenient to set very high intake air temperatures in a lab environment, but if we think ahead to a transient vehicle application, what intake temperature response rate is required at different loads to support the strategy? Additional incremental steps to

improving indicated thermal efficiency are not the pathway to implementation, but instead the barriers, such as transient response of boundary conditions and tolerance to the variability of market fuels, should be addressed.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer very much liked the collaboration that is an integral part of PACE. The integrated efforts of the various National Laboratories and stakeholder participants is greater than the sum of previous independent efforts.

Reviewer 2:

Collaborations on each of the three projects are good.

Reviewer 3:

The team has good synergy between ignition (Ekoto), pattern recognition (Kaul), and CA50 control of gasoline compression ignition (Dec). Please show if GCI can be used at high loads.

Reviewer 4:

Overall, the collaboration is good considering the difficulties between different topics. But, more interactions and coordination are encouraged.

Reviewer 5:

The coordination seems adequate, but these are three very different tasks. More coordination of how these relate to each other may be necessary, or how they should be moved closer to other activities within PACE. It looks as if each specific task has reasonable collaboration with its own relevant partners.

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

Reviewer 1:

The reviewer affirmed very thorough future work.

Reviewer 2:

Using the barrier discharge igniter in a pre-chamber is very interesting. The reviewer looked forward to seeing the results of this project.

Reviewer 3:

The reviewer asserted that identifying an appropriate surrogate fuel should remain a high priority.

Reviewer 4:

Slide 4 and Slide 20 give enough detail to show that the future research is reasonably planned and thought out with minimal risk.

Reviewer 5:

Future work needs to broaden the scope to address questions related to commercial implementation over a broad range of operating conditions and not another dilution tolerance sweeps or incremental increase in indicated specific fuel consumption (ISFC).

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

Reviewer 1:

The project is highly relevant to the overall DOE objectives. This is an important area to explore to keep pushing for efficiency improvement.

This project is highly relevant to the DOE objective of enabling dilute gasoline combustion. It is also highly relevant to industry. The next cycle prediction (Kaul's work) would be extremely useful to improve engine performance.

Reviewer 3:

The close collaboration between the different participants and their connection to DOE and Industry, through USDRIVE and USCAR via the various tech teams, keeps the focus of this work relevant.

Reviewer 4:

Improvements in engine efficiency addresses DOE goal of reduced energy consumption.

Reviewer 5:

It is clear that improving ignition systems can improve engine efficiency in either lean-burn or EGRstoichiometric operation. It is also clear how the machine learning task contributes to realizing higher efficiency combustion strategies in the real world. It is not completely clear if the multi-mode ACI task is relevant, but the fuel-specific areas of this task are relevant to the broader PACE goals.

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

Reviewer 1:

The project overall is on track with good resources.

Reviewer 2:

The resources and the team in place appear to be adequately resourced to tackle the challenges of this project.

Reviewer 3:

It appears to the reviewer that funding is adequate.

Reviewer 4:

The budget looks to be appropriate for the future tasks and future milestones. Additionally, the National Laboratory facilities and the HPC resources are clearly sufficient.

Reviewer 5:

There was no indication that the funding level was insufficient.

Presentation Number: ace149 Presentation Title: Cold-Start Physics and Chemistry in Combustion Systems for Emissions Reduction Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

Presenter

Scott Curran, Oak Ridge National Laboratory

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-33 - Presentation Number: ace149 Presentation Title: Cold-Start Physics and Chemistry in Combustion Systems for Emissions Reduction Principal Investigator: Scott Curran (Oak Ridge National Laboratory)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The project team well understands technical barriers to the reduction of cold-start combustion and emissions. The project is planned well for addressing key issues of cold-start emissions through single cylinder engine testing and numerical simulation of a PACE surrogate with PAH mechanism. It seems feasible that the project can be executed well in both testing and simulation, and the project team could provide invaluable information to overcome the barriers. However, it is not certain if soot modeling can be accurate for a wide range of cold-start operation as the current surrogate fuel showed a big difference with the reference fuel RD5-87 in higher exhaust heat flux range.

Reviewer 2:

The approach to use both simulation and experiment to better understand the physics of cold start is sensible. This project is using engine experiments, benchtop experiments (at Yale), and simulations—this should be a recipe for success. It also appears that some work on the Argonne engine to allow for proper exhaust cam timing would benefit this project and bring it more in-line with the other aspects of the project.

Reviewer 3:

The focus on development and understanding around cold-start performance is a relevant topic. The challenges, and clear technical barriers, are not laid out in great detail, though this may largely be a result of the overall PACE focus on experimental programs providing data to build out model capabilities. Clarity on what barriers need addressing within the modeling work are not highlighted. This again may be a function of

the overall PACE effort and structure of the AMR presentations. On an individual project basis, the approaches being taken are on target and, as best can be ascertained from the level of detail allowed in this format, feasible for the resources and tools available.

Reviewer 4:

The project may be overreaching on objectives and experiencing a creep in scope by tackling active prechamber ignition for cold start and the development of a transient test protocol. The project should first aim to understand the physics and chemistry of the incumbent cold-start techniques being employed by OEMs. This basically involves injection (quantity and timing), spark timing, and other basic engine control variable changes to speed up catalyst heating. The ACEC Cold Start protocol is a very good place to start gaining this understanding. Then, later, advanced ignition systems and transient understanding can be developed.

Reviewer 5:

The focus on catalyst heating conditions is critical for any new combustion technology to enter production. The approach is generally solid, but the reviewer had some concerns. The ANL heat flux sweep is anemic. Typical turbo engine without an auxiliary method to heat the catalyst would need to operate in the approximately 8 kilowatt (kW)/L range. The ACEC protocol recommended range of 3-10 is to see how capable the approach is across this range. Where does the stability begin to fall apart? The ANL baseline approach might benefit from a more sophisticated injection method (split injection, stratified injection) to enable higher heat fluxes. The spark around top dead center (TDC) is typical for a PFI type of homogeneous charge system. The reviewer commented that, typically, there is an inability to retard spark past TDC without combustion stability issues.

The reviewer liked seeing the skip fire approach. Steady state cold fluids are known to underestimate the emissions that depend on wall impingement. Internal temperatures are too high. It does a reasonable job at capturing the stability and heat flux capability though.

With respect to the operating conditions for soot, catalyst heating conditions are important but maybe more important are the higher loads seen around 20-30 seconds on the FTP cycle. The customer requests torque. Mass flow, fuel flow increases, and the combustion chamber is still relatively cold. Consider adding a higher speed and load condition to the work.

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

Reviewer 1:

Overall, the progress that has been made is very good. Both steady-state and transient operations of single cylinder engines (SCEs) at three participating National Laboratories were being performed. ANL made progress in testing baseline SI cold-start test although exhaust heat flux range was low. ORNL characterized cold start emissions using both baseline and PACE surrogate fuels on a converted SCE from a 4-cylinder engine. SNL tried to test transient cold start operation, which seems the most valuable test but also hard to control the operation. LLNL developed a PAH mechanism and validated against data from diffusion flame tests.

Reviewer 2:

There are good accomplishments considering a Q3 of FY 2019 start.

Reviewer 3:

The accomplishments in this project have been pretty good—the engines, burners, and simulations have produced some interesting results and some understanding has been gained. However, exhaust heat flux in the Argonne engine is well below the target (due to a fixed cam not allowing EVO), limiting its effectiveness. But, the resources applied do not seem to match up with expected results. There still seems to be some improvements to be made in the experimental validation and matching results from facility to facility.

The Oak Ridge data for the ACEC Cold Start test look very much on par and as expected. Good to see the PACE surrogate performing well. Can this engine be used to study the effect of injection and spark parameters on engine performance during the ACEC Cold Start test? The Argonne data do not seem to be in the ballpark of the ACEC Cold Start test expectations. Perhaps changing the cams will resolve the situation. It is suggested that the guidelines set for the engine performance for the test protocol be first met satisfactorily before investigating an active pre-chamber advanced ignition system.

Reviewer 5:

The 2019 milestone of commissioning a series of off-the-shelf instruments is viewed as a very weak milestone, especially since it is the only listed milestone for a project funded at \$400,000. Moving forward, this reviewer would have liked to see a more meaningful measurement of progress.

The reviewer was concerned to see the lower than desired exhaust heat flux in the ANL engine experiments. This should be rectified so that all experiments across the different National Laboratories are proceeding with similar cold-start conditions. The reviewer realized that this issue was not likely apparent ahead of experiments, but it should be addressed and corrected moving forward.

There is solid initial work at ORNL to establish and characterize baseline cold-start conditions in their engine. There are significant variation and scatter in some of the emissions data presented from this baseline testing on Slide 10. This would be good to resolve in future experiments and characterize whether this is due to combustion and fuels, or simply experimental uncertainty. Results from SNL efforts focus on new experimental technique development. Future results need to focus on phenomenon explanation and details, not further experimental tweaks.

Yield sooting index (YSI) measurement validation is "complete," but the simulated YSI for tetralin, a key component planned for use to represent heavy, high boiling point components, is off by nearly 35% from the experimental measurement. It is not clear how this is a successful validation, given the offset and importance of this molecule to the PACE surrogate. Does matching engines improve validation data? It may improve validation on a single geometry, but CFD sub-models should be agnostic to engine geometry and type.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

There appears to be excellent coordination and collaboration among the team members on this project. The benchtop and simulation work appear to be particularly well coordinated. The engine progress was also significant, and the communication appeared to be good.

Reviewer 2:

There are four National Laboratories participating in this project, and they are all working toward a common goal for the PACE program. They seemed to work closely internally and also externally for exchanging experimental data for model validation work.

As far as testing all different SCEs at different sites goes, they need to have a common definition or calculation of test data collection and processes for such parameters as indicated mean effective pressure (IMEP), brake mean effective pressure (BMEP), burn rate, CA50, cycles for coefficient of variation (COV) IMEP, exhaust heat flux, NO_x correction, soot measurement, etc., for testing all different SCEs at different sites.

Reviewer 3:

Very good collaboration exists between ORNL, ANL, and Sandia for the engine experiments. Modeling efforts have started but are experiencing some difficulties (ACE145).
Reviewer 4:

The structure of PACE promotes excellent collaboration. Be sure to stay connected to the fuel spray portion of PACE. Fuel impingement is critical for HC and soot production during cold start. Is the baseline wall wetting (due to the injection approach) a good place to start to look for improvements? Is your baseline wall impingement representative of a typical cold-start calibration? Wall impingement from an intake stroke injection will be different from a late compression stroke injection that might be employed to stabilize combustion during catalyst heating.

Reviewer 5:

Collaboration appears mostly on paper for this project. The different National Laboratory efforts are focused on completely different subjects under the same general focus area. Very little collaboration across the team is apparent. This may stem in part from the overall PACE structure and how presentations were bundled for this AMR. However, overall participation in the PACE umbrella program should not be viewed as the sole necessary collaboration across project teams. Some outside collaboration is noted, but generally limited. For some of the external collaborations, it is not clear that the collaborative work applies to this particular effort.

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

Reviewer 1:

Selected future research topics from all four teams look quite reasonable and moving forward to meet the project goal and support PACE program goals.

Reviewer 2:

The proposed future work appears to be fairly well coordinated and connected to the progress made this year. The new exhaust manifold for the ORNL engine should help provide improved measurements. The prechamber results from the Argonne engine should be especially interesting if they can get it up and running properly.

Reviewer 3:

The reviewer said to continue to pursue a skip fired protocol.

Reviewer 4:

Presumably the modeling efforts, once some of the initial challenges mentioned in ACE145 are resolved, will keep in step with the experiments.

Reviewer 5:

Proposed future work looks reasonable as a next step for this particular area, although the connection to CFD model development is not immediately clear. As the effort moves forward, it will be useful to detail how the results from these efforts feed into the model development and enhancement. The parametric study on prechamber geometry, while addressing a key potential barrier to pre-chamber adoption, seems like it is only part of the necessary study. Engine hardware design is always a compromise between different driving factors. In this case, does a pre-chamber optimized for cold start still deliver the lean or dilute operation performance that is a prime driver for using pre-chambers? This effort should be ideally expanded to demonstrate if there is a tradeoff between cold-start performance and the other enabling characteristics for pre-chamber use.

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

Reviewer 1:

This project supports the overall DOE objectives in providing low emissions dilute combustion strategies in cold start and operation and modeling capabilities.

Reviewer 2:

Yes, this project directly supports the overall DOE goals—reducing cold-start emissions by better understanding the fundamental mechanisms behind the formation of fuel films and locally rich operation.

Reviewer 3:

The project is directly connected to DOE objectives on improving vehicle emissions. As engine and aftertreatment effectiveness increase and emissions regulations grow ever more constraining, the bulk of emissions occurs during cold-start operation. Understanding details of operation during cold start is crucial for developing strategies to reduce emissions further under these conditions.

Reviewer 4:

The reviewer asserted that the project is directly relevant to putting clean and efficient ICEs into LD fleets.

Reviewer 5:

Understanding the base spark ignition cold start is more important. The application of an active pre-chamber is of lower priority.

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

Reviewer 1:

The amount of effort, facilities, and funding appears to be consistent with a project this size.

Reviewer 2:

The reviewer commented sufficient. The PI did not indicate additional resources would improve the outcome.

Reviewer 3:

Each team seems to have adequate resources for engine testing or simulation. ANL needs to extend the engine testing range to higher exhaust heat flux but it is more on the technical side.

Reviewer 4:

Funding looks appropriate for the scale of the effort associated with each subtask. The funding going toward validation of a PAH and soot model against experimental data looks high for this particular scope. Increased funding for the pre-chamber effort should be considered if the scope increases to look at tradeoffs in design for cold-start conditions versus lean or dilute performance.

Reviewer 5:

More of the resources should be focused on understanding the baseline cold-start strategy and looking for opportunities for improvement before applying advanced ignition concepts or complicating the test protocol any further.

Presentation Number: ace150 Presentation Title: Enabling Low-Temperature Plasma (LTP) Ignition Technologies for Multi-Mode Engines through the Development of a Validated High-Fidelity LTP Model for Predictive Simulation Tools Principal Investigator: Nick Tsolas (Auburn University)

Presenter

Nick Tsolas, Auburn University

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-34 - Presentation Number: ace150 Presentation Title: Enabling Low-Temperature Plasma (LTP) Ignition Technologies for Multi-Mode Engines through the Development of a Validated High-Fidelity LTP Model for Predictive Simulation Tools Principal Investigator: Nick Tsolas (Auburn University)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The reviewer said remarked that this is a very solid approach to developing an LTP model and comparing the current available commercial software.

Reviewer 2:

Overall, this work is well designed and is addressing key technical barriers that could allow for the development of advanced ignition systems. Each of the four work packages is very well planned and executed.

It is not clear how the four efforts in this work are interconnected, if they are in fact interconnected at all. If they are, it would be beneficial to communicate these connections visually to show how the four efforts ultimately are integrated to help develop improved ignition systems. If they are not interconnected, this reviewer suggested trying to integrate portions of them into one another, even if it is at the latter stages of the validation or trial efforts.

Reviewer 3:

The combination of simulation and experimentation, including combustion vessel studies, is an acceptable overall approach but seems to stop short of engine validation. Still, the technical, phenomenological insights should be valuable. The U.S. DRIVE Roadmap recommends evaluating plasma ignition, among others. This presentation would be better if it included a slide on the overall status of plasma ignition and what other

barriers besides simulation exist. For example, are these systems in use and what is the record of success? The approach is missing an industry collaborator or potential manufacturer.

Reviewer 4:

It is unclear why the team needs both an exascale solver based on AMReX and VizGlow. Can one solver be chosen to avoid proliferation and development of different solvers?

Reviewer 5:

This project is aimed at developing a computational tool for simulating LTP ignition of hydrocarbon fuels. It includes both experimental and computational pieces in the overall approach. It is a bit unclear to the reviewer why two computational frameworks—AMReX and VizGlow/CONVERGE—are needed. Are both tools adequate for the project? Both tools have advanced mesh refinement (AMR) and have significant parallelization capability. It needs to be made clear that the work in both codes is not redundant. The reviewer's fear was that AMReX is developed for this project, but then this tool is not transferred or used by OEMs actually designing engines. The experimental approach appears to be reasonable.

Reviewer 6:

This is a fairly new project and the proposed approach seems plausible. A question was raised during the discussion whether VizGlow work and AMR software work are duplicative, for which the PI replied that one of the co-PIs believes that VizGlow has some inherent issues. This reviewer indicated that since the plasma ignition models are not well understood, it is a worthwhile endeavor to use both tools; but, at the end of the work, the team should point out the strengths and weaknesses of each tool as the predicted results will be validated with experiments.

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

Reviewer 1:

The project is in early stages, but the team members have exhibited good progress and have generated useful results. The experimental apparatus is moving along well.

Reviewer 2:

This project kicked off in January 2020 and was impacted by the COVID-19 pandemic. While the progress is behind the planned schedule, it is progressing appropriately given the circumstances.

Reviewer 3:

Progress is limited due to the pandemic, but progress is being made on the modeling work.

Reviewer 4:

Solid progress has been made at all teams although the project just got started. Some experimental delays due to the pandemic are understandable.

Reviewer 5:

Of course, the experimental initiative has been delayed due to COVID-19; however, some progress has been made on the computational side. This project has only just started in January of this year and so not a lot of progress is expected. Having said that, chemical mechanisms have been evaluated and reduced, and some parametric studies have been performed.

Reviewer 6:

The reviewer noted that it is too early to gauge this, especially with the interruptions caused by COVID-19.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

This is a very good team, comprised of two National Laboratories and two universities.

Reviewer 2:

There is good collaboration between all the teams involved in the project.

Reviewer 3:

The roles of each team member are sufficiently clear. There is some debate about which software foundation is best but seems likely to be worked out. The lack of an industry partner or advisory panel is noted. There is a private sector company pursuing commercialization of plasma ignition, also under DOE funding, which perhaps should be acknowledged.

Reviewer 4:

This project is a collaboration of two National Laboratories and two universities and is leveraging the expertise of each individual organization. Referencing prior comments, the reviewer suggested it would be beneficial to increase coordination of these efforts, or to communicate them more clearly if they already exist. Additionally, it would be helpful to engage with industry (e.g., a Tier 1 supplier of ignition systems) to inform the work and facilitate potential commercialization.

Reviewer 5:

The direct linkage of the work being conducted at the University of Texas at Austin and ANL is unclear. How do these modeling efforts overlap with each other?

Reviewer 6:

Not applicable was indicated by this reviewer.

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

Reviewer 1:

The reviewer commented the next step plan seems reasonable.

Reviewer 2:

If complex fuels (e.g., gasoline) were able to be evaluated experimentally with the gas chromatography mass spectroscopy (GC-MS) in the Auburn work, it could be instructive to understand what a complex fuel breaks down into – even if detailed kinetic modeling is not possible for that fuel. In other words, characterization and speciation of complex fuels experimentally might inform the experiments and modeling of the simpler fuels in this work, at least based on the understanding of this reviewer.

Reviewer 3:

Only 5% of the project has been completed since the project started in January 2020, and much of the experimental effort has been delayed due to COVID-19. So, in essence, the near entirety of the project is future work and the original scope should be maintained.

Reviewer 4:

There was no "Future Research" slide, but the reviewer assumed efforts will be made to accelerate the experimental measurements when possible.

Reviewer 5:

Since the project is only 5% complete, practically all research is "future." However, there still should have been a slide and few points made about research for the next year. The reviewer presumed this was an oversight and will be corrected next time.

Reviewer 6:

The reviewer asserted that this is one area that needs some improvement. Tables are provided with tasks and milestones, but it would be better to see more details about the future tasks, their barriers, and alternate pathways.

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

Reviewer 1:

This work fully supports DOE's objectives and is filling gaps in knowledge that could lead to improved engine efficiency via the development of advanced ignition systems.

Reviewer 2:

The current work is relevant to the overall DOE objectives and has the potential to contribute to different projects.

Reviewer 3:

Yes, this project supports the overall DOE objective of designing more efficient and cleaner engines.

Reviewer 4:

Technical developments from this project can assist PACE deliverables.

Reviewer 5:

Engines that use highly dilute mixtures, or attempt to ignite mixtures at very high pressures, or difficult-toignite fuels can benefit from better, more robust ignition systems. The U.S. DRIVE Roadmap recommended such.

Reviewer 6:

Absolutely. As we are looking for efficient engines with air or EGR dilution, it is important to understand the physics behind alternative ignition mechanisms such as LTP. The intersection of LTP and EGR will be interesting, and the emergence of radicals and EGR species and their interaction will be challenging. For example, NO_x (in EGR) is known to have an impact on ignition delay.

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

Reviewer 1:

The resources and team executing this work are sufficient for achieving the project milestones in a timely fashion.

Reviewer 2:

The team has sufficient resources.

Reviewer 3:

From the amount of information that was presented to the reviewer, the reviewer believed that the resources for this project are sufficient.

Reviewer 4:

There are no resource issues except some measurement delays, which are set to resume.

Reviewer 5:

The budget information is a little vague. Is the National Laboratory funding \$300,000 total, or per year, or per lab? Given that the project output is computational methods and data (not a prototype system), the resources seem satisfactory.

Reviewer 6:

The reviewer remarked that it is too early to comment as much of the project is yet to be accomplished.

Presentation Number: ace151 Presentation Title: Hierarchically Informed Engineering Models for Predictive Modeling of Turbulent Premixed Flame Propagation in Pre-Chamber Turbulent Jet Ignition Principal Investigator: Haifeng Wang (Purdue University)

Presenter

Haifeng Wang, Purdue University

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-35 - Presentation Number: ace151 Presentation Title: Hierarchically Informed Engineering Models for Predictive Modeling of Turbulent Premixed Flame Propagation in Pre-Chamber Turbulent Jet Ignition Principal Investigator: Haifeng Wang (Purdue University)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

Starting from a very detailed and accurate simulation and then paring down to an engineering level simulation all the while comparing to bench rig and engine test results is an excellent approach.

Reviewer 2:

The project is well designed to improve the predictive accuracy and efficiency of turbulent combustion submodels for the simulations of premixed flame propagation initiated by pre-chamber turbulent jet ignition, from DNS to LES to RANS. However, the newly developed model should be validated based on experimental results, in addition to DNS.

Reviewer 3:

The team seeks to leverage DNS simulations to improve LES and RANS models. However, will the proposed power-law scaling account for turbulence-chemistry interaction in the RANS framework?

Reviewer 4:

The technical barriers specified were to establish the modeling tools for rapid screening design and to build a robust ignition system with less variability. The approach of working with DNS for a turbulent jet ignition (TJI) model—LES simulation supported by statistics properties from DNS and final RANS simulation aided by the LES—is generally okay and acceptable. However, the technology transformative connections are not clear. For example, what type of specific data and specific sub-models, other than power-law scaling, will be

utilized from DNS to LES to RANS and the ranges of Karlovitz number under the highly stretch flame occurring in the typical engine condition? Individual Objectives defined in Slide 3 seem to stand alone without the profound connection among them. There is no return feedback algorithm to improve the DNS sub-model development from Argonne (LES and RANS) to Purdue (DNS) as the flow chart describes in Slide 5. The reviewer indicated that the LES and RANS simulations at Argonne have a very weak connection with DNS work, especially because the targets and goals being investigated are unclear. The reviewer also indicated that feedback for each simulation to improve the sub-models being investigated was lacking.

Reviewer 5:

The reviewer worried that the approach for this project is too complex with DNS, LES, and RANS all part of the methodology. If the project were successful in taking DNS to LES, that in itself would be a success. In addition, how much more effort should we be putting into RANS models? If the goal is exascale, then the accuracy of LES simulations should be leveraged.

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

Reviewer 1:

This project seems to be on track, with the Q1 milestone completed and the others on schedule for this year.

Reviewer 2:

The project started early this year. As planned, the PI completed hypothesis testing of the existence of powerlaw scaling of sub-filter scaling mixing in high-Karlovitz turbulent jet flames from both global and local perspectives.

Reviewer 3:

It would be good to show a comparison of predictions of a flame with and without the addition of the powerlaw scaling.

Reviewer 4:

The reported progress does not seem to be very extensive and is not understandable by someone who is not a CFD expert.

Reviewer 5:

Technical progress and accomplishment on this project are too early to judge since this project has just started in January 2020. However, it looks like DNS work mainly focuses the power-law scaling sub-model development under the high-Karlovitz turbulent premixed flame in order to provide the statistics properties for the LES simulation only. In reality, most of engine combustion conditions are under high pressure and lean combustion, which may significantly affect the burning process at the flame front due to the non-unity Lewis number effect. The power-law scaling model seems to be overly simplified, and the effect of Lewis number on the DNS flame simulation needs to be considered when the high mixing occurs at the flame interface.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Collaboration with ANL for engine data and a Purdue colleague for bench rig data is good.

Reviewer 2:

The collaboration level in simulation seems to be adequate between Purdue and Argonne while the reviewer anticipated that it may be problematic for DNS validation at engine conditions due to the lack of high-pressure TJI data.

Reviewer 3:

The Purdue-Argonne team is a strong one. Sandia is also listed a partner, but the reviewer did not see any of the budget going toward it. How do they fit in?

Reviewer 4:

The project started early this year, so it is difficult to assess the level of collaboration. The reviewer hoped that PIs can strengthen the collaborations with the auto OEMs or other companies who are working on TJI.

Reviewer 5:

Is the modeling work targeting a specific type of TJI or is it generalized? Can the species composition in the TJI rig be controlled?

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

Reviewer 1:

Since this is a 15-minute presentation, the presentation provided very limited information about the future plan. But, it seems well planned based on the "Milestones" of the project. Again, PIs should consider validation based on real engine results.

Reviewer 2:

The proposed future research for this project is nicely laid out in a logical and organized manner. It would be nice to see some alternate development pathways, however, especially for a project like this that relies on a fairly complex approach.

Reviewer 3:

It is not clear when work with the engineering level simulation will be undertaken. This is an important step toward helping engine developers design new engines with TJI.

Reviewer 4:

What is the plan to incorporate machine learning shown in Slide 5? What ML approach is being used and specifically how will it be linked to the RANS engine simulation? Will ANL also simulate the TJI rig?

Reviewer 5:

To the reviewer, the future plan is not concrete in a way because there seems to be a very weak connection between DNS versus LES and RANS. The reviewer believed that the future success depends on the collaboration between the experimental effort for new validation method and the work on a minimum tuning parameter model with fast turnaround of computation time, especially LES and RANS simulations.

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

Reviewer 1:

The reviewer believed that this project does support the overall DOE objectives. This is summarized by the two U.S. DRIVE Roadmap barriers listed on the Overview slide: "Understanding and robust modeling tools for rapidly screening proposed designs based on sound metrics are lacking"; and "More robust ignition systems for lean and EGR, as well as boosted conditions that reduce combustion variability are needed". This work attempts to overcome those barriers for TJI combustion.

Reviewer 2:

TJI is another approach at enabling dilute, high-efficiency gasoline engine technology toward meeting the U.S. Department of Energy's efficiency goals. It does support DOE goals.

Reviewer 3:

The technical work has linkage to the PACE program.

Reviewer 4:

Accurate engineering level simulation tools will help engine designers develop more efficient engines, and this will help reduce energy consumption.

Reviewer 5:

From a broad perspective, the reviewer responded yes. However, in order to improve the sub-model development, experimental data validation at high pressure and high EGR conditions is needed for DNS.

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

Reviewer 1:

The reviewer believed that the resources for this project to achieve the stated milestones are sufficient.

Reviewer 2:

The resources are sufficient.

Reviewer 3: Resources are sufficient.

Reviewer 4:

The resources for simulation appear to be adequate.

Reviewer 5:

The team has the necessary resources to conduct the proposed research. However, the reviewer hoped DOE can provide additional funding to support model validation with real engine results.

Presentation Number: ace152 Presentation Title: Development of High-Fidelity and Efficient Modeling Capabilities for Enabling Co-Optimization of Fuels and Multi-Mode Engines Principal Investigator: Matthias Ihme

(Stanford University)

Presenter

Matthias Ihme, Stanford University

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-36 - Presentation Number: ace152 Presentation Title: Development of High-Fidelity and Efficient Modeling Capabilities for Enabling Co-Optimization of Fuels and Multi-Mode Engines Principal Investigator: Matthias Ihme (Stanford University)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

A solid and efficient combustion model is definitely needed for the multi-mode combustion. The chemistry is key for high-energy ignition modeling. The approach is sound and reasonable.

Reviewer 2:

The approach is a good one and leverages the expertise of the team members well. It is particularly nice to see consideration of heat transfer taken into account in the simulations as this can be a significant loss to efficiency. The focus on high-performance computing and optimization of the methods is also critical, so coordination with Argonne in that respect is important.

The only piece of the approach that is currently missing is the lack of treatment of radiation. The PI indicated that it may not be necessary due to the dilute conditions and soot, but it is actually those dilute conditions that cause gas-phase radiation and the resultant re-distribution of temperature to be quite important. The PI pointed to the work from Dr. Dan Haworth's group—this will be important to consider going forward. Fortunately, the PI also mentioned a collaboration with Dr. Volker Sick, who has worked with Dr. Haworth's group in the area of radiation and wall heat transfer in the past. It would be prudent to determine whether gas-phase radiation will be a contributor to temperature re-distribution and then also wall heat transfer early in the project to improve the impact of the work down the road.

Reviewer 3:

Multi-mode combustion is the chief focus of DOE VTO, and the project tries to address the challenges through fundamental studies including Pareto-efficient combustion, chemical reduction strategies for plasma ignition, a non-equilibrium wall model for heat transfer, and, finally, multi-mode engine simulations on an exascale platform. All these tasks are critical, and a fundamental understanding is necessary.

Reviewer 4:

The reviewer thought this project sounds impressive, but wondered how relevant it is. For example, do we need the "Pareto-efficient combustion model" to simulate these conditions? What is the benefit of developing Nek5000 when industry does not use this tool for designing engines? Do not get the reviewer wrong, the reviewer thought that all of the work being done under this project is likely high quality—the reviewer's concern is more about if it is needed.

Reviewer 5:

Does the Pareto-efficient combustion model run on GPUs? If not, would there be a significant speed advantage? Also, how does the Pareto-efficient combustion model compare to LLNLs Zero-RK approach?

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

Reviewer 1:

Solid progress has been made for various topics in the project.

Reviewer 2:

The project does a nice job laying out the technical accomplishments that have been completed so far by each of the collaborators.

Reviewer 3:

The team is making progress in all technical areas. The team should include a timeline or chart showing when each of the tasks will be complete.

Reviewer 4:

The project has only recently started, and the initial accomplishments in the first approximately8 months have been good. The use of methane for the multi-mode combustion simulations at the outset is a bit limiting, given the uniqueness of methane ignition chemistry and the need for more complex fuels in real engine configurations, but it is good to hear that the PIs have plans to move quickly to iso-octane. Concurrent development and implementation of models into the Nek5000 framework is important.

Reviewer 5:

The project started in October 2019 and has less than a year under the belt. About 15% of the work is completed and seems to be on track. The reviewer thought a better assessment of the progress could be done at next year's AMR.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer found very solid and extensive collaboration and coordination with other institutions.

Reviewer 2:

This is a strong team comprised of Stanford University, the University of Connecticut, and Argonne. There is also coordination with Sandia, the University of Illinois Urbana-Champaign, the French National Centre for Scientific Research, and the University of Michigan at Ann Arbor.

Reviewer 3:

There seems to be good collaboration across the team, and a good team has been assembled to tackle all of the issues outlined in the project. The reviewer encourages further interactions with Isaac Ekoto as well as the simulation team at Argonne in the area of ignition, as there has been a significant research focus in that area over the past few years as part of this portfolio. The continued connection with experimental data is important.

Reviewer 4:

This is a small team compared to several other collaborations seen in ACE. Some industry collaboration for the team would be helpful to have some ground-truthing of the results achieved here. The team should also see if there could be potential collaboration with Convergent Science or other CFD provider to see if reduced order models could be implemented in their solvers, especially for plasma ignition.

Reviewer 5:

Why is there no engagement with Argonne National Laboratory on ignition modeling? How does the proposed ignition model described here differ from what is being done at Argonne?

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

Reviewer 1:

The project tasks lend well to improving the Nek5000 engine simulations.

Reviewer 2:

The next steps of the project area seem logical and the work to date sets up a good foundation on which to build toward these ambitious goals. As mentioned previously, the PIs are encouraged to consider the effects of radiation, especially since the development of non-equilibrium wall modeling is an explicit goal of the project. Otherwise, the remainder of the tasks are sound.

Reviewer 3:

The proposed future work sounds reasonable. Is there a plan to merge to one platform for model cross-validation at a certain point?

Reviewer 4:

Since the project is only about 15% complete, much of the originally proposed work is still future work. As of now, the future work seems realistic and relevant. A better assessment could be done at next year's AMR.

Reviewer 5:

The team does a good job outlining the proposed future research, but again the reviewer questioned how necessary much of it is.

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

Reviewer 1:

Absolutely. These are the kind of activities that DOE needs to be funding at the fundamental level in universities and National Laboratories.

Reviewer 2:

The project goals can be leveraged to support the PACE program.

Reviewer 3:

This project supports the overall DOE objectives by developing improved models and algorithms to enable reliable predictions to support the Co-Optima program.

Reviewer 4:

This project particularly supports DOE goals of development of models and methods for high-performance computing. The knowledge about combustion processes will also be important, and the PIs are encouraged to continually be aware of the other work going on in the Co-Optima and PACE projects as there are a lot of connections that could be made.

Reviewer 5:

Yes, the project is highly relevant, especially in its more accurate sub-models to support different projects. For example, the advanced combustion model would be a good candidate for the cold-start project, etc.

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

Reviewer 1:

Both financial and personnel resources are sufficient. Computing resources for the project are critical and also sufficient.

Reviewer 2:

Resources are appropriate for a project that is predominantly modeling and simulations.

Reviewer 3:

The project has sufficient resources.

Reviewer 4: The resources are sufficient at this stage.

Reviewer 5:

The resources are sufficient for this project.

Presentation Number: ace153 Presentation Title: Chemistry of Cold-Start Emissions and Impact of Emissions Control Principal Investigator: Melanie Moses-DeBusk (Oak Ridge National Laboratory)

Presenter

Melanie Moses DeBusk, Oak Ridge National Laboratory

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

All reviewers indicated that the project was relevant to current DOE objectives. All reviewers also indicated that the resources were sufficient.

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



Figure 1-37 - Presentation Number: ace153 Presentation Title: Chemistry of Cold-Start Emissions and Impact of Emissions Control Principal Investigator: Melanie Moses-DeBusk (Oak Ridge National Laboratory)

Reviewer 1:

The research plan is carefully designed and systematically executed.

Reviewer 2:

This project is well designed and doing a good job of speciating cold-start HC (and particulate) emissions from two late model pick-ups.

Reviewer 3:

The approach is good that HC speciation is explored and analyzed in multiple ways. It would be interesting to see how catalyst companies design the HC trap based on this understanding. Further, as tailpipe emissions regulations are becoming stringent, it is really important to understand details of exhaust and tailpipe emissions.

Reviewer 4:

The project specifically addresses the following barrier identified in the U.S. DRIVE Roadmap: "Similar to design of HC Traps for gasoline exhaust temperature ranges, HC Traps must be designed for effective control of specific HC species that are present in gasoline engine exhaust." The reviewer's impression is that the overarching goal of the project is to measure engine-out HC speciation, TWC-out speciation, and HC-trap out speciation. While these will be useful data, it would be good to know how these data are to be used. That is, will the speciation data be used to design HC traps? Will there be any modeling efforts?

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

Reviewer 1:

The team reported on the laborious work of collecting and analyzing the emission molecules (especially HCs) from the critical first 250 s during typical engine cold start on representative vehicle platforms. The analyses are rigorous and are well supported by abundant data.

Reviewer 2:

Overall progress appears to be on track to meet the stated timeline.

Reviewer 3:

The project is up to schedule and delivered the results with satisfaction. It would be beneficial if particle number (PN) also would be categorized by PN size.

Reviewer 4:

Detailed cold-start hydrocarbon speciation has been completed on two pick-ups from an engine-out location and after the close-coupled catalysts.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The reviewer remarked that there is good collaboration with the Ford and Umicore partners on this project.

Reviewer 2:

ORNL and Umicore teams seem to be well coordinated for this project, with the consultation support from Ford and others.

Reviewer 3:

Collaborations between National Laboratories and industry are shown to be effective.

Reviewer 4:

The project appears to be coordinated well across the various participants, although the bulk of the work is being done by ORNL. Regarding the collaboration with the CLEERS community for sharing of results, is there any plan to share the collected data (or a subset thereof) through the CLEERS database? This type of data is difficult to find outside of industry.

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

Reviewer 1:

Future research is planned for GPF impact on the cold-start emissions. Approach and work content are good.

Reviewer 2:

The project will logically next look at cold-start HC speciation changes after the addition of an underfloor HC adsorber and an underfloor HC adsorber plus GPF. The project will also complete cold-start and re-start HC speciation for a hybrid vehicle application. It would be interesting to see how re-starting HC speciation may change with the time between re-starts in a hybrid vehicle. It also appears that HC adsorber studies will include engine aging of the HC adsorber using the U.S. DRIVE storage aging protocol (50 hour [h]) cyclic aging at 700°C). It would be interesting to speciate HCs post-trap after 25 h and then 50 h of aging to characterize aging impacts on the HC adsorber function.

Reviewer 3:

The proposed future work is sensible and addresses several barriers, including the "rolling cold start" challenge with hybrid vehicles. If there are any decision points (Go/No-Go decisions) or alternate development pathways considered, they are not apparent in the presentation.

Reviewer 4:

Considering the data availability to the public and conclusion applicability to the U.S. automotive industry as a whole, the team needs to go beyond the demonstration of successful data collection (the work can be done by OEMs) by looking into the collected data from the chemistry perspective of how these emission characteristics evolve with vehicle propulsion systems, mileage, and aftertreatment system designs. Such more insightful knowledge as a know-how database can ultimately help the design of more advanced ACE systems, which also echoes the title of the project.

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

Reviewer 1:

This project directly supports the VTO mission to develop cost effective aftertreatment technologies that further reduce emissions.

Reviewer 2:

This project will add important understanding to the development of HC adsorber technology.

Reviewer 3:

It is important to understand the details of emissions from engines and the role of various components. Most of the studies focused on NO_x and PM, but this study is complementary and provides much refined details about HCs and PN.

Reviewer 4:

Having a thorough understanding of the specific chemistry for most of (if not all) the HCs species emitted during the cold start is pivotal in enabling targeted development of catalytic materials and systems to handle the emissions.

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

Reviewer 1:

This project appears to have sufficient resources to complete the studies planned with HC adsorbers on the selected pick-ups and to characterize cold-start and re-start HC emissions from a hybrid vehicle.

Reviewer 2:

Sufficient resources were contributed by DOE for this work.

Reviewer 3:

Resources for this project appear to be sufficient.

Reviewer 4:

The project coordinates the resources to ensure the completion of the project very well on the hardware side. As suggested, the know-how chemistry should be emphasized by the completion of the project.

Presentation Number: ace154 Presentation Title: Heavy-Duty Hybrid Diesel Engine with Front-End Accessory Drive-Integrated Energy Storage Principal Investigator: Chad Koci (Caterpillar)

Presenter Chad Koci, Caterpillar

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-38 - Presentation Number: ace154 Presentation Title: Heavy-Duty Hybrid Diesel Engine with Front-End Accessory Drive-Integrated Energy Storage Principal Investigator: Chad Koci (Caterpillar)

Question 1: Approach to performing

the work—the degree to which technical barriers are addressed, the project is well-designed and wellplanned.

Reviewer 1:

The approach is very good. The analysis, which led to the identification of how best to apply hybridization, was well done and resulted in identifying the approach that is being taken—hybridized front-end accessory drive (FEAD). It appears to be a very good example of analysis-led design.

Reviewer 2:

The project approach is rather complete, encompassing air handing systems to meet engine downsizing targets, waste heat recovery, parasitic loss reduction, and hybrid powertrain integration. Overall performance targets are clear: 17% percent improved fuel efficiency and reduction of cost of ownership.

Reviewer 3:

The project has sharpened its focus and resources to develop the heavy-duty hybrid diesel (H2D2) for the offroad application. The project has a good systematic approach of using technologies to increase the powersystem efficiency through engine downsizing and integration of hybrid front-end accessory drive, including high-speed flywheel (HSFW), turbocharger, and motor-generator unit (MGU). It is clear that a very good integration of many technologies shows promise for significant reduction in fuel consumption while this requires very careful matching of the operating characteristics of each component of the multiple technologies being implemented. The approach being followed here is a systematic and fundamentally based. Given that, the reviewer would have liked to see the data that led to the technical decisions, especially for the thermofluid/simulations and waste heat recovery methods. For example, the reviewer questioned the air delivery system improvement of 30% improved power density, and inquired about the specific engine combustion technology adopted to maintain the same level of durability shown in the reference engine.

Reviewer 4:

The analysis-led design approach being implemented in this project, which heavily leverages analytical tools in the early phase if the program is to select and validate system architecture decisions, is fundamentally sound. However, some of the architecture selections, like the use of turbo-compounding as well as the use of both flywheel and motor generator unit, are puzzling since they introduce more complexity than is required.

Reviewer 5:

It was not clear to the reviewer what the distinction is between research and the normal engine development work that Caterpillar does anyway.

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

Reviewer 1:

The simulation results have shown some encouraging outcomes that have supported the Go/No-Go decisions for the selected architecture.

Reviewer 2:

The project is on task relative to the statement of work (SOW) schedule. The postponement of the first Go/No-Go decision was to enable some additional analysis to be performed and is not affecting the progress of the project. The hybridization system has been identified, along with its components and the logic for its operation. The downsized engine has been identified, and the team is proceeding with set-up and testing.

Reviewer 3:

There has been good progress as the project completes its first year. Some of the reported delays were explained in regard to the overall concept selection and optimization. No delay was reported on the Go/No-Go decision. The presentation makes a good case for the importance of the supervisor-manager and explains the challenges of providing power through the base engine (now download) and from the hybrid and the SuperTurbo power plant. Power system predictions are also included and broken down by category.

Reviewer 4:

In the first year of the project, key items were identified to develop the high-efficiency power system and complete the individual component analysis. It seems the Phase 1 engine was built, and therefore, the project has made significant progress that largely exceeds expectations. However, the reviewer would have liked to see the detailed breakdown of the fuel efficiency table on Slide 12 compared to the cost and performance achievements. The reviewer also would have liked to see results from the thermo-fluid, structure, and dynamic simulations in order to address the air handling requirement in the power system. In the presentation, it is not clear how to increase the efficiency over start/stop implementation.

Reviewer 5:

It was not clear to the reviewer what the distinction is between research and the normal engine development work that Caterpillar does anyway. For example, the reviewer could not figure out if the downsized concept engine was already in development before the project started, but it was shown as an accomplishment. In addition, the reviewer assumed most components put together in the projects are developed by suppliers.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Reasonable levels of collaboration and coordination have been demonstrated between Caterpillar, SuperTurbo Technologies, the University of Texas at Austin, and some vendors.

Reviewer 2:

There appears to be strong collaboration between Caterpillar and the suppliers and DOE.

Reviewer 3:

Work by project partners is indicated throughout the presentation.

Reviewer 4:

The collaboration level seems to be adequate but requires more data exchange and feedback among the academic and industry partners. In particular, the work from the University of Texas at Austin is not well defined.

Reviewer 5:

The reviewer did not see anything here about the collaborative work between parts. For example, what was the role of the University of Texas at Austin?

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

Reviewer 1:

The work is well outlined. The work will be taking place in the main subsystems and hybrid integration.

Reviewer 2:

With the analysis done and build-up underway, future work has been clearly identified. The team looks to be on track for their December Go/No-Go decision on proceeding with durability testing.

Reviewer 3:

The future plans are to continue working on the extension of the Phase 1 concept demonstrator engine-only testing and major subsystem analysis. In general, the project's work continues to design the high-efficiency power system through the downsized engine development. In particular, the durability of the downsized engine will be challenging because of the 30% increased power density.

Reviewer 4:

What the reviewer saw from future work is just normal engine development work.

Reviewer 5:

The proposed future research has effectively planned the appropriate tasks and decision points to achieve the project objectives. However, alternate development pathways to mitigate durability concerns as a result of increased power density (cylinder head structural integrity, bearings, crankshaft, etc.) have not been clearly identified. This H2D2 engine is being designed for Caterpillar's wheel loader, excavator, and articulated dump truck. Hybrid systems are usually designed for a given duty cycle. What application duty cycle is being selected for this architecture design? The PIs should consider whether the selected application duty cycle will create a challenge for a different application duty cycle.

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

Reviewer 1:

Yes, this project supports the overall DOE objectives because it plans to deliver a more fuel-efficient power solution that will have a substantial impact in reducing the total cost of ownership for off-road applications than current Tier 4 diesel engines.

Reviewer 2:

The project seems to be well aligned with DOE objectives by focusing on high-capability air handling equipment and waste heat recovery and reduction in fuel consumption.

Reviewer 3:

It appeared to the reviewer that overall work is relevant.

Reviewer 4:

Heavy-duty, off-road equipment is a critical aspect of our infrastructure and economic well-being. It is also a non-trivial consumer of hydrocarbon fuels, and it is likely to be dependent on IC engines fueled with liquid energy carriers for decades to come. Reducing its CO_2 footprint is important.

Reviewer 5:

Is there any engine development work not in line with DOE objectives of higher efficiency, lower emissions, low cost, and better reliability?

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

Reviewer 1:

The project is 35% complete and on plan with the current funding level.

Reviewer 2:

It appears that the project is progress on schedule with the current resources.

Reviewer 3:

Resources appear adequate.

Reviewer 4:

The resource appears to be sufficient.

Reviewer 5:

It was not clear to the reviewer why this project received so much DOE funding compared with funds received by National Laboratories and academia for more important work and better results. Is all the work developed by National Laboratories and academia benefiting all industry partners?

Presentation Number: ace155 Presentation Title: Low-Mass and High-Efficiency Engine for Medium-Duty Truck Applications Principal Investigator: Qigui Wang (General Motors)

Presenter

Qigui Wang, General Motors

Reviewer Sample Size

A total of six reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-39 - Presentation Number: ace155 Presentation Title: Low-Mass and High-Efficiency Engine for Medium-Duty Truck Applications Principal Investigator: Qigui Wang (General Motors)

Question 1: Approach to performing

the work—the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

It is good to see that previous DOE program accomplishments are able to contribute to this new project, particularly the propulsion materials and lightweight materials projects referenced.

Reviewer 2:

The reviewer appreciated the team looking at two engine configurations in the first phase of this project. The approach seems appropriate for the technical objectives.

Reviewer 3:

The approach is comprehensive. The use of two new engine configurations at the early stage and then relying on an analytical approach to down-select the engine are technically sound approaches. It would be interesting to see in the next annual report how the integrated computational materials engineering (ICME) approach would be applied in order to accelerate development, reduce risk, and enable tailored properties that lead to cost effective mass reduction.

Reviewer 4:

The project is in its beginning stage. Targets are clearly identified. The project captures two phases (four tasks), encompassing research and development, followed by validation and demonstration. New combustion technologies are outlined. Advanced materials and manufacturing technologies are outlined.

Reviewer 5:

The approach is generally good, but there is not enough definition on the exact approach to give a very solid review. The reviewer chalked that up to this being a pretty new project and looks forward to the next update.

Reviewer 6:

Although very early in the project, already known barriers and challenges were not highlighted much. For example, initial crankshaft analysis demonstrated strength improvement but little weight saving. Peak cylinder pressures need to go up by roughly 50%, but block and head strengths are going to need much more work. Comparing naturally aspirated versus boosted engine designs is a very good thing. Combustion challenges to meet the efficiency target are formidable—even more so with the weight reduction target. The reviewer realized that this is very early in a 4-year project and many big problems have to be solved. The reviewer was just looking for a bit more on the size of the challenge and potential barriers.

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

Reviewer 1:

There has been some evident progress in the studies of materials changes to save weight. It is difficult to quantify exactly how fast things should move during a project startup. The reviewer hoped that in the next meeting we can get a better evaluation of the technology development for the combustion system and materials development.

Reviewer 2:

The project is too new to provide much feedback on accomplishments. Ensuring it will fit in the vehicle and projecting the potential weight savings did show significant progress.

Reviewer 3:

The project has just started, so there is not much in the way of accomplishments. The team seems to have a solid plan and is making progress on early requirement setting and research of materials.

Reviewer 4:

The reviewer referenced prior comments and indicated that the project team appears to have a good start and a feasible plan, but wanted a bit more relative to the challenges and barriers.

Reviewer 5:

Good progress has been made in layout and performance simulation of engine architectures, and weight reduction is also moving forward, too. It would be interesting to see whether the cast aluminum engine block can be realized in the next annual report, which can significantly reduce the engine weight. What is Phase 2 Greenhouse Gas Emissions Model (GEM)? Would that be the EPA Phase 2 GEM, which is a vehicle model?

Reviewer 6:

Technology accomplishments included layout and performance simulation of the engine architecture (sweeping engine size parameters—not identified nor ranges identified) via Phase 2 GEM. The baseline was done with the 2015 GM MD truck engine. Some one-dimensional (1-D) engine performance simulations were shown. The physical engine layout of the cab was presented. Mass reduction opportunities are shown, with correlation to the impact to the particular components. Key components, such as block and crankshaft, are included.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

The team member responsibilities appear to be well defined.

Reviewer 2:

Work by project partners is indicated throughout the presentation.

Reviewer 3:

It seems that all partners have contributed to the program.

Reviewer 4:

There is a nicely organized team with university, supplier, and National Laboratory partners. In future years, please be sure to indicate the specific accomplishments that each contributed.

Reviewer 5:

Universities and ECK Industries Inc. seem to have their teams identified and work documented. Is there any chance any customer groups can be added in an advisory mode, such as commercial truck fleets or municipal customers? The reviewer believed this would be very beneficial and likely one or more of those groups would be happy and even honored to participate.

Reviewer 6:

It is not obvious that any work has been done at the outside partners yet. There is a list of collaborators with some defined tasks, but it is hard to see what is being done across the team. The reviewer would have liked to see more explanation of how the work split has been accomplished.

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

Reviewer 1:

The proposed future work is very well defined.

Reviewer 2:

The work plan is good, and the reviewer was confident that it will result in a project success. Once there is more concrete definition of the path forward, it will be easier to evaluate the work plan against the distance to the target.

Reviewer 3:

Future work as outlined in the presentation is logical. More detailed internal project plans should highlight barriers and potential alternatives as soon as feasible to identify potential changes to the technology path.

Reviewer 4:

The work is well outlined and will be taking place in the main subsystems. Some consideration is being given to cost-effectiveness (this is tough as no criteria are given), and a little more detail on the down-selection could be given.

Reviewer 5:

The remainder of FY 2020 and FY 2021 research plans look good, although it is not really clear what the criteria for technology down-selection going into phase 2 will be based on if both meet the FOA minimum targets.

Reviewer 6:

A high level was presented, but on only one slide. The reviewer wished that the team had given more detail on the work planned as the project is in such an early stage and is a relatively big project (\$10 million). This should be a bigger part of what is presented at an AMR.

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

Reviewer 1:

The project meets the DOE mission of reduced energy consumption and will contribute to the energy security of the United States.

Reviewer 2:

The reviewer believed this project does support the DOE objectives of improving emission and weight in the 3500-truck class of vehicle.

Reviewer 3:

Higher efficiency SI engines for medium-duty applications are a huge potential environmental benefit; this is a well-placed program.

Reviewer 4:

This project supports the overall DOE objectives because of 10% fuel efficiency improvement.

Reviewer 5:

Overall, the work is relevant.

Reviewer 6:

The trucks that this engine will go into will have high volumes and are second to Class 8 tractors in their impact on U.S. emissions and petroleum use.

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

Reviewer 1:

The budget and spend rate look fine.

Reviewer 2:

Resources appear adequate.

Reviewer 3:

The reviewer stated that the project team has all it needs to complete the program.

Reviewer 4:

At this point in a very new project, there appear to be sufficient resources to reach the stated milestones and they are appropriately challenging.

Reviewer 5:

The reviewer remarked that it is too early in the project to evaluate.

Reviewer 6:

The reviewer commented that it is difficult to tell. The reviewer will assume yes, but no evidence or even a comment to such is in the package or mentioned in the review.

Presentation Number: ace156 Presentation Title: Next-Generation, High-Efficiency Boosted Engine Development Principal Investigator: Michael Shelby (Ford)

Presenter

Michael Shelby, Ford

Reviewer Sample Size

A total of five reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-40 - Presentation Number: ace156 Presentation Title: Next-Generation, High-Efficiency Boosted Engine Development Principal Investigator: Michael Shelby (Ford)

Question 1: Approach to performing

the work—the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

Although this project has already selected the engine, the approach is quickly working on detailed technologies to deliver on the objectives.

Reviewer 2:

The approach looks solid with an initial single-cylinder engine, moving to multi-cylinder engine, and then moving to vehicle level. Extensive modeling and analysis will be key to the success of this project to meet its aggressive goals, which far exceed the minimum FOA requirements (23% fuel economy improvement versus 10%).

Reviewer 3:

The technical barriers to completing the work were clearly articulated as well as the approach to address those items. The project appears to be feasible relative to the fuel economy goal, but meeting the weight saving goal would appear to be very difficult given the plans laid out, even with the deletions of components outlined. Just reaching the fuel economy goal is a very formidable challenge.

Reviewer 4:

It would be helpful to provide more description of the approach taken in this project. One slide to summarize the entire approach is too simplified. Also, it would be helpful to add more description of the approach on how the weight reduction goal can be achieved.

Reviewer 5:

The project is really tightly focused on addressing the project goals of mass reduction and engine efficiency improvement. All of the technologies identified appear to be a stretch from where we are today for production applications, but none appears to require a yet-undiscovered solution to be able to be brought to near-production.

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

Reviewer 1:

A nice level of detail is provided here, and there is really good progress for the project being at such an early stage. This significant progress seems to have been enabled by the extensive modeling effort (1D and 3D).

Reviewer 2:

For being 6 months in, a lot appears to have been accomplished in terms of nailing down hardware paths and starting to build up test facilities to support the development. These accomplishments gave the reviewer the confidence that there will be ample time for development before the multi-cylinder engine builds need to start.

Reviewer 3:

The project appears to be on schedule, but the milestones for 2020 listed were a little sparse. Analysis work was mentioned (e.g., 14:1 compression ratio [CR]) but does not really appear on the milestones chart until later. Perhaps that is too much detail for a 30-minute report.

Reviewer 4:

The team has obviously jumped on the opportunities having already spent 15% of the program budget. The accomplishments are broad, and many are giving multiple technology opportunities to meet the objectives.

Reviewer 5:

Much progress has been made during the first few months of the project, including compression ratio evaluation, combustion system, and low heat capacity coating. However, progress on the weight reduction is lacking, perhaps due to the early stage of the project. It would be hoped that more progress in weight reduction can be seen in the next annual review.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

It seems that both of the two key partners have contributed to the progress of this work.

Reviewer 2:

The reviewer expected the collaboration to be quite good, given the definition of the partner tasks. It looks like there has not been a ton of joint work to date, but the tasks that involve the partnerships are starting up so we should see a lot more as we go toward the next review.

Reviewer 3:

This looks like a strong team, with a significant dependence on FEV to provide solutions in many key engine design areas. In future AMR presentations, please be sure to specifically call out which team member and accomplishment is attributed to. A university partner would be nice to have on the team, particularly in the three-dimensional (3-D) modeling work, considering the complexity of modeling the pre-chamber.

Reviewer 4:

Clearly there is a good deal of coordination going on within Ford. The other partners seem to be just getting started at this time.

Reviewer 5:

FEV and Oak Ridge seem to have their teams identified and work documented. Is there any chance any customer groups can be added in an advisory mode, such as commercial truck fleets or municipal customers? The reviewer believed this would be very beneficial and likely one or more of those groups would be happy and even honored to participate.

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

Reviewer 1:

There are well documented future plans to reach design decisions on time.

Reviewer 2:

The path forward looks really interesting; there are lots of technology paths that are under current research in the DOE that will be brought into this project to see how they work in a production-style development program. The milestones are well defined and look achievable.

Reviewer 3:

Appropriate decision points have been set. However, being so early in the project, it is very hard to evaluate how the team will compensate for the inevitable challenges as they present themselves.

Reviewer 4:

What are the criteria for engine concept selection between the three-spark plugs and pre-chamber? Are cost and reliability the determining factors if performance is equivalent?

Reviewer 5:

The proposed future research is defined well on the performance side, but the proposed new technologies on the engine would increase the challenge of meeting the weight reduction goal. This would become even more challenging since the engine platform of this project is based on an existing engine, which has significant limitations on the weight reduction. It would be helpful if the future work can address this outstanding issue.

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

Reviewer 1:

The project directly feeds into the VTO programmatic goals for efficiency improvement.

Reviewer 2:

The reviewer thought that this project is right in line with the DOE objectives.

Reviewer 3:

This engine would be intended for some of the largest volume LD vehicles on the market; achieving the efficiency improvements targeted would have a huge impact on U.S. fuel consumption and CO₂ emissions.

Reviewer 4:

These pickup trucks are second to Class 8 tractors for emissions and U.S. petroleum impacts. Reductions here are key for the climate and U.S. businesses.

Reviewer 5:

This project will be able to support the overall DOE objectives if the team can achieve its aggressive fuel economy improvement and weight reduction goals.

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

Reviewer 1:

The budget level and spend rate look good relative to the project scope and progress.

Reviewer 2:

Resources appear to be sufficient at this time.

Reviewer 3:

The reviewer said that the project team should have all it needs to complete the program at this time.

Reviewer 4:

There was no mention of resources in the slides or in the review. The reviewer realized that Ford has had ongoing projects for these engines over the years with the DOE, but resource plans should be in a review for projects at this stage.

Reviewer 5:

It is difficult to evaluate at the early stage of the project.

Presentation Number: ace157 Presentation Title: Low-Temperature Gasoline Combustion for High-Efficiency Medium- and Heavy-Duty Engines Principal Investigator: John Dec

(Sandia National Laboratories)

Presenter

John Dec, Sandia National Laboratories

Reviewer Sample Size

A total of four reviewers evaluated this project.

Project Relevance and Resources

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



Figure 1-41 - Presentation Number: ace157 Presentation Title: Low-Temperature Gasoline Combustion for High-Efficiency Medium- and Heavy-Duty Engines Principal Investigator: John Dec (Sandia National Laboratories)

Question 1: Approach to performing the work—the degree to which

technical barriers are addressed, the project is well-designed and well-planned.

Reviewer 1:

The approach of complementing analysis with experiments is fundamentally sound, and the PIs have done a good job in identifying the relevant tasks for achieving the project objectives.

Reviewer 2:

The project has clearly defined objectives, and the research activities are laid out well to progress toward achieving those objectives.

Reviewer 3:

At the detail level, this work is very well designed, planned, and executed. A concern of this reviewer is that to ensure that the results of this work can ultimately address key technical barriers and be impactful is that perhaps a bit more effort to assess the overall feasibility of the additive-mixing fuel injection (AMFI) approach is warranted. Specifically, some effort to assess how well this approach works for what would be expected to be the variation of market fuels in the United States is warranted. It is of no value if this approach is not robust enough to work for a broad range of fuels.

Reviewer 4:

The use of LTC to meet the upcoming efficiency and emissions targets is very sound. However, there is significant uncertainty that an AMFI system will ever be commercially viable (it looks like the OBD problem from hell) and the NO_x numbers that need to be considered are NOT EPA 2010 but rather the ultra-low NO_x proposed regs in California (nominally, 0.02 g/kW-h). The ultra-high efficiencies achieved in these LTC

strategies tend to make the exhaust temperatures a challenge for keeping SCR warm. This is an issue that would be good to address in the future. In addition, the efficiency comparisons were made to engines that currently achieve significantly longer durability and reliability targets than automotive engines, which substantially degrade their peak efficiency performance. A better comparison for this research-level efficiency would be the efficiencies reported by the SuperTruck teams, since durability is less of a concern in those projects.

The previous work in phi-sensitivity also indicates that phi-sensitivity is enhanced by elevated pressure. Has there been any attempt to use pressure control at TDC (whether by boost or CR, similar to Miller cycle) to manage ignition characteristics instead of 2-ethylhexyyl nitrate (EHN)?

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

Reviewer 1:

The results showing that LTGC-AMFI can operate over the entire load-speed map of the EPA Generic 7 L diesel with higher BTE are very encouraging.

Reviewer 2:

The investigators have been able to develop approaches (LTGC-AMFI) to overcome the challenges of reaching the objectives of operating over the entire operating map of the engine. Technically, this is a significant accomplishment. Overall, the progress is very good.

Reviewer 3:

Some slight delays were encountered due to the COVID-19 pandemic, but nonetheless this project is progressing well and on track. A minor question and/or comment from this reviewer is to clearly elucidate if and/or how the project team accounted for operation of all the accessory components in estimating BTE. The BTEs that are being reported are very high; thus, it would help make people confident in the results to understand how accessory components were accounted.

Reviewer 4:

The technical accomplishments are quite impressive. Substantial progress toward the goals has been made. There have been several test matrices run that have highlighted the ability of this combustion system to provide very high efficiency and a very low emissions signature. One thing that would be very useful is a sensitivity study on the EHN dosing since, in a standard configuration, there will be six of these devices that need to operate and all of them need to operate within very tight limits to ensure that each and every cylinder is operating within acceptable limits. Even one of six cylinders operating slightly out of limits will create compliance/OBD problems.

Question 3: Collaboration and Coordination Across Project Team.

Reviewer 1:

Fantastic collaboration and coordination between two National Laboratories, three industry partners, and three universities.

Reviewer 2:

This project appears to have excellent collaboration and coordination among partners. There are OEMs and suppliers involved, other National Laboratories, and universities. Their efforts appear to be reasonably well coordinated and enhancing of each other.

Reviewer 3:

The project appears to be well connected and engaged with industry, National Laboratories, and universities.

Reviewer 4:

Collaboration is extensive and well coordinated.

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

Reviewer 1:

The future work plans should facilitate continued successful progress

Reviewer 2:

There is a good list of future tasks being proposed that builds on the accomplishments that have been demonstrated so far in the project. However, there are a couple of open questions that the PIs should address. First, can we reach 0.2 g/horsepower (hp)-h NO_x with low-temperature gasoline combustion without excessive HC and CO emissions compared to traditional diesel? Second, most of the challenges being faced in the industry are at low load NO_x, but the PIs are using EHN, which makes more NO_x.

Reviewer 3:

The proposed future work on the AMFI system is reasonable, although there should be a backup plan due to the significant uncertainty that AMFI will ever be robust enough for technology transfer, not to mention the substantial resistance of customers to carrying three consumable fluids (gasoline, DEF, and EHN). Alternate methods of controlling the reactivity in a more robust manner should be explored.

Reviewer 4:

The proposed future work is logical to progress the combustion approach, but effort may be better if reframed or utilized in other directions. The work ought to be compared to state-of-the-art diesel engines that are in production and compare engine-out emissions levels (especially at low load) relative to a state-of-the-art diesel. This comparison should include HC and CO in addition to the existing focus on NO_x and soot. Related to this, efforts must focus on showing pathways to future emissions compliance, not relative to 2010 emissions levels. Finally, as previously mentioned, an effort to show that the AMFI approach works for a spectrum of fuels would also be beneficial.

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

Reviewer 1:

This project supports the overall DOE objectives because it is exploring combustion system technologies that can achieve high thermal efficiency compared with traditional diesel while limiting emissions.

Reviewer 2:

This project definitely supports the overall DOE objectives of high efficiency, low emissions combustion systems.

Reviewer 3:

This project is aligned with DOE's objectives as it aims to develop a more efficient engine.

Reviewer 4:

The project is explained well in the relevance slide.

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

Reviewer 1:

Progress is excellent and the resources seem adequate.

Reviewer 2:

The project is 53% complete and on plan with the current funding level, which has been consistent over the past couple of years.

Reviewer 3:

The project resources are sufficient for timely project execution.

Reviewer 4:

The resources appear to be sufficient to maintain progress and timeline.

Acronyms and Abbreviations

1-D	One-dimensional
3-D	Three-dimensional
A/F	Air-fuel ratio
A/F	Amplitude-frequency
ACC	Adaptive cruise control
ACE	Advanced Combustion Engine
ACEC	Advanced Combustion & Emissions Control
ACI	Advanced compression ignition
AEC	Advanced Engine Combustion
AI	Artificial intelligence
Al ₂ O ₃	Aluminum oxide (alumina)
AMFI	Additive-mixing fuel injection
AMR	Annual Merit Review
ANL	Argonne National Laboratory
ARB	Air Resources Board
BEA	Zeolite beta
BMEP	Brake-mean effective pressure
BP	Budget period
BSFC	Brake-specific fuel consumption
CA50	Crank angle at 50% mass fraction burned
CAE	Computer-aided engineering
CARB	California Air Resources Board
CCE	Closed-cycle efficiency
CCV	Closed-crankcase ventilation
Cd	Coefficient of drag
CDC	Change-data capture
CDC	Conventional diesel combustion
CDTI	Clean Diesel Technology, Inc.

Ce	Cerium
CeO ₂	Cerium oxide (ceria)
CFD	Computational fluid dynamics
CH_4	Methane
CHT	Conjugate heat transfer
CI	Compression ignition
CLEERS	Crosscut Lean Exhaust Emissions Reduction Simulations
CNG	Compressed natural gas
CO_2	Carbon dioxide
COV	Coefficient of variation
CR	Compression ratio
CRADA	Cooperative research and development agreement
C _{rr}	Coefficient of rolling resistance
Cu	Copper
DEF	Diesel exhaust fluid
DFT	Density functional theory
DISI	Direct-injection spark ignition
DNS	Direct numerical simulations
DOC	Diesel oxidation catalyst
DOE	U.S. Department of Energy
DPF	Diesel particulate filter
DRIFTS	Diffuse reflectance infrared Fourier-transform spectroscopy
E10	10% ethanol content gasoline
ECFM	Extended coherent flame model
ECN	Engine Combustion Network
ECU	Engine control unit
EERE	Energy Efficiency and Renewable Energy
EGR	Exhaust gas recirculation
EHN	2-ethylhexyl nitrate
------------------	---
EPA	U.S. Environmental Protection Agency
FCA	Fiat-Chrysler Automobiles
FE	Fuel economy
FE	Fuel efficiency
Fe	Iron
FEAD	Front-end accessory drive
FOA	Funding opportunity announcement
FTP	Federal Test Procedure
FWC	Four-way catalyst
FY	Fiscal year
g	gram
GCI	Gasoline compression ignition
GCMS	Gas chromatography mass spectroscopy
GDI	Gasoline direct injection
GEM	Greenhouse gas Emissions Model
GHG	Greenhouse gas
GM	General Motors
GPF	Gasoline particulate filter
GPU	Graphics processing unit
GVW	Gross vehicle weight
GVWR	Gross vehicle weight rating
H_2	Hydrogen
H2D2	Heavy-duty hybrid diesel
H ₂ O	Water
НС	Hydrocarbon
HCCI	Homogeneous charge compression ignition
НСТ	Hydrocarbon trap

HD	Heavy-duty
HNCO	Isocyanic acid
HP	Horsepower
HPC	High performance computing
HSFW	High-speed flywheel
HSS	High-strength steel
HTA	Hydrothermally aged
HVAC	Heating, ventilating, and air conditioning
IC	internal combustion
ICE	Internal combustion engine
ICME	Integrated computational materials engineering
ID	Ignition delay
IMEP	Indicated mean effective pressure
IP	Intellectual property
ISFC	Indicated specific fuel consumption
JM	Johnson Matthey
K	Potassium
kW	Kilowatt
L	Liter
LANL	Los Alamos National Laboratory
lb	Pound
LD	Light-duty
LES	Large eddy simulation
LEV III	Low-emission vehicle level III
LLNL	Lawrence Livermore National Laboratory
LSPI	Low-speed pre-ignition
LTC	Low-temperature combustion
LTNA	Low-temperature NO _x adsorber

LTP	Low-temperature plasma
m	Meter
MCCI	Mixing-controlled compression ignition
MGU	Motor-generator unit
MHDV	Medium- and heavy-duty vehicle
Micro-CT	Micro-computed tomography
ML	Machine learning
mm	Millimeter
Mn	Manganese
MON	Motor octane number
MOU	Memorandum of understanding
MY	Model year
N ₂ O	Nitrous oxide
NACFE	North American Council for Freight Efficiency
NG	Natural gas
NGV	Natural gas vehicle
NH ₃	Ammonia
NN	Neural network
NO	Nitric oxide (nitrogen monoxide)
NO ₂	Nitrogen dioxide
NO _x	Oxides of nitrogen
NP	Nano-palladium
NREL	National Renewable Energy Laboratory
OBD	On-board diagnostics
OC	Oxidation catalyst
OCE	Open-cycle efficiency
OEM	Original equipment manufacturer
ORNL	Oak Ridge National Laboratory

OSC	Oxygen storage capacity/component
Р	Phosphorous
PACE	Partnership for Advanced Combustion Engines
РАН	Polycyclic aromatic hydrocarbon
PC	Pre-chamber
PCC	Predictive cruise control
Pd	Palladium
PFI	Port fuel injection
Pi	Principal investigator
PMI	Particulate matter index
PN	Particle number
PNA	Passive NO _x adsorber
PNNL	Pacific Northwest National Laboratory
Pt	Platinum
P-T	Pressure-temperature
Q	Quarter
Q&A	Question and answer
R value	Resistance to heat flow
R&D	Research and development
RANS	Reynolds-averaged Navier-Stokes
RCM	Rapid compression machines
Rh	Rhodium
RMS	Root mean square
RON	Research octane number
S	Second
S	Sulfur
SAC	Single-atom catalyst
SCE	Single-cylinder engine

SCO	Selective catalytic oxidation
SCR	Selective catalytic reduction
SCRF	Selective catalytic reduction on filter
SI	Spark ignition
SNL	Sandia National Laboratories
SOW	Statement of work
Spaci-MS	Spatially resolved capillary inlet - mass spectroscopy
SSZ	Alumina silicate zeolite
ST2	SuperTruck 2
SULEV	Super ultra-low emissions vehicle
SwRI	Southwest Research Institute
Т	Temperature
ТСО	Total cost of ownership
TDC	Top dead center
Tech	Technical
TJI	Turbulent jet ignition
TWC	Three-way catalyst
U.S. DRIVE	U.S. Driving Research and Innovation for Vehicle efficiency and Energy sustainability
UHC	Unburned hydrocarbons
UPS	United Parcel Service
USCAR	United States Council on Automotive Research
UVA	University of Virginia
V	Volt