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Refining Economics of U.S. Gasoline: Octane Ratings and Ethanol Content

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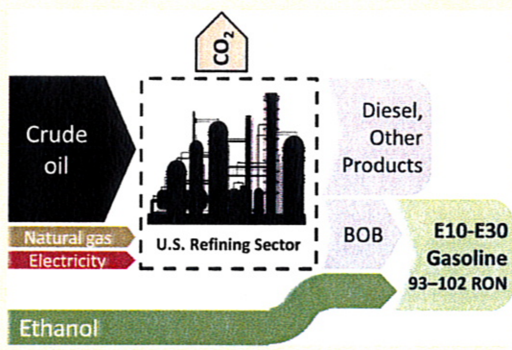
Supporting Information

ABSTRACT: Increasing the octane rating of the U.S. gasoline pool (currently ~93 Research Octane Number (RON)) would enable higher engine efficiency for light-duty vehicles (e.g., through higher compression ratio), facilitating compliance with federal fuel economy and greenhouse gas (GHG) emissions standards. The federal Renewable Fuels Standard calls for increased renewable fuel use in U.S. gasoline, primarily ethanol, a high-octane gasoline component. Linear programming modeling of the U.S. refining sector was used to assess the effects on refining economics, CO_2 emissions, and crude oil use of increasing average octane rating by increasing (i) the octane rating of refinery-produced hydrocarbon blendstocks for oxygenate blending (BOBs) and (ii) the volume fraction (Exx) of ethanol in finished gasoline. The analysis indicated the refining sector could produce BOBs yielding finished E20 and E30 gasolines with higher octane ratings at modest additional refining cost, for example, ~1¢/gal for 95-RON E20 or 97-RON E30, and 3–5¢/gal for 95-RON E10, 98-RON E20, or 100-RON E30. Reduced BOB volume (from displacement by ethanol) and lower BOB octane could (i) lower refinery CO_2 emissions (e.g., ~ 3% for 98-RON E20, ~ 10% for 100-RON E30) and (ii) reduce crude oil use (e.g., ~ 3% for 98-RON E20, ~ 8% for 100-RON E30).



■ INTRODUCTION

Octane rating specifications for standard grades of U.S. gasoline (regular, midgrade, and premium) have not changed since the 1970s, when leaded gasoline was phased out, leading to reductions in gasoline antiknock index (AKI) and compression ratios (CR) for naturally aspirated engines. AKI is the average of research octane number (RON) and motor octane number (MON)). But, since the 1970s, there have been great changes in technologies, standards, and regulations applicable to vehicles, oil refining, and fuels.

Auto manufacturers have improved performance and complied with higher fuel economy standards for new U.S. car and light-duty trucks using a variety of design changes, including gradually increasing engine CR. Higher CRs have been enabled by new engine technologies (adaptive spark control, variable valve timing, and fuel injection) and by new combustion chamber designs featuring high turbulence, central spark plug location, and optimized cooling. New vehicle technologies have also contributed (hybridization, turbocharging, downsizing, lightweight materials, and improved aerodynamic drag and rolling resistance).

Over the same time period, refineries have increased energy efficiency, reduced operating costs, met more stringent fuel standards (e.g., low-sulfur gasoline and diesel fuel), accommodated increasing volumes of ethanol in the gasoline pool,

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and are now reducing the gasoline/distillate ratio of the U.S. refined product slate in response to changes in demand. U.S. gasoline now meets stringent regulations for volatility (as measured by Reid Vapor Pressure (RVP)), sulfur content, and benzene content.

The U.S. Renewable Fuel Standard (RFS2) mandates[1] have triggered large increases in ethanol use; essentially all U.S. gasoline is now E10. RFS2 calls for further annual increases in ethanol use through 2022, although it is not clear how additional ethanol volumes will be accommodated in the gasoline pool, given current regulations governing gasoline and the limited compatibility of the refueling infrastructure and the light-duty vehicle fleet with ethanol content greater than E10.

More change is coming as the automotive industry gears up to meet new federal corporate average fuel economy (CAFE) and GHG standards.[2] The new standards become more stringent each year, reaching a fleet average of 54.5 mpg in 2025 (about double the current standard). Meeting these standards will require advanced vehicle and engine technologies and, possibly, new fuels.

One approach under consideration is to further increase gasoline engine CRs to achieve higher thermal efficiency and therefore higher vehicle fuel economy and lower GHG emissions. For example, increasing the CR from 10:1 to 12:1 could increase efficiency by 5−7%, or by 6−9% for 13:1, depending on attributes of the vehicle, engine, fuel, and drive cycle.[3,4] However, higher CRs require higher-octane fuel to prevent knocking at high load. Increasing CR by 1 number (e.g., from 10:1 to 11:1) requires an increase of 2.5 to 6 RON in the fuel (e.g., from 92 RON to 94.5−98 RON),[3−5] depending on cylinder displacement and geometry and engine technology (e.g., direct injected or port fuel injected, turbocharged or naturally aspirated).

As ethanol use has increased in the past decade, the U.S. refining industry has reduced the average octane rating of the hydrocarbon portion of gasoline (the BOB) by approximately 2−2.5 AKI to take advantage of ethanol's high octane rating while meeting the minimum octane standards for the finished gasoline.[5]

The potential for realizing higher gasoline octane ratings depends on refining techno-economics and federal and state standards on gasoline properties and composition. However, significantly higher gasoline octane ratings can be achieved by (i) increasing the octane rating of hydrocarbon gasoline to the extent feasible (e.g., to values typical 10 years ago) and (ii) increasing ethanol content from the current 10 vol % to 20−30 vol % (assuming federal regulations were modified to allow such fuels). Ethanol has a high volumetric blending octane value in gasoline: ∼115−135 RON, depending on the ethanol concentration and BOB RON and composition (Supporting Information (SI) Section 4.6).[6,7]

Ethanol also has a high latent heat of vaporization and high sensitivity (RON minus MON), contributing to improvements in knock resistance in direct-injection and turbo-charged engines, allowing further increases in CR.[3,4] Ethanol can also increase efficiency in part-load operation, regardless of engine architecture.[8,9]

Finally, increasing the ethanol content in gasoline blends could reduce the "well-to-wheels" (WTW), life-cycle GHG emissions from light-duty vehicles, with the magnitude depending on the carbon footprint of ethanol production, fuel properties (e.g., carbon content), and engine efficiency benefits.

The use of high-RON gasolines would contribute to the vehicle industry's ability to meet future CAFE and GHG standards, but the production of such fuels would impose costs on the refining industry. Older WTW studies are outdated, do not consider GHG implications in the U.S. setting, and do not consider ethanol use at present or projected U.S. levels. The 1970s oil embargo and lead phase-out spurred studies[10,11] of optimal octane ratings for unleaded U.S. gasoline, considering both refining sector effects and vehicle efficiency. Reviewing these studies, the U.S. Environmental Protection Agency (EPA) concluded[12] that "the current rating of 91 RON/83 MON for unleaded gasoline does not appear strictly appropriate on a permanent basis." In the 1980s, a European oil industry study[13] evaluated gasoline octane ratings in light of their lead phase-out. In that study, oil consumption was the key metric and neither GHG emissions nor ethanol as a high-octane blending component were considered. A more recent European analysis[14] considered cases with 100-RON gasoline and E20 gasoline, reporting higher refinery CO_2 emissions and cost in the former case and lower CO_2 emissions and cost in the latter. In 2005, a Japanese auto-oil industry research group concluded that increasing the RON of Japanese gasoline from 90 to 95 could provide a WTW CO_2 emissions reduction and that ethanol blending had greater potential than refinery changes.[15] However, that study considered vehicles designed for the Japanese market, Japanese refineries and fuels, and ethanol content was limited to 3 vol %.

A recent paper by Speth et al.[16] addressed economic and GHG implications of increasing U.S. gasoline RON from regular- to premium-grade in the context of future CAFE standards and reported significant associated reductions in WTW CO_2 emissions and cost. Further addressing the lack of relevant analysis, this paper examines the implications for the U.S. refining industry of increasing the octane rating and/or the ethanol content of U.S. gasoline. It assesses the investment requirements, refining cost, and other consequences in the U.S. refining sector of producing a national gasoline pool meeting minimum RON standards from 93.2 (the approximate current average) to 102, with ethanol concentrations from 10 to 30 vol %, both as nationwide midlevel blends (E10 to E30) and as combinations of E85 and E10. Fuel properties are estimated to enable WTW assessments of the associated GHG emissions.

METHODS

The analysis employed regional refinery linear programming (LP) modeling to estimate the effects on the U.S. refining sector of producing a single future national gasoline that (i) meets a uniform minimum octane rating (RON) standard, (ii) contains ≤10 ppm sulfur (the new national Tier 3 standard),[17] and (iii) satisfies existing federal, California, and industry gasoline standards. Linear programming has long been the preferred method for analyzing technical and economic aspects of refining operations.[18,19] A refinery LP model yields an optimal value for an economic objective function, subject to a set of constraints denoting product demands, crude oil availability, refinery process capacities and capabilities, and energy and material balances.

In this study, the objective function to be minimized was total refining cost (the sum of direct operating costs and capital charges for new investments) incurred in producing the same slate of primary refined products with specified properties including octane rating. In this product slate, the volumes of all primary refined products were fixed in all cases (as required for

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cost minimization). (See SI Section 4.5.) The methodology for estimating capital charges associated with installing new refining process capacity is discussed in SI Section 4.8 and is similar to that used in the U.S. Department of Energy's Liquid Fuels Market Model.[20]

The analysis assessed refining operations in a future year (2017) for each of three regional refining aggregates, defined in terms of U.S. Petroleum Administration for Defense Districts (PADDs, SI Section 1). PADDs 1−3 were treated together because of their similar refinery characteristics; PADDs 4 and 5 were treated individually because their refining operations and economics differ significantly. Regional results (presented in SI Section 5.3) were aggregated to a national level.

Model Cases. Table 1 shows the scenarios in the analysis, each consisting of a combination of current gasoline octane

Table 1. Modeled Fuel Scenarios

			ethanol blend			
			E10	E10	E20	E30
	sulfur		1 psi RVP waiver			
case	(ppm)	RON	yes	no	no	no
calibration cases (2010)	30	93.2	•	N/A	N/A	N/A
reference cases (2017)	10	93.2	•	•	•	•
study cases (2017)						
E10, E20, E30	10	95	•	•	•	•
	10	98	•	•	•	•
	10	100	•	•	•	•
	10	102	•	•	•	•
E10/E85 combinations	10	93.2[a]	N/A	N/A	•	•

[a]RON of the E10 portion is the same as the Reference cases.

ratings or prospective national RON standard (95 to 102 RON), ethanol concentration (10, 20, or 30 vol %), and RVP waiver assumption. Two additional scenarios representing joint production of E10 and E85 with total ethanol volumes matching that required for national E20 and E30.

Calibration cases validated the regional refining models by demonstrating that their outputs closely match reported data on refining sector performance in 2010, including retail gasoline property data.[21] (See SI Section 4.1).

Reference cases represented production of projected refined product volumes in the study year (2017) assuming nationwide E10, E20, or E30 with *unchanged octane ratings*, and subject to all other fuel regulations and industry standards currently in place or scheduled to be in place by 2017, including the Tier 3 gasoline sulfur limit (10 ppm average).[17] The Reference cases embody octane ratings corresponding to the current average for the U.S. gasoline pool: 87.6 AKI, corresponding to 93.2 RON. For PADD 4, the baseline includes an AKI of 85 (not 87) for Regular-grade gasoline.

Study cases assessed the techno-economic refining sector effects, relative to the corresponding Reference cases, of meeting higher national RON standards with specified ethanol concentrations and blending approaches (as nationwide E10, E20 or E30 or as E10/E85). In the E10/E85 cases, ethanol constituted 20 vol % or 30 vol % of the U.S. gasoline pool, but with the ethanol blended in combinations of E10 and E85 in amounts to provide equal total delivered energy. The ethanol content of E85 was 74 vol %[22] and RVP was 8.0 psi for both winter and summer, with light naphtha as hydrocarbon blendstock.

Model Assumptions. Consistent with federal, state, and industry standards for E10,[23] finished gasoline in all Reference and Study cases also met the following property limits: MON > 82, sulfur <10 ppm average, summer RVP (7 psi in California and federal RFG areas; 9 psi elsewhere), Driveability Index <1250, and benzene <0.62 vol %, average.

Uncertainty in future RVP regulations was considered. Under the federal Clean Air Act,[24] E10 is allowed a 1 psi RVP waiver, relaxing the applicable summer RVP standard by 1 psi, in regions not otherwise subject to lower RVP standards. This waiver reduces refining costs. Higher ethanol blends including E20 and E30 are ineligible for the RVP waiver and were modeled accordingly. The E10 cases were modeled both with and without the RVP waiver; the former to represent current regulations and the latter to avoid conflating the refining cost of summer RVP control with that of producing high-RON fuels.

All Reference and Study cases reflect (i) regional refined product volumes for 2017 estimated from national projections from the U.S. Energy Information Administration (EIA), (ii) an average crude oil price of $96/b, and (iii) an average natural gas price of $5.19/Mcf, all drawn from EIA's Annual Energy Outlook 2011.[22] Reference cases for each refining region maintain approximately constant domestic gasoline output in terms of *energy delivered* (BTU/year) across *all* ethanol concentrations. The total annual volume of finished gasoline increases with increasing ethanol content, reflecting ethanol's lower energy content relative to hydrocarbon gasoline. The Study cases corresponding to each Exx Reference case maintained the same finished gasoline volume.

In all cases, the regional refining models represented refinery production of gasoline blendstocks for oxygenate blending (BOBs). A BOB (SI Section 1) is a gasoline blendstock purpose-produced for blending with ethanol in specified proportions (downstream of the refinery). The resulting finished gasoline meets the specified octane rating standard and all other specifications.

The refinery LP models incorporate ethanol's octane contribution estimated using the molar concentration blending method,[6,7] expressed as volumetric blending octane values that decrease with increasing RON of the finished gasoline blend (SI Table S6). This method provides a conservative representation of ethanol's blending value in typical U.S. gasoline.[7] The blending RVP for ethanol was incorporated as a declining function of ethanol content from E10 to E30[25] (SI Section 4.6).

Model Outputs. The estimated refining sector effects (relative to the appropriate Reference case) for each Study case include the required RON and MON of the BOBs, industry-wide average annual additional refining cost (ARC), per-gallon ARC, refining industry investment, crude oil input to the refining sector, natural gas and electricity use, refining sector CO_2 emissions, average operating severity and total throughput of refinery reformer units, refinery sales of distressed blend-stocks, resulting effects on BOB properties (aromatics content, density, energy content), and consumer savings associated with energy density. Reported refining cost and refinery CO_2 emissions results are average national full-year *differences* between values for Study cases and their corresponding Reference cases.

The methodology for computing refining sector CO_2 emissions (described in SI Sections 2 and 3) was as in a prior study by Hirshfeld and Kolb.[18] The estimated CO_2 emissions apply only to the refining sector; they *do not* represent complete life cycle emissions for fuels (e.g., natural gas) purchased by refineries and used to provide refinery energy.

The estimated changes in refining costs apply only to BOB production and do not depend on the price of ethanol, because ethanol use is constant across the Reference case and Study cases *within* a given ethanol blending scenario (E10, E20, or E30).

The higher ethanol concentration cases assume that implementation barriers are managed; total U.S. ethanol supply (from all sources) increases to support nationwide demand; federal and state regulations governing ethanol/gasoline blends are modified to allow such concentrations; and vehicle fleet and infrastructure capability are in place. Likewise, the E10/E85 cases assume sufficient ethanol supply, numbers of flexible fuel vehicles (FFVs), and E85 fueling stations, and a regulatory framework to support energy parity (or better) retail E85 pricing.

RESULTS

Key results, presented here, include refining economics, CO_2 emissions, petroleum consumption, and BOB properties. Additional and more detailed results are given in SI Section 5 and SI Appendix C.

Refining Economics. The estimated average additional refining costs (ARC, ¢/gal of BOB)—*relative to the corresponding Reference case*—of producing gasoline BOBs for each case are shown in Figure 1. These estimated costs are independent of ethanol price. They are volume-weighted national averages for the refining regions analyzed and include changes in investment costs and annual operating costs. For a given ethanol content, the refining cost increases with increasing RON standard at an accelerating rate. However, for a given RON standard, the associated ARC decreases with increasing ethanol content. These trends exist for every refining region.

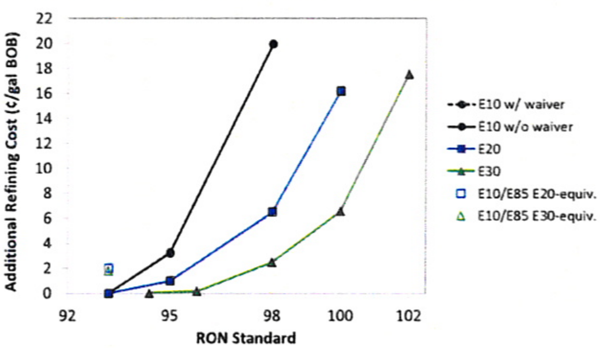

Figure 1. Estimated additional refining cost (¢/gal BOB) for different finished gasoline RON standards, total U.S. year-round average, relative to the respective Reference cases.

The highest point shown on each curve represents the maximum RON considered feasible for production as the primary gasoline throughout the U.S., using only ethanol and refinery-produced gasoline blendstocks (i.e., with no purchased high-octane blendstocks). These limits come primarily from limitations in U.S. refineries' existing octane-generating capacity needed to produce high-octane BOBs. However, the *maximum* RON standards likely to be attainable nationwide increase with available ethanol content, namely 98-RON E10, 100-RON E20, and 102-RON E30.

The analysis suggests that the refining sector could produce BOBs for national 95-RON E20 or 97-RON E30 gasoline pools at an ARC of approximately 1¢/gal of BOB. This small cost increase reflects the fact that these BOBs have octane ratings similar to that of the BOB currently used for Regular-grade E10. The refining sector could produce national BOB pools for (i) 95-RON E10, 97-RON E20, or 100-RON E30 gasoline pools at ARCs of approximately 5¢/gal, and (ii) 96-RON E10, 99-RON E20, or 101-RON E30 gasoline pools at an ARCs of approximately 10¢/gal.

The cost estimates incorporate both volume and octane rating effects on refining costs. Increasing the *ethanol content* in finished gasoline at constant octane (e.g., E10 95 RON → E20 95 RON) reduces refining costs through two effects. The required octane rating of the BOB declines (Figure 2), reducing the refining cost, and the necessary volume of the gasoline BOB declines (to accommodate the additional ethanol). Increasing the *octane rating* of gasoline at constant ethanol content (e.g., E20 95 RON → E20 98 RON) increases refining costs, likewise through two effects. The required BOB octane rating and associated refining cost increase, while the volume of BOB declines slightly, because its energy density increases with increasing RON. Additional details are provided in SI Section 5.2.

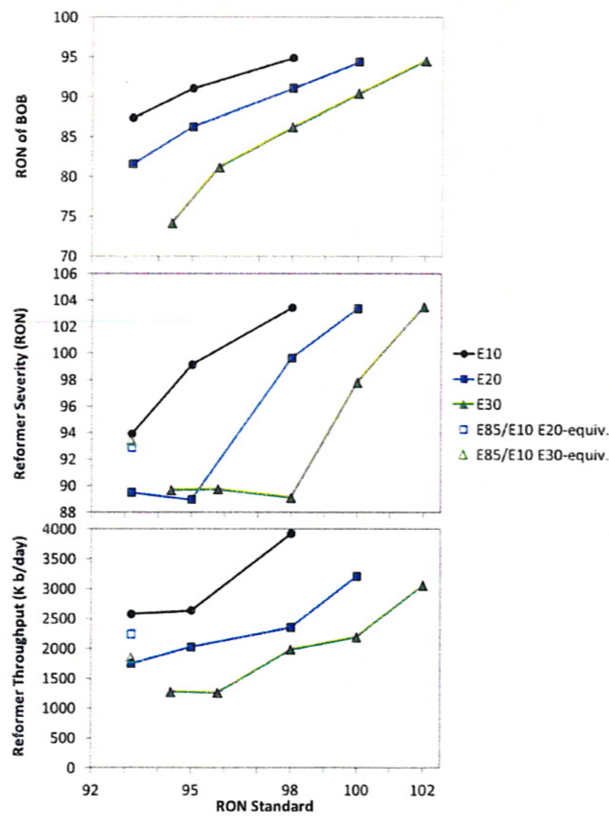

Figure 2. Estimated RON of gasoline BOBs and U.S. total reformer throughput and average severity as functions of RON standard and ethanol content.

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Table 2. Key Results of Refinery Modeling, Year-Round Average, Total U.S

	finished gasoline pool								BOB pool		
study case[a]	RON	volume (MM b/d)	energy density (MM btu/b)	aromatics content (vol %)	Δ refinery invest.[b] ($billion)	Δ refining cost[b] ($billion/y)	Δ ARC[b] (¢/gal)[c]	energy density savings[b] (¢/gal)[c]	RON	MON	crude oil use (MM b/d)
E10	93.2	8.54	5.017	19.0	base	base	base	base	88.8	82.1	14.57
w/RVP waiver	95	8.54	5.025	21.6	4.45	3.84	2.9	0.6	91.1	83.1	14.69
·	98	8.54	5.075	28.6	27.07	23.52	18.0	4.0	94.9	87.1	15.31
E10	93.2	8.54	5.021	19.1	base	base	base	base	88.8	82.1	14.63
·	95	8.54	5.032	21.7	4.36	3.79	2.9	0.8	91.1	83.0	14.75
·	98	8.54	5.082	28.6	25.07	23.49	18.0	4.2	94.9	87.0	15.39
E20	93.2	8.83	4.839	12.5	base	base	base	base	83.3	79.9	13.82
·	95	8.83	4.849	13.8	0.18	1.04	0.8	0.6	86.3	79.4	13.88
·	98	8.83	4.863	18.9	5.92	7.02	5.2	1.7	91.1	83.2	14.13
·	100	8.83	4.904	22.9	17.28	17.51	12.9	4.3	94.4	86.7	14.45
E85/E10 E20eq	n/a[d]	8.82	4.859	15.6	0.79	2.20	1.6	0.9	n/a[d]	n/a[d]	13.95
E30	94.4	9.17	4.671	9.0	base	base	base	base	77.9	78.8	13.08
·	95.8	9.17	4.671	9.0	0.84	0.13	0.1	0.0	81.2	75.7	13.03
·	98	9.17	4.686	11.8	1.04	2.44	1.7	1.0	86.2	79.6	13.16
·	100	9.17	4.694	15.3	4.37	6.42	4.6	1.7	90.4	82.8	13.34
·	102	9.17	4.738	20.1	14.48	17.27	12.3	4.4	94.5	87.0	13.71
E85/E10 E30eq	n/a[d]	9.14	4.686	12.3	1.19	1.73	1.2	0.2	n/a[d]	n/a[d]	13.13

[a]All cases are without RVP waiver unless indicated otherwise. [b]Amounts are relative to the corresponding reference case (~93 RON) with the same ethanol content. [c]Amounts are ¢/gal of finished gasoline. [d]E10 and E10 BOB octane ratings are the same as the E10-only case w/o RVP waiver. The BOB for E85 is assumed to be light naphtha with approximately 71 RON and 70 MON.

Figure 2 shows the estimated BOB RON, average reformer severity, and total reformer throughput as functions of the finished gasoline RON and ethanol content. For a given ethanol content, the BOB octane rating is increased mainly by increasing the concentration of reformate, leading to greater aromatic hydrocarbon content (SI Table S15), higher crude oil consumption, and higher refinery energy use and CO_2 emissions.

(The estimation of BOB RON values using the linear molar blending method,[6] as described in SI Section 4.6, gives a conservative estimate of BOB RON. However, different BOB compositions can have second-order effects yielding higher RON than predicted by this approach.[7,26] Combining the synergistic ethanol blending effects reported by Anderson et al.[7] with the BOB RON values in Figure 2 yields higher finished gasoline RON values for all fuels in the study, with larger effects for E20 and E30 fuels than for E10. A key implication is that higher-octane blends would be more attractive than shown here, because they would require lower-RON BOBs).

The increases in ARC in most of the higher-RON cases are partially offset by the value of the gasoline's increased energy density (Table 2), stemming mainly from increases in aromatic hydrocarbon content. Increased energy density increases vehicle fuel economy and reduces the fuel volume consumed.

Table 2 includes a summary of key refining economics results, reported in terms of annual national values. Costs in Table 2 are incremental changes relative to each Reference case; Reference case costs are provided in SI Table SI−C1.

Estimated refinery investment required increases rapidly with RON standard for each ethanol content but decreases with increasing ethanol content for each RON standard. Most of the indicated investment goes to increase octane-generating capacity, mainly in reforming and pentane/hexane isomerization (the latter an octane-enhancing process that isomerizes *n*-paraffins to *i*-paraffins). Large increases in investments for the highest RON cases—more than $25 billion for E10 and $15 billion for E20 and E30, respectively—indicate that further increases in the RON standard (beyond those shown in Figure 1) would likely be infeasible with existing refining technology.

Estimated annual refining costs are the sum of capital and fixed charges for refinery investments and additional refining operational costs. The latter includes costs from increasing reformer severity and throughput, other octane-yielding refining operations, and loss in revenue associated with rejected low-octane refinery streams sold at a distress price (SI Section 4.5). The estimated annual refining costs and ARCs (¢/gal) exhibit the same trends as refinery investments with respect to RON standard and ethanol content.

Comparison of the refining economics for the E10/E85 Study cases with their corresponding E20 and E30 Reference cases indicates that average U.S. refining costs would be about 1.6¢/gal and 1.2¢/gal (of finished gasoline) higher if ethanol was blended in combinations of E10 and E85 rather than in national E20 or E30, respectively, with the *Reference case octane rating*. These incremental costs are approximately equal to that for producing nationwide 95-RON E20 and 97-RON E30, respectively.

The additional refining costs in the E10/E85 cases stem from "octane give-away" in E85: E85's octane rating is higher than that required by applicable fuel specifications, while it could be fully utilized for E20 or E30. (Current FFVs cannot fully utilize E85's high octane rating, because they must also function well using Regular-grade gasoline. Future vehicles optimized for E85 might realize greater benefit.) Refiners generally take full advantage of ethanol's octane value in the production of suboctane BOBs for E10; in the Reference cases it is assumed that they would follow the same practice in producing E20 or E30.

As a sensitivity analysis, the effect on estimated refining costs of changes in the assumed prices of crude oil and natural gas was determined. As discussed in SI Section 5.5, the ARC would be increased by increasing crude oil price due to increased crude oil demand. In contrast, the ARC would be decreased by increasing natural gas price because of increased production of low-value refinery streams used as refinery fuel instead of natural gas, and increased reformer production of hydrogen, displacing hydrogen produced from natural gas. Also, incremental costs of finished gasoline, assuming a given ethanol price, are provided in SI Table S16. Not surprisingly, higher ethanol price increases the incremental cost of finished gasoline production, in step with increasing ethanol content.

Refining Sector Crude Oil Use. Estimated changes in total refinery crude oil throughput, relative to the E10 Reference case, are shown in Figure 3. The E20 and E30 cases indicate

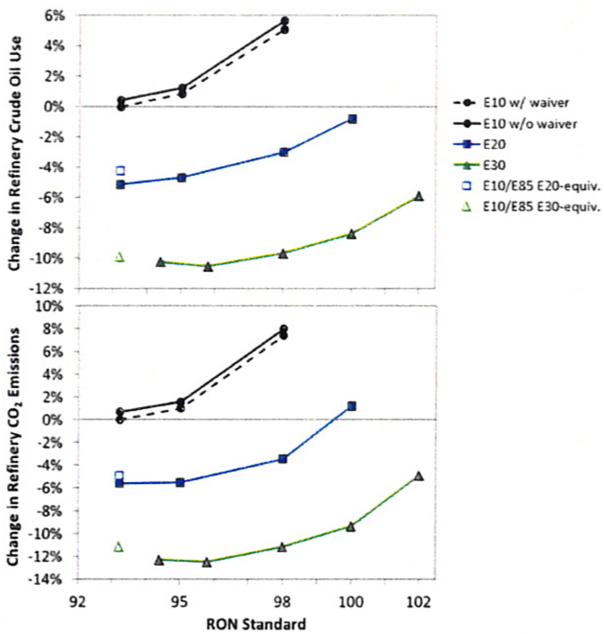

Figure 3. Estimated percent change in total U.S. refinery crude oil use (top) and CO_2 emissions (bottom) relative to E10 Reference case with RVP waiver, year-round average.

reductions of about 5% and 10%, respectively, in crude oil use. Reduced refinery demand for crude oil generally provides a net WTW reduction in oil use, because gasoline production consumes more oil than production of most alternative fuels.[27] These percentage changes are higher if attributed solely to the change in gasoline BOB production (i.e., by a factor of approximately 2, the ratio of total refinery product divided by gasoline BOB quantity).

Crude oil use increases with increasing RON (for a given ethanol content) because this requires higher RON for the corresponding BOBs, typically accomplished through increased reformer throughput and/or severity, both of which increase crude oil consumption. The additional consumption is negligible in Study cases with reformer throughput and severity comparable to their corresponding Reference case (Figure 2). Specifically, 95-RON E20 and 98-RON E30 involve increases in crude oil use of approximately 0.5%, and 1%, respectively, relative to their Reference cases (which have lower RON). Production of higher-RON BOBs calls for larger increases in crude throughput.

Refining Sector CO_2 Emissions. Changes in estimated annual refinery CO_2 emissions relative to the E10 Reference case are shown in Figure 3. Refinery CO_2 emissions decrease with increasing ethanol content in the finished gasoline pool. Conversely, at constant ethanol content, refinery CO_2 emissions increase with increasing RON of the finished gasoline pool, primarily reflecting increased refinery energy use to increase the RON of the BOB pool.

The analysis indicates that the refining sector could produce national BOB pools for 95-RON E10, E20, or E30 finished gasoline with increases in refinery CO_2 emissions $\leq$1% relative to their Reference case octane ratings. Producing national BOB pools for 98-RON E20 or E30 would entail increases in refinery CO_2 emissions of 2.3% and 1.3%, respectively. To yield a net reduction in WTW CO_2 emissions, these increases in refinery CO_2 emissions would have to be more than offset by vehicle CO_2 emissions reductions from higher engine efficiency enabled by these fuels.

Finished Gasoline Pool Properties. To conduct a complete WTW analysis for CO_2 emissions, changes in finished fuel properties are needed, including carbon/hydrogen (C/H) ratio, energy content (lower (net) heating value), and density. Fuel properties were estimated from results returned by the LP models (SI Section 4.7) and are given in SI Table S18 for both gasoline BOB and finished gasoline pools. In general, the C/H ratio and lower heating value of finished gasoline increase with increasing finished gasoline RON (at constant ethanol content) and decrease with increasing ethanol content (at constant finished gasoline RON). Density increases with RON whether accomplished through increased content of aromatic hydrocarbons or ethanol.

Vehicle tailpipe CO_2 emissions (assuming constant engine efficiency) are proportional to a fuel's energy-based carbon content (gC/MJ, Figure 4), calculated from carbon weight

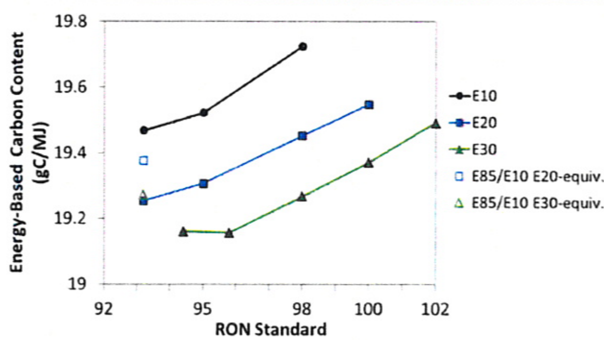

Figure 4. Energy-based carbon content of finished fuel pools (with no RVP waiver), defined as the ratio of carbon weight fraction and energy content on a lower-heating value basis. (Values for E85/E10 scenarios are weighted averages of E10 and E85 in the total fuel pool).

fraction and energy content (MJ/kg). This parameter increases with RON (for a given ethanol content) and decreases with ethanol content (for a given RON). For example, compared with the E10 Reference case, the energy-based carbon content of 98-RON E10 is 1.2% higher and that of 95-RON E30 is 1.6% lower. These differences reflect the greater energy-based carbon content of aromatic hydrocarbons relative to nonaromatic hydrocarbons and ethanol.

■ DISCUSSION

Increasing the octane rating of U.S. gasoline would enable higher engine efficiency, facilitating compliance with federal fuel economy and greenhouse gas (GHG) emissions standards for light-duty vehicles. It would also have significant implications for the U.S. refining sector, whether the higher octane ratings were achieved through more severe refining operations, increased use of ethanol, or both.

This analysis applied linear programming modeling of the U.S. refining sector to assess the effects on refining economics, crude oil use, CO_2 emissions, and gasoline pool properties of increasing the average octane of the U.S. gasoline pool (currently ~87.5 AKI, corresponding to 93.2 RON) to as high as 102 RON by increasing the octane rating of refinery-produced BOBs and/or the ethanol content in finished gasoline.

This analysis concludes that the U.S. refining sector could produce national BOB pools for 95-RON E20 and 97-RON E30 finished gasoline pools with < $1 billion of investment in additional refining capability and at an ARC of ~1¢/gal (including return on investment). The ARC for these BOBs is low because they would have octane ratings (~92 RON) close to that of the current U.S. E10 BOB pool. Similarly, the U.S. refining sector could produce national BOB pools for 95-RON E10, 98-RON E20, or 100-RON E30 gasoline pools with ~$4–$6 billion of investment and at an ARC of ~3–5¢/gal. Achieving still higher octane ratings for finished gasoline would incur progressively higher investment and ARC until practical limits of refining capability were reached. The price of ethanol relative to gasoline and crude oil are key determinants of the relative costs of the various finished fuels (SI Tables S16 and S17).

Producing E20 and E30 gasoline pools would incur somewhat lower refining costs, petroleum use, and CO_2 emissions than using the corresponding volumes of ethanol in combinations of E10 and E85. The difference stems from the "octane give-away" associated with E85 (whose octane rating is higher than that required by fuel specifications), whereas ethanol's octane can be fully utilized in producing BOBs for E20 or E30.

The study considered higher-RON E10 blends produced with and without the 1 psi waiver for summer RVP currently allowed for most U.S. gasoline (other than reformulated gasoline). Eliminating the RVP waiver would call for a compensating reduction of ~1 psi in the RVP of the affected E10 BOBs. In a given refinery, the ARC of this additional RVP control could be significant. However, on a year-round, national basis, the ARC of this additional RVP control would be small, because (i) it would be required only in the summer gasoline season and (ii) the RVP waiver is not available for federal and California reformulated gasoline (which account for more than one-third of the U.S. gasoline pool).

The analysis showed that, for a given ethanol content, refinery CO_2 emissions and crude oil use increase with finished gasoline RON, reflecting higher refinery energy use and higher reformer severity and throughput needed to produce a BOB pool with higher RON. For a given RON, refinery CO_2 emissions and crude oil use decrease with increasing ethanol content in the gasoline pool, due primarily to the reduction in BOB volume and RON.

The analysis did not include the option to utilize certain high-octane gasoline blendstocks not used now in the U.S., though some have been in the past, including hydrocarbons (iso-octane, iso-octene), alcohols (methanol, iso-butanol), and ethers (MTBE, ETBE, TAME), all with RON of 100 or more.[28,29] A national high-RON gasoline standard (coupled with increased supplies of natural gas liquids resulting from the expansion of U.S. natural gas production) could call out supplies of these high-octane blendstocks, which in turn could improve the economics of the high-RON gasoline standards, with or without additional ethanol use.

The cost estimates for E20 and E30 blends include neither additional costs that would be incurred in the distribution system, refinery to pump, to accommodate higher ethanol content fuels (e.g., replacement of tanks, lines, and pumps at terminals and filling stations) nor savings that might be realized because a national RON standard would reduce the number of gasoline grades in commerce. Nor do these estimates reflect any assessment of market conditions, such as supply/demand balances, that might influence retail gasoline prices in a given period.

Producing national E20 and E30 gasoline pools would require (i) changes in the regulatory framework governing ethanol use to allow such midlevel ethanol blends, (ii) sufficient additional ethanol production to support nation-wide production of these blends, (iii) changes in the distribution infrastructure to handle midlevel ethanol blends, and (iv) a vehicle fleet capable of using these fuels.

For vehicle manufacturers to optimize engine designs to use the combustion advantages of higher-RON, higher-ethanol content fuels, these fuels would have to be readily available nationwide and competitively priced with other liquid fuel alternatives, particularly during a transition to a national high-RON E20 or E30 standard. The transition would require concerted actions by multiple stakeholders, including fuel producers, fuel distributors and retailers, vehicle manufacturers, and government agencies. However, such transitions have been accomplished in the past to realize longer-term, system-wide benefits (e.g., transition to unleaded gasoline).

Understanding the implications for the refining sector is fundamental to assessing the feasibility and potential of future U.S. gasoline with higher octane ratings and/or higher ethanol content. This study provides a techno-economic assessment of this subject to address the lack of such information in the open literature. Higher-octane (95 RON) E10 gasoline was determined to be technically feasible, without considerable additional cost, CO_2 emissions, or petroleum consumption for refineries. Higher ethanol content (E20, E30) could provide a viable path to fuel with still higher octane ratings (98 RON) with reduced petroleum consumption and lower refinery CO_2 emissions. Considering the significant efficiency increases demonstrated for higher-CR engines,[3,4] these results suggest that further consideration (e.g., WTW life-cycle analyses[16]) of higher-octane gasoline in the U.S. is warranted.

■ ASSOCIATED CONTENT

Supporting Information

Further details on the methodology, detailed regional and national-level results, sensitivity analyses, and discussion. This material is available free of charge via the Internet at http://pubs.acs.org/.

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Notes

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