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Promoting Increased Ethanol Utilization Through Development of Renewable Super Premium Fuel and Investigation of Blending Natural Gasoline into FFV Fuel:

Project Plan

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OAK RIDGE NATIONAL LABORATORY
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Bioenergy Technologies Program

Promoting Increased Ethanol Utilization Through Development of Renewable Super Premium Fuel and Investigation of Blending Natural Gasoline into FFV Fuel

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BACKGROUND

The use of fuel ethanol in the US has grown dramatically over the past decade and with ethanol easily the largest volume of any biofuel. In 2012, the United States consumed only 0.058 billion gallons of E85, whereas over 13 billion gallons of ethanol were produced and over 130 billion gallons of gasoline were consumed. However, it will be difficult to achieve markedly higher levels of ethanol consumption because a regulatory blend wall is encountered with E10 and E15, and E85 consumption remains extremely limited (<1% of ethanol consumption). This comes at a time cellulosic ethanol and other advanced biofuels are poised to become a commercial reality but that promise could be limited if a viable market does not exist for these renewable biofuels.

Concurrent with the need for increasing renewable fuel consumption, original equipment manufacturers (OEMs) of automobile light-duty engines are pursuing a complete portfolio of technologies to reduce CO_2 emissions, including technologies reliant on higher compression ratios and fuels with improved anti-knock properties, such as gasoline with significantly increased octane numbers.

Recently published data from the Department of Energy (DOE) laboratories[1,2,3,4], OEMs[5], and discussions with the US Environmental Protection Agency (EPA) suggest the high potential of a new "Renewable Super Premium" (RSP) fuel with 25–40 vol % of ethanol to assist in reaching RFS2 and greenhouse gas (GHG) goals. This fuel was named internally simply to distinguish this potential fuel and project from other ethanol blends or high-octane fuels. In this project plan, we are referring to the fuel as Renewable Super Premium or RSP as the name now has recognition; it will be re-named in the future. This mid-level ethanol content fuel, with a research octane number (RON) of near 100, appears to enable efficiency improvements in a suitably calibrated and designed engine/vehicle system that are sufficient to more than offset its lower energy density[6] This would negate the tank mileage (range) loss typically seen with ethanol blends in gasoline and ethanol-tolerant vehicles. The prospects for such a fuel are additionally attractive because it can be used legally in 17 million flexible-fuel vehicles (FFVs) currently on the road. Thus the FFV fleet can serve as a bridge by providing a market for the new fuel immediately, so that future vehicles will have improved efficiency as the new fuel becomes widespread. In this way, RSP can simultaneously help improve fuel economy and increase ethanol usage in the United States by creating a growing market for an ethanol blend >E10.

RSP could be complementary to the biomass-derived "drop-in" fuels being developed by DOE and others. The octane level for any drop-in biomass-derived fuel and the chemical octane needed to enable improved fuel economy are important considerations, regardless of RSP. RSP offers a nearer-term opportunity to expand the use of ethanol, and it highlights the benefits of higher octane in a fuel. At E10, neither the advantageous nor disadvantageous properties of ethanol are particularly noticeable. At high-level blends (E85) for typical FFVs, the potential benefits of high octane number cannot offset the loss in

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[1] Splitter, D.A., and Szybist, J.P., "Experimental Investigation of Spark-Ignited Combustion with High-Octane Biofuels and EGR. 1. Engine Load Range and Downsize Downspeed Opportunity," *Energy & Fuels*, 28(2): 1418-1431, 2014, doi:10.1021/ef0401574p

[2] Splitter, D.A., and Szybist, J.P., "Experimental Investigation of Spark-Ignited Combustion with High-Octane Biofuels and EGR. 2. Fuel and EGR Effects on Knock-Limited Load and Speed," *Energy & Fuels*, 28(2): 1432-1445, 2014, doi:10.1021/ef401575e

[3] Szybist, J., Foster, M., Moore, W., Confer, K. et al., "Investigation of Knock Limited Compression Ratio of Ethanol Gasoline Blends," SAE Technical Paper 2010-01-0619, 2010, doi:10.4271/2010-01-0619.

[4] Splitter, D. and Szybist, J., "Intermediate Alcohol-Gasoline Blends, Fuels for Enabling Increased Engine Efficiency and Powertrain Possibilities," *SAE Int. J. Fuels Lubr.* 7(1):2014, doi:10.4271/2014-01-1231

[5] Anderson, J.E., DiCicco, D.M., Ginder, J.M., Kramer, U., Leone, T.G., Raney-Pablo, H.E., and Wallington, T.J., "High Octane Number Ethanol-Gasoline Blends: Quantifying the Potential Benefits in the United States," *Fuel* 97: 585-594, 2012.

[6] Jung, H., Leone, T., Shelby, M., Anderson, J. et al., "Fuel Economy and CO2 Emissions of Ethanol-Gasoline Blends in a Turbocharged DI Engine," *SAE Int. J. Engines* 6(1):2013, doi:10.4271/2013-01-1321.

tank mileage (octane number benefits are nonlinear and diminish at blends >40% ethanol), and pricing practices do not appeal to consumers.

A recent Oak Ridge National Laboratory (ORNL) study shows that mid-level ethanol blends can yield high-RON fuels even if relatively low-octane hydrocarbon streams such as straight run gasoline (SRG, with an RON of around 60–65) are used. FFV blends with SRG and 51% ethanol provide superior engine knock resistance compared with premium unleaded gasoline. The experiments were conducted in a single-cylinder research engine.[7] Low-octane natural gasoline has become relatively inexpensive compared with other hydrocarbon blendstocks, as the supply is increasing dramatically as a result of increased shale gas production in the United States. The use of natural gasoline and other similar low-cost blendstocks for blending RSP might therefore lead to a significant reduction in retail price and increased use of this fuel. As demonstrated in a recent National Renewable Energy Laboratory (NREL) publication, the 91 RON level typical of finished regular gasoline today could be met by blending natural gasoline with approximately 30 vol % ethanol[8].

There are numerous challenges to realizing the RSP vision, as well as questions about whether such a fuel would lead to favorable fuel economy and GHG emissions on a life-cycle basis. The current research program is investigating these challenges with the following objectives:

- Quantify the efficiency and GHG benefits of dedicated RSP vehicles
- Conduct a complete well-to-wheel analysis to understand the tradeoffs between improvements in tailpipe CO_2 emissions versus GHGs generated in petroleum fuel and bioethanol production and distribution
- Determine the state of the legacy refueling infrastructure and compatibility with RSP
- Examine the properties of ethanol blends with low-cost blendstocks, such as natural gasoline and renewable naphtha
- Assess whether the knock resistance of ethanol blends is adequately represented by the RON and motor octane number (MON) octane specifications
- Assess market barriers to the introduction and successful use of RSP
- Investigate the performance benefits of RSP in legacy FFVs, and the possible use of natural gasoline and other low-cost blendstocks in E85, to help provide a "bridge" to RSP implementation or an incentive to the petroleum industry

The purpose of this project is to evaluate this potential opportunity and assess the likelihood that RSP will be successful in the marketplace in the near to medium term. This project will provide additional strategic information assessing the potential for RSP and additional technical information to quantify some of the perceived advantages of its use. The project goal is to determine whether RSP is "worth the risk" for the nation and help articulate a suitable path to introduce the fuel. It will examine how the proper knock resistance level can be obtained through ethanol concentrations and altering the petroleum blendstock. Lessons learned from previous attempts to introduce ethanol fuels into the marketplace will be applied. The project team will constructively engage stakeholders while providing an unbiased technical assessment. At the conclusion of this effort in early FY 2016, sufficient information should be available to decide if it makes sense to further the RSP concept or if the effort should cease. If more investigation is warranted, specific research that needs to be pursued within the Bioenergy Technologies Office (BETO) and the Vehicle Technologies Office (VTO) will be articulated.

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[7] Szybist, J. and West, B., "The Impact of Low Octane Hydrocarbon Blending Streams on the Knock Limit of "E85"," *SAE Int. J. Fuels Lubr.* 6(1):44-54, 2013, doi:10.4271/2013-01-0888

[8] Alleman, T.L., McCormick, R.L., Yanowitz, J. "Properties of Ethanol Fuel Blends Made with Natural Gasoline" in preparation.

This research program will provide a quantitative picture of the barriers to adoption of RSP and the highly efficient vehicles it enables, and of the potential environmental and economic benefits of this technology. It will include the following efforts.

- Gain a broad understanding of economic and regulatory barriers to adoption of RSP by four key stakeholder groups: fuel producers/distributors, fuel retailers, vehicle manufacturers, and consumers (Task C). Each group is subject to different federal and state regulatory requirements and has different economic constraints. This effort is supported by other subtasks:
  - Determine the extent to which existing infrastructure is compatible with RSP-range (25 to 40%) ethanol blends, whether emerging infrastructure components are compatible, and whether there is a blend-level breakpoint at which infrastructure compatibility is less an obstacle (Task B).
  - Develop a preliminary description of the key knock resistance properties of RSP to obtain a full understanding of both regulatory and ASTM standard development issues with regard to defining and introducing this fuel (Task H).
  - Experimentally validate and measure the performance benefits of RSP in current FFVs (Task F). Consider the potential to blend this fuel using low-cost gasoline blendstocks (Task E). These are key transition technologies to fully optimized vehicles and RSP.
  - Experimentally validate and measure efficiency and performance benefits of RSP in a dedicated vehicle (Task G). This vehicle-level demonstration complements ongoing engine-based studies researching the benefits of increased octane and compression ratio.
- Study the impacts on the petroleum refining sector and life-cycle environmental benefits across the US economy of broad adoption of RSP and the highly efficient vehicles it will enable (Task D). This effort is supported by analysis results under other subtasks:
  - Ascertain the shares of RSP and non-RSP demand of light-duty vehicle fleet (Task C). These shares determine the refinery operations and the gasoline components in the refinery linear programming (LP) models.
  - Define fuel property requirements for RSP. These constrain the properties of the hydrocarbon blendstock, which can have a large effect on life-cycle energy use and GHG emissions (Tasks E, F, G, and H).
  - Develop initial estimates of vehicle efficiency improvements based on the literature to support the life-cycle analysis (Tasks F and G).

The interdependent tasks listed in the following table are under way to better define the opportunity. The purpose of this project plan is to help harmonize the collaborative efforts of the national laboratories and communicate the goals of the combined effort. This document does not replace or obviate the individual laboratory annual operating plans (AOPs). Annual spending plans, budgets and quarterly milestones are detailed in each laboratory AOP.

Task	Description	Lead
A	**Develop RSP Program Plan:** Work with DOE and key stakeholders to develop a more detailed test plan directed at providing technical data to eliminate barriers to commercialization. Ensure regular and consistent communication among the team and vested stakeholders	ORNL/ NREL/ANL
B	**Infrastructure Assessment**: Work with stakeholders to consider fuel storage and dispensing infrastructure compatibility with RSP in legacy systems	**NREL**/ ORNL
C	**Market Analysis:** Assess economic and regulatory barriers to introduction of RSP into the market and evaluate options for addressing transition issues (assuming the laboratory research being done in parallel is successful in identifying a suitable blend/technology). This task will engage stakeholders in identifying barriers and the innovations to overcome those barriers. This work will provide feedback to the lab research, as well as engage stakeholders in identifying and supporting win-win deployment solutions	**NREL**/ ORNL/ANL
D	**Well To Wheels Analysis**: Conduct a well-to-wheels analysis of various options with input from related tasks. Determine changes in GHG and energy when production, delivery, and utilization are all considered	**ANL/**NREL/ ORNL
E	**Low-Cost Potential RSP Blendstock(s):** Evaluate natural gasoline fuel quality based on a mini-survey of eight samples obtained from a range of sources, with a focus on sulfur and benzene content, as well as vapor pressure, distillation curve, octane numbers, and detailed hydrocarbon analysis. Assess the performance properties of blends of ethanol (E30–83) with a range of natural gasolines and renewable naphtha blendstocks (having acceptable sulfur and benzene content), including vapor pressure, distillation, octane numbers, water separation, and cold temperature phase separation. Develop a model for predicting the vapor pressure of natural gasoline–ethanol blends from the vapor pressures of the two blend components	ORNL/ NREL
F	**Effects of RSP on Legacy FFVs:** Determine the effects of high-octane gasoline blends such as E20–E40 on legacy "ethanol tolerant" FFVs. Demonstrating a performance benefit in legacy FFVs offers an opportunity to revise marketing approaches for using ethanol blends in the legacy FFV fleet; doing so would bolster the infrastructure to enable fueling future vehicles designed for this fuel.	**ORNL**
G	**Efficiency Gains of RSP in Dedicated Vehicle**: Quantify the fuel economy benefits of high-octane ethanol fuel blends at the vehicle level. Significant fuel economy improvements are possible from the combination of improved engine thermal efficiency and improved system efficiency from downspeeding and downsizing. NREL will fully characterize the fuels used in vehicle testing by ORNL, including quantification of both octane number and heat of vaporization.	**ORNL**
H	**Descriptive Properties for Engine Knock Resistance:** Develop a description of fuel knock resistance than considers the octane number, heat of vaporization, fuel distillation curve, and burning velocity.	**NREL**/ ORNL

DISCUSSION OF TASKS

Task A. Develop Renewable Super Premium Program Plan

ORNL, Argonne National Laboratory (ANL), and NREL will work with DOE and key stakeholders to update the project plan and specific tasks for FY 2015 based on data and analysis performed in FY 2014.

This task will include communication between the national laboratories and DOE-BETO as well as engagement of the external stakeholders. At this time, monthly teleconferences among the national laboratory participants and BETO are envisioned, although the timing may be adjusted as necessary. External stakeholders that will be engaged include but are not limited to the Renewable Fuels Association, the petroleum equipment industry, Underwriters Laboratories, the petroleum refinery industry, the automobile industry, and EPA (both the Office of Air Quality and the Office of Underground Storage Tanks). We will use existing relationships with these communities to elicit feedback and candid assessments of the opportunities and barriers associated with RSP. An overriding goal will be to determine the realistic opportunity and quantify the technical and nontechnical barriers.

This project is currently planned for FY 2014 and 2015 funding. A key project outcome is to generate sufficient data and plans to critically evaluate the potential for RSP fuel in the marketplace. At the end of quarter 1 of FY 2016, we plan to communicate the results of this effort to BETO and others, along with our best recommendation for pursuing RSP as a new fuel in the United States. The combined team is committed to producing a joint comprehensive report on fuel properties, tradeoffs among ethanol blend levels, miles-per-gallon fuel economy, GHG emissions, infrastructure cost, hydrocarbon blendstock cost, and other factors. It will include recommendations for future analysis and research at the end of December 2015.

Task B. Infrastructure Assessment

Objective

The objective of this task is to work with stakeholders to consider fuel storage and dispensing infrastructure compatibility with RSP in legacy systems. The results were published in an NREL report.[9]

This task will identify the issues associated with storing and dispensing a new fuel in the existing infrastructure, considering both the aboveground and the underground equipment. Both NREL and ORNL have significant interactions with these communities from their experience with E15 research. NREL will use its contacts within the supplier community and ORNL will contact the materials community to discern the issues, identify the barriers, and assess the likelihood that RSP will be acceptable for use with legacy industry equipment and what equipment upgrades are necessary. The industry is still in a state of flux with regard to the increased use of biofuels in general, so it may be that RSP will not be an insurmountable additional burden. Existing Underwriters Laboratories listing requirements have a specific protocol for fuels with ethanol concentrations of 25% or less, so the advantages of accepting that upper limit will be explored. ORNL will focus on the materials influence of RSP fuels to assess the impact of this suggested fuel on the infrastructure, and NREL will examine the fuel from the viewpoint of the supplier community.

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[9] Moriarty, K., Kass, M., Theiss, T. "Increasing Biofuel Deployment and Utilization through Development of Renewable Super Premium: Infrastructure Assessment" Technical Report, NREL/TP-5400-61684, November 2014.

The analysis generated under this task is critical input to Task C (Market Analysis), and the national laboratory project leaders will work to ensure close collaboration between the leaders of these tasks. The results will also inform Task G (Efficiency Gains of Renewable Super Premium in Dedicated Vehicles) and Task H (Descriptive Properties for Knock Resistance) in that those tasks may include E25 in the test matrix if it becomes clear that infrastructure hurdles for that ethanol blend level are significantly lower than the hurdles for higher blends.

A key outcome from FY 2014 studies is the realization that the underground equipment is already largely compatible with RSP (either E25 or E40), although some stations will have more difficulty than others in identifying the specific equipment used in order to demonstrate compliance. Aboveground equipment may have to be replaced, and the replacement cost will depend on the ethanol content of the fuel. E25 above-ground equipment is only slightly more expensive than traditional dispensers, but any fuel blend over E25 will require an E85 dispenser, which is significantly more expensive. In FY 2015, NREL will examine the readiness of blending terminals to supply RSP.

ORNL will re-examine some previous materials results to evaluate previous findings regarding resin compatibility with E25. The resin itself did not perform particularly well in the compatibility studies, and research to obtain additional understanding is warranted.

Issues with fueling infrastructure and RSP appear to be somewhat overstated, and a workshop or information-sharing discussion is planned to communicate results with key external stakeholders. The workshop will include discussions with stakeholders on any remaining issues, as well as outreach and education regarding previous relevant research findings. The workshop is as yet unscheduled and will be co-hosted by NREL and ORNL.

Task C. Market Analysis

Objective

This task will assess the economic and regulatory barriers to the introduction of RSP into the market and evaluate options for addressing transition issues (assuming the experimental research being done in parallel is successful in identifying a good blend/technology). It will seek to understand the attractions and deterrents of RSP for key stakeholder (market) groups and assess market potential. It will allow an initial assessment of the market effects and benefits of RSP with regard to enhancing ethanol use; achieving the RFS2 (or variant goal) in a timely, cost-effective way; and reducing fuel costs, providing consumer and economy-wide benefits.

The project team will work with relevant stakeholders to explore the barriers they face to RSP use in addition to the promise that RSP holds for them. It will seek ways of enhancing the RSP business case that circumvent difficulties faced by E85 and E15. This task will examine the four major stakeholder groups impacted by RSP (fuel producers/ distributors, fuel retailers, vehicle manufacturers, and consumers), chart the dynamic relationship between them, and develop market scenarios for each one. Direct communication with stakeholders will be used to gather pertinent information for successful implementation of RSP. The team will identify the barriers with realistic market scenarios, avoiding the trap of optimistic listening.

Economic modeling of the transition and the anticipated endpoint can highlight penetration hurdles and provide justification and motivation for continuing with RSP development by quantifying its benefits to key players. Economic modeling will allow representation of system-wide or market economic issues for RSP, and exploration of the potential demand for and supply of RSP under various conditions (technological, market, and policy). This study provides an essential “feedback loop” for the laboratory research. NREL and ORNL will utilize existing economic modeling tools (e.g., BioTrans, Biomass

Scenario Model [BSM], and other models) to evaluate the market pull of RSP. Minimum modifications will be made to these models to accommodate RSP. The models will be compared against each other to help bound the problem and gather additional insight into the influence of the modeling assumptions and approaches. The outcome will not be an economic projection of the market demand of RSP but rather an assessment of barriers, benefits, parametric sensitivities, conditions necessary for successful implementation, and the likelihood that the latter will occur.

This task is supported by several other tasks that provide critical input and baseline information, including Task B (Infrastructure Assessment), Task F (Effects of Renewable Super Premium on Legacy FFVs), Task G (Efficiency Gains of Renewable Super Premium in Dedicated Vehicles), and Task H (Descriptive Properties for Knock Resistance).

Key findings from the market assessment task in FY 2014 include the following:

Large-scale adoption of RSP will require the participation of four main stakeholder groups: drivers, vehicle manufacturers, fuel retailers, and fuel producers (gasoline and ethanol). Their participation is predicated upon benefiting from RSP. Drivers stand to benefit from projected fuel cost savings, reduced price volatility, increased torque in performance applications, and the energy security and environmental attributes associated with RSP. Vehicle manufacturers could benefit from RSP as a means to meet fuel economy requirements and as a way to increase torque in performance applications. Fuel retailers could fetch higher per-gallon margins from RSP than from gasoline, could see an increase in visits to their stores because of the lower price of RSP versus gasoline, and could use RSP as a means to differentiate their stations from the competition. Fuel producers stand to benefit from RSP as a way to comply with RFS2, both because the boost in ethanol demand could come at a strategic time for the transition to cellulosic ethanol and because it could enable the use of less expensive blendstocks.

Despite the potential benefits of RSP, many hurdles must be resolved before it is adopted at large scale. Thirty of these hurdles were identified through stakeholder interviews and a literature review. These hurdles were categorized according to their formidability, the stakeholder groups they primarily impact, and their realm (i.e., logistical, economic, regulatory, or behavioral). Ninety potential resolutions to these hurdles were also identified and explored. Complementary subsets of these resolutions were grouped into eight deployment scenarios.

The eight deployment scenarios were modeled by the Automotive Deployment Options Projection Tool (ADOPT) to estimate the adoption rate of RSP vehicles (RSPVs). All scenarios achieved a high percentage (77–98%) of the light-duty vehicle stock by 2050. ADOPT estimated that high oil prices could increase the rate of RSPV adoption, particularly if RSP is an E40 blend. In general, more RSPVs are adopted if RSP is an E25 blend, because vehicle manufacturers would need more E25 than E40 vehicles to meet Corporate Average Fuel Economy (CAFE) requirements. RSPVs were found to reduce the number of advanced powertrains, such as hybrid electric vehicles, because they could present a less expensive option for vehicle manufacturers to meet their CAFE requirements.

The estimated vehicle sales and stock from ADOPT were then used as inputs for scenario analyses to further explore the potential impacts of RSP on other areas of the fuel supply chain. Two models were used: BSM and BioTrans. The market modeling analyses concurred that feedstock availability and cost are not expected to be obstacles to the substantial adoption of RSP fuel. In many cases, RSP fuel costs were low enough that substantial market share was attained in the models, provided the refueling infrastructure is developed. RSPV purchases were likewise not a limiting factor to the size of the RSP market in most scenarios.

The combined system analyses also indicate that RSP use can be limited by the maximum rate at which industry can construct new biorefineries and by inadequate investment in retail infrastructure in some scenarios. Uncertain incentives, from either the market or policy, can deter retailers from installing RSP-compatible equipment. The high capital costs for individual retailers in certain scenarios may be prohibitive for investment, particularly for those stations that are not high-volume sellers. This outcome suggests a need for some level of support, at least in the early phase of development.

For steady development of the RSP market, consistent growth paths are needed for RSPV stock and the capacity of the RSP supply chain. The scenarios considered in this study had mixed success in achieving this growth symmetry. Scenarios that introduce RSP in stages, encourage or require new dispensers to be RSP-compatible, and focus on an E25 blend (instead of E40) achieve the greatest RSP production. Incremental investment costs tend to be higher as the speed of introduction is increased.

Based on these findings, FY 2015 activities under this task will produce the following results:

- Analysis of the interrelationships between the vehicle and fuel supply industries under various deployment, incentive, and external condition (e.g., oil price) scenarios through industry research and through linking existing biomass-to-biofuels supply chain models (BSM and BioTrans) and vehicle projection models (ADOPT and MA3T).
- Analyze the multiple options for CAFE regulations to address RSP and the resulting effects on the size of the RSP market.
- Converge on a central adoption scenario and conduct sensitivity analyses to prioritize methods for overcoming market penetration hurdles.
  - Sensitivity analyses for given variables will be run either by the combined ADOPT/BSM models or BioTrans/MA3T models, depending on which model combination is best suited to the variable.
- Summarize the costs and benefits of choosing specific blend levels of ethanol.
- Perform discounted cash flow analyses of key players attempting to bring RSP to market and sensitivity analyses of which parameters lead to profitability:
  - refueling stations
  - various fleets
  - independent drivers

  OEMs or fuel producers will not be studied because their economics are too proprietary

Task D. Well-To-Wheel Analysis of High-Octane Spark-Ignition Engine Fuels

Objective

RSP is under consideration by auto makers for purposely designed spark-ignition engines (beyond current FFVs) with increased energy efficiency. In particular, several options for making RON 100 fuel may be considered, including E10, E20, E30, and E40 blends. Gasoline blending stocks for these different levels of ethanol will require different refining operations in petroleum refineries. Addressing these various blending options is especially important given that US refineries may face the increased use of both heavy crudes, such as oil from the Canadian oil sands, and very light crude shale oil from shale formations such as Bakken and Eagle Ford. In addition, the predicted changeover in product slates to reduce gasoline production and increase diesel production will need to be considered.

The objective of the well-to-wheels analysis is to model petroleum refining to produce RON 100 final gasoline products with a range of ethanol blending levels and gasoline blendstocks. The energy and GHG emission intensity differences among these options from petroleum refinery LP modeling, together with upstream production of different crude types and ethanol, will be incorporated into the GREET model for well-to-wheels simulations of energy and GHG effects.

Furthermore, ORNL estimates of potential energy efficiency improvements in advanced vehicles, using these premium fuel options and current gasoline blends with lower octane levels, will be incorporated into GREET for well-to-wheels simulations. The upstream production differences and vehicle operating efficiency differences with different blending levels of ethanol and different hydrocarbon blending stocks will be key considerations of the well-to-wheels analysis.

Task D Subtask 1: Petroleum Refining Modeling of Producing RSP with Different Ethanol Blending Levels (e.g., E10, E25, and E40)

Refinery energy consumption to produce hydrocarbon blendstocks for blending with ethanol to make RSP gasoline may be greater than the energy consumption to make gasoline (E10) with the same fuel specifications (due to the difficulty in meeting the RVP standards). The impact of producing RSP could be greater for gasoline blendstocks with higher levels of ethanol (e.g., E30, E40). That is, refineries may need to be configured to produce gasoline blendstocks to address the vapor pressure of final gasoline products, among other fuel specification issues of various product pools. On the other hand, the impact of increased octane number from higher ethanol blends in gasoline products on life-cycle GHG emissions has not been addressed. It is currently unknown whether the GHG benefits of increasing the use of ethanol, with its high octane, would be offset by the increase in refinery GHG emissions (due primarily to vapor pressure control). A study by the Japan Clean Air Program suggests that the refinery GHG increase is larger than the decrease from using ethanol[10]. On the other hand, a study by OEMs showed that higher ethanol blending reduces the life-cycle GHG emissions and petroleum consumption, but increases the cost[11]. This proposed task intends to answer this question with additional rigor by using refinery LP models to simulate a variety of refinery configurations for various RSP gasoline production scenarios. It builds on the current work conducted by ANL investigating diesel fuel cetane/sulfur premium production. With a recruited reputable company with extensive understanding of refinery operations and LP modeling experience, several different ethanol blending levels that meet the octane level of RON 100 are selected, and hydrocarbon and ethanol routes to increased octane are compared. The goal is to estimate life-cycle energy use and GHG emissions for different routes of producing gasoline products to meet required fuel specifications (e.g., RON and RVP), with and without increased ethanol blending levels and market shares.

Key findings from this subtask in FY 2014 include

- Overall refining efficiency was unchanged for all evaluated blending levels and market shares with the imposed constraint of not allowing capital expansion (e.g., adding hydrocrackers or reformers).
- As ethanol blending level increases, more gasoline blendstocks are shifted from RSP gasoline to export gasoline. Interestingly, the efficiency of refining the total gasoline blendstocks (domestic regular and RSP gasoline plus export gasoline) was also unchanged with different ethanol blending levels and market shares. However, many changes in gasoline components (e.g., reformate, alkylate, naphtha) were observed in the domestic gasoline blendstock and export gasoline pools. This is likely a result of simply moving RSP gasoline components displaced by ethanol into the export pool.

[10] Koseki, K., 2014. JCAP Study, in: SAE 2014 High Octane Fuels Symposium. Presented at the SAE 2014 High Octane Fuels Symposium, Washington, DC.

[11] Hirshfeld, D.S., Kolb, J.A., Anderson, J.E., Studzinski, W., Frusti, J., 2014. Refining Economics of U.S. Gasoline: Octane Ratings and Ethanol Content. Environ. Sci. Technol. 48, 11064–11071. doi:10.1021/es5021668

- The refinery configurations with the imposed constraint on capital expansion were unable to produce a fuel with a target RON value of 100 using only 30% ethanol blending level due to high costs of meeting RON and RVP constraints.

Task D Subtask 2: Examination of Production of Crude Types and Ethanol

In the next 25 years, crude oil inputs to US petroleum refineries will go through significant changes. On the one hand, California will continue to use its own heavy crude and Canada could increase its oil sands production from the current level of 1.9 million barrels per day (BPD) to a level of more than 5 million BPD by 2030[12]. More oil sands products (i.e., synthetic crude oil and bitumen) are intended for export to the United States markets. On the other hand, US domestic production of light crude from places such as the Bakken and Eagle Ford Plays is expected to increase significantly. ANL will address the production of these various crude types and their energy and GHG emissions. The mix of different crude types that are fed into US refineries in Task D, Subtask 1, will be evaluated. The upstream production-related energy use and GHG emissions of these crude types will be incorporated into the GREET model for well-to-wheels simulations of RSP gasoline.

Ethanol production routes will also experience changes. Over the next 25 years, cellulosic ethanol production is likely to increase as a result of cellulosic ethanol technology advancement and to meet RFS2 cellulosic ethanol requirements. Meanwhile, corn ethanol production is expected to improve in terms of energy efficiency and GHG intensity, as experienced in the past 20 years. With its ongoing efforts to address emerging issues for cellulosic and corn ethanol for BETO, ANL will assess these changes in ethanol production and incorporate them into GREET well-to-wheels modeling of RSP gasoline.

Key outcomes from this subtask in FY 2014 include the following:

- Oil sands pathways in GREET were expanded to include the following four production pathways: Mining+SCO, Mining+Bitumen, In-Situ+SCO, and In-Situ+Bitumen.
- The energy and GHG intensities associated with the production operations and land use changes of these four oil sands production pathways were estimated and incorporated into the GREET model.
- The projections for the oil sands shares from these four pathways in crude oil inputs to US refineries were updated and incorporated in the GREET model.
- Corn and cellulosic ethanol production pathways were updated and incorporated in the GREET model for WTW simulations of RSP gasoline pathways.

Task D. Subtask 3: GREET Configuration and Well-To-Wheels Simulations

Task G led by ORNL under this project will evaluate vehicle performance changes and potential fuel efficiency gains with RSP gasoline. For the near term, vehicle fuel economy gain estimates with RSP were developed from public literature sources for incorporation into GREET model.

With a newly configured GREET model, well-to-wheels simulations will be conducted for different fuel options meeting RON 100. Well-to-wheels energy and GHG emission results will be produced from the simulations for various RSP production routes and market scenarios, and various vehicle fuel economy gains.

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[12] U.S. EIA, 2013. Annual Energy Outlook 2013 (No. DOE/EIA-0383(2013)). U.S. Energy Information Administration, Washington, D.C.

This task is supported by several other tasks that provide critical input and baseline information, including Task A (Develop RSP Program Plan), Task C (Market Analysis), and Task G (Efficiency Gains of Renewable Super Premium in Dedicated Vehicles).

The following are key findings from this subtask in FY 2014:

- Well-to-wheels results are dominated by ethanol blending levels and RSP market shares, i.e., impacts of refinery operation changes on well-to-wheels GHG emissions are much smaller compared to the impacts of ethanol blending levels and market shares.
    - E10, E25 and E40 RSP can reduce well-to-wheels GHG emissions by up to 3%, 6% and 9% relative to the non-RSP baseline case, respectively. The maximum RSP shares for the reductions are 30%, 65% and 70% for E10, E25 and E40 RSP, respectively, and 5% MPGGE gain by RSP vehicles is assumed.
- Vehicle efficiency gains and upstream (e.g., oil sand shares) impacts on well-to-wheels GHG emissions are also significant.
    - The reduction in GHG emissions by E40 RSP relative to the non-RSP baseline case increases from 9% to 12% by assuming 10% MPGGE gain by RSP vehicles instead of 5% MPGGE gain.

Based on these results, FY 2015 activities under this task will focus on the following:

- Updating the refinery LP modeling, including consideration of cost analysis and capital expansion. This subtask will also examine the impact of light and heavy crude inputs to refineries (e.g., Bakken and Eagle Ford light crudes and Canadian oil sands heavy crudes); the impact of prices of crude, ethanol, and various refinery products (e.g., domestic regular and RSP gasoline and export gasoline); and the impacts of product slate changes (e.g., naphtha sales to the international market, gasoline/diesel ratio).
- Updating upstream of crude and ethanol. This subtask will investigate the production of light crude from Bakken and Eagle Ford, and update ethanol production.
- Generating updated GREET well-to-wheels simulation results.

Task E. Low-Cost Potential RSP Blendstocks

Objective

The objective of this task is to complete the following four activities:

- Examine the ranges of composition and properties for natural gasoline sold in the US market.
- Determine the properties of blends of various natural gasolines and ethanol at different blend levels.
- Develop a model to predict natural gasoline–ethanol blend vapor pressure.
- Determine the effects of natural gasoline on FFV emissions. EPA's recent Notice of Proposed Rule Making (NPRM) is requesting comment on the development of an emissions test fuel for FFVs.

Samples of natural gasoline will be obtained from eight sources covering the range available in the market. These will be assessed for chemical composition using detailed hydrocarbon analysis (ASTM D6730: High-resolution gas chromatography to identify individual components of gasoline) and by benzene analysis (ASTM D3606). Sulfur, vapor pressure, and RON will be determined by appropriate ASTM methods.

A subset of these samples meeting the current benzene limit and the proposed Tier 3 sulfur limit, and covering the range of composition and properties, will be blended with ethanol at 30, 51, 70, and 83 vol %. The vapor pressure, RON, and MON will be measured. For the E30 blends, NREL will also measure the distillation curve (D86) and vapor lock protection class ($T_{v/l=20}$). NREL has used a modeling approach based on the Wilson equation and on considering the gasoline as a pseudo-component to successfully predict the vapor pressure of gasoline–alcohol blends to within 0.7 kPa. That is more precise than the repeatability of the vapor pressure measurement method (2 kPa for ASTM D6378[13]) This method will be applied to the blends to determine its suitability for predicting Reid vapor pressure (RVP). Under this scenario, for the E30–83 blend, it would not be necessary to measure the RVP of the final blend, but only the RVP of the natural gasoline blend component, to predict the compliance of the blended product with EPA maximum and ASTM minimum RVP requirements. If this modeling approach is not successful, other approaches will be examined with stakeholder input. Vapor pressure, distillation curve, and vapor lock protection class will be used to predict the drivability of these blends.

Key outcomes from the FY 2014 research are the following:

- Natural gasoline consists of 80–95% paraffinics, 5–15% naphthenics, 3% or less aromatics, and the balance olefins. Paraffins were typically n-pentane and iso-pentanes.
- Benzene content ranged from approximately 0.1 to 1.2 wt %, so blends of E30 and E40 would meet EPA limits for benzene content in gasoline. Sulfur content ranged between 4 and 145 ppm. Assuming an ethanol content of 51 vol %, a natural gasoline blendstock would be required to have 20 ppm sulfur or less for the finished fuel to meet the EPA Tier 3 gasoline sulfur limit.
- The RON for the natural gasoline ranged from 67 to 72. When it is blended with ethanol, the 91 RON level typical of finished regular gasoline would be met with approximately 30 vol % ethanol.
- Vapor pressure (ASTM D5191-13) ranged from 12.9 to 14.55 psi. Because of the high vapor pressure, over 70 vol % ethanol could be blended into flexible fuel while still meeting the class 4 (wintertime) minimum vapor pressure requirement of 9.5 psi. For blending of class 1 (summertime) flexible fuel, a minimum of 74 vol % ethanol was required to stay below the 9 psi upper limit on vapor pressure.
- Modeling of vapor pressure using UNIFAC- and Wilson equation–based approaches provided good agreement with experimental data only below 50 and above 70 vol % ethanol. Because empirical parameters in these models are based on data for ethanol blended with conventional blendstocks, the models might be improved if they were recalibrated based on data for ethanol–natural gasoline blends.

Based on these results, FY 2015 activities under this task will focus on the following activities:

- Develop fuel property data for the high-level ethanol case using low-cost blendstocks (including renewable naphtha and other drop-in hydrocarbons, if available; natural gasoline; and butane). The objective of using these hydrocarbon streams is to utilize their unique properties in a way that maximizes the renewable ethanol content of the finished fuel and that facilitates much higher ethanol levels than does blending with conventional gasoline.
- Perform finished fuel blending analysis to identify the most cost-effective blending strategies for RSP production. Using proposed finished fuel properties for RSP blends, available property data for fossil and biomass-derived blendstocks, and blendstock rack costs, the RSP team will perform theoretical blending cost analyses with a hydrocarbon fuel blending model developed for BETO at NREL to identify the lowest-cost approaches for blending RSP at different ethanol levels.

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[13] Christensen, E., Yanowitz, J., Ratcliff, M., McCormick, R.L. "Renewable Oxygenate Blending Effects on Gasoline Properties" Energy Fuels 25 (10) 4723–4733 (2011).

Task F. Effects of Renewable Super Premium on Legacy Flex Fuel Vehicles

Objective

Task F will determine the performance benefits of high-octane gasoline blends such as E20–E40 for legacy ethanol-tolerant FFVs. Demonstrating a performance benefit for legacy FFVs offers the opportunity to revise marketing approaches to using ethanol blends in the legacy FFV fleet, bolstering the infrastructure to enable the fueling of future vehicles designed for this fuel.

FFVs used only 58 million gallons of ethanol in 2012. Limited ethanol use in FFVs is often attributed to limited E85 infrastructure. Unfavorable pricing (on a $/BTU or $/mile basis) and a 25% reduction in miles per gallon cannot be overlooked as important contributors to the limited use of "fuel for FFVs." If a new RSP for future vehicles is on the horizon, it could be beneficial to begin building out the fueling infrastructure now. Offering a new ~E30 blend as "renewable super premium for your FFV" could help the industry increase the infrastructure and sell additional ethanol now, if the fuel were priced and marketed appropriately. EPA's Tier 3 NPRM proposed to allow OEMs to request approval for an alternative certification fuel, such as a high-octane E30 blend. Before vehicles requiring this fuel can be offered for sale, the fuel needs to be widely available (much as unleaded gasoline was made available in 1975 before vehicles requiring it were sold, or ultra-low sulfur diesel fuel was available in 2006 before the sale of 2007 diesel engines that required it). Seventeen million FFVs on the road today can legally use an E30 blend, but consumers need some incentive to purchase the fuel.

This project aims to establish the performance benefits of an RSP-like fuel in the legacy FFV fleet. As a stand-alone effort, four FFVs will be tested to represent multiple FFV OEMs and available engine technologies. Some manufacturers are already advertising increased torque and power output for their FFVs when they are fueled with E85, and prior work has shown that small amounts of ethanol can have a large effect on improving the anti-knock properties of the fuel. Therefore, a performance benefit is likely; this task will quantify the benefit.

The following are key findings from the FY 2014 research:

- A GMC Sierra FFV and a Chevrolet Impala FFV demonstrated a solid acceleration performance improvement with 100 RON E30 compared with 87 AKI E10. These GM FFVs use normally-aspirated gasoline direct-injection engines.
- Preliminary analysis of results for a Chrysler minivan and a Ford F150 pickup with port-fuel injection engines showed a less significant performance improvement. Data analysis for these vehicles is ongoing and a report is planned in FY 2015.

Task G. Efficiency Gains of Renewable Super Premium in A Dedicated Vehicle

Objective

Task G will quantify the CO_2 emissions benefits of ethanol fuel blends at the vehicle level. Significant CO_2 reductions are possible from a combination of improved engine thermal efficiency and improved system efficiency from downspeeding and downsizing.

Discussion

Ethanol is a superior spark ignition engine fuel when engines are designed for it; however, its use in regular gasoline–ethanol blends at 10 or 15 vol % or in ethanol-tolerant FFVs that are optimized for gasoline do not allow its superior properties to be exploited. Recent research (highlighted at the 2013

High Octane Fuels Symposium) suggests that a new fuel with 20–40% ethanol could enable greatly improved thermal efficiency in future downsized, downspeeded, boosted engines and result in fuel economy on par with E10 fuel in conventional vehicles (volumetric fuel economy parity). In addition to the potential for consumer acceptance of such a high-performance fuel, a reduction in GHG emissions would be expected. The fuel would have the added benefit of contributing to Energy Independence and Security Act compliance.

ORNL has acquired a relevant test vehicle for this effort. The vehicle is equipped with a turbo-charged gasoline direct-injection engine. The OEM has committed to providing technical support such as engine controls, an instrumented cylinder head, and high-compression pistons. The baseline, or first phase of the effort, will involve the stock engine build. Fuel blends with a range of RONs and ethanol content will be used in the first phase, ranging from 87 AKI to 100 RON and with ethanol contents up to 40%. In the second phase, higher-compression pistons will be installed and experiments repeated with several of the fuel blends.

Experiments will include triplicate tests of the Federal Test Procedure (FTP, or city cycle); the US06 high-speed, high load test; and a torque curve measurement for each fuel. The FTP, used for estimating "city" fuel economy, consists of transient stop-and-go driving under fairly light engine loads. The US06 test involves much more aggressive acceleration and power demands (under these conditions, manufacturers often must retard combustion phasing to avoid knock, sacrificing thermal efficiency). These two cycles will capture the typical range of vehicle operation and highlight the efficiency benefits of high-octane fuels when knock is avoided. Engine downsizing will be simulated by repeating experiments at higher test weights. The current experiment scope is one vehicle with OEM support and one compression ratio change. The main focus of this study will be to evaluate and quantify the improved efficiency (fuel economy) with an improved high-octane fuel, highlighting the benefits of ethanol. The vehicle experiments will be conducted throughout FY 2015 and reported in early FY 2016. NREL will support the study with fuel blend guidance and fuel analyses.

The following were significant activities in FY 2014.

- A 2013 Cadillac ATS vehicle was purchased and baseline fuel economy and emissions were measured with certification gasoline.
- OEM support was secured to facilitate changing the compression ratio and ignition timing.
- The vehicle is equipped with a 2.0 liter turbocharged, gasoline direct-injection engine and manual 6-speed transmission. The manual transmission will enable ready adjustment of shift schedules for downspeeding.
- An instrumented cylinder head was provided by the OEM partner. The cylinder head has been installed on the engine to enable cylinder pressure measurements.
- Spare sets of wheels and tires and a taller differential gear have been acquired to facilitate downspeeding

Task H. Descriptive Properties for Knock Resistance

Objective

RSP specification is made challenging by the fact that knock resistance for ethanol blends is a function of both octane number and heat of vaporization (HOV; evaporative charge cooling). A performance-based metric for charge cooling (as opposed to requiring a specific ethanol content) may be required by ASTM but does not yet exist, making this a high-priority task for the introduction of RSP. The research will include an assessment of various methods of measuring or capturing the HOV and octane number effects in fuel knock resistance, and validation of these measurements in single-cylinder engine experiments. The fuel property methods include distillation curve and HOV calculation from the Clausius-Clapeyron Equation, and HOV measurement by differential scanning calorimetry (DSC) or other methods. Additional approaches will be identified in this research. A small number of engine tests will be performed using an existing engine setup and will simply validate that a measured fuel parameter is predictive of knock resistance.

Significant findings from the FY 2014 research include the following:

- Blends of ethanol at 10 to 50 vol % were prepared with three gasoline blendstocks and a natural gasoline. RON and MON, as well as other performance properties, were measured. HOV was estimated from a detailed hydrocarbon analysis (DHA) as well as by using a DSC/thermogravimetric analysis (DSC/TGA) method. A striking feature of the DHA results was the insensitivity of HOV to the hydrocarbon blendstock for temperatures up to 150°C—that is, all gasoline blendstocks tested had essentially the same HOV. Additionally, all four gasoline blendstocks had the same response for HOV when blended with ethanol. Should this prove true for a larger set of gasoline blendstocks, then there is no need to measure HOV: it can simply be calculated or looked up on a chart as a function of temperature and ethanol content.
- Measurement of knock-limited spark advance in a single-cylinder engine suggested that the knock resistance of high-HOV E25 and E50 was not captured by the octane index defined as OI=RON – K S, but that agreement could be improved by adding a term related to HOV.

Based on these results, FY 2015 research will focus on improving the precision of measurement of HOV by DSC/TGA, and particularly on measuring HOV as a function of the fraction evaporated. This information is important to automobile OEMs for calibrating dedicated RSP vehicles for cold weather starting and possibly for other purposes that have not yet been identified. To more fully predict fuel economy benefits from using RSP, it is important to quantify any knock resistance benefits associated with ethanol that may not be fully captured in standard RON and MON measurements for vehicle design. NREL will also provide ORNL with a detailed knock resistance characterization for fuels being tested in other tasks of this project.

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