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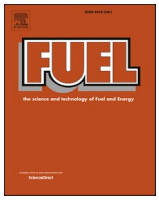

Full Length Article

Economic analysis of the benefits to petroleum refiners for low carbon boosted spark ignition biofuels

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ABSTRACT

A refinery modeling framework is developed to estimate the benefits of blending high-quality biofuels directly with refinery gasoline components to produce premium grade fuels. The results offer a change in paradigm - instead of biofuels being competitors to fossil fuels, biofuels can add value to refineries' product slates, because of their favorable properties. This potential value can be characterized by calculating the breakeven value (BEV), as defined below. The proposed modeling framework incorporates extensive data from (1) projected product demands over the next few decades, (2) crude oil and refinery products pricing, and (3) fuel specifications. The complete refinery models serve as a basis for assessing the value of biofuels, assuming profitability remains the same for representative petroleum refinery configurations. Resulting valuations varied widely with BEVs observed between $10-$120/bbl given the considered blending levels and crude prices. Further, BEV was correlated with the fuel octane ratings such as octane numbers (research, RON and motor octane numbers, MON) and both antiknock index (AKI, average of RON and MON) and sensitivity (S, difference between RON and MON), with a slightly higher correlation with the sensitivity. However, the expected decrease in gasoline demand for the upcoming years could negatively impact biofuels demand and value, in a business-as-usual scenario. The analysis also showed high valuations in smaller refineries since they can enhance the capabilities for producing specialty, high-value fuels/products, and introduce high octane-barrels into otherwise constrained blending operations. Additional implications towards refiners include opportunities to rebalance operations, access to high-value fuel markets, and synchronization with broader transportation industry trends. Furthermore, results indicate the value of Co-Optima boosted spark ignition (BSI) efficiency gains can extend to refiners to incentivize decarbonization and diversified feedstock production.

Abbreviations: BSI, Boosted Spark-Ignition; GHG, Greenhouse Gas; CAFÉ, Corporate Average Fuel Economy; RON, Research Octane Number; MON, Motor Octane Number; AKI, anti-Knock Index; S, Sensitivity; EPA, Environmental Protection Agency; ETC, Ethanol; IPR, Isopropanol; NPR, *N*-propanol; IBU, Isobutanol; DII, Di-isobutylene; CYC, Cyclopentanone; FUR, Furans Mixture; BOB, Before Oxygenate Blend; RBOB, Reformulated Before Oxygenate Blend; RVP, Reid Vapor Pressure; LCA, Life Cycle Assessment; PIMS, Process Industry Modeling System; PADD, Petroleum Administration for Defense Districts; LPG, Liquefied Petroleum Gas; AEO, Annual Energy Outlook; ADOPT, Automotive Deployment Options Projection Tool; NREL, National Renewable Energy Laboratory; BPD, Barrels-*per*-day; WTI, West-Texas Intermediate; OPIS, Oil Price Information Service; API, American Petroleum Institute; TAN, Total Acid Number; BTX, Benzene, Toluene, Xylenes; PCA, Principled Component Analysis; BEV, Break-Even Value; PIONA, *N*-paraffins, Isoparaffins, Olefins, Naphthenes, and Aromatics; MSP, Minimum Selling Price; TEA, Techno-Economic Analysis; BBS, Bio-Blendstock; DOE, Department of Energy; LSR, Light Straight Run Naphtha; FCC, Fluid Catalytic Cracking; ASTM, American Society for Testing and Materials.

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1. Introduction

The transportation sector is one of the largest contributors to global anthropogenic greenhouse gas (GHG) emissions, and in the United States (US) alone, accounted for over 28 % of total GHG emissions in 2018 [1,2]. There is a mounting concern to reduce the GHG emissions associated with gasoline and diesel fuels as well as improve the efficiency of combustion engines. The research and development of sustainable biofuels which demonstrate a synergistic performance improvement when used in co-designed engines was conducted through the Co-Optimization of Fuels & Engines (Co-Optima) project [3,4]. Light-duty biofuels to be consumed in boosted spark ignition (BSI) engines are considered in this analysis while heavy-duty biofuels for mixing-controlled compression ignition (MCCI) engines are similarly analyzed in Ref [5]. Light-Duty BSI biofuels, owing to their superior fuel properties such as higher-octane ratings, can be designed for use in low-emission vehicle engines with potential efficiency improvements up to 15 % [6,7].

Commercially available gasoline is a mixture of several blendstocks, produced from a variety of separation and upgrading refinery operations that are ultimately blended into a gasoline pool and then finished by adjusting composition and using a suitable additives package, for attaining government established (e.g., ASTM D4814) and market required (e.g., octane rating) specifications. These blendstocks cover a range of components from butanes to heavy naphtha sourced from crude distillation (straight run), fluidized catalytic crackers, hydrocrackers, cokers, visbreakers, alkylation, isomerization, and reforming units. Some of these naphtha fractions undergo hydrotreatment, mainly to ensure sulfur content is low enough for meeting that specification. Table A1 (in SI) summarizes the typical volume concentration of these traditional gasoline blendstocks, the ranges of their octane values, and the sources of their production in the refinery.

Progressively stringent fuel standards and heightened regulatory requirements are forcing gasoline producers to modify their operations which creates a unique opportunity for the expanded use of biofuels in refinery operations. Advancements in fuel economy standards, known as Corporate Average Fuel Economy (CAFÉ) standards [8], and the proposal from automobile manufacturers to create Research Octane Number (RON) 95 as the new uniform standard for gasoline will require an increased share of high octane blendstocks, such as reformate, in the fuel mix [9]. The rising price of octane over the last five to six years stemming from an increasing demand for premium gasoline and the increasing consumption of light shale oil [10] indicates that refineries are already facing operational constraints [11,12]. Additionally, the U.S. Environmental Protection Agency (EPA) introduced Tier 3 regulations that require all gasoline sold in the US to meet a 10-ppm annual sulfur average criterion [13]. Tighter sulfur restrictions could render some refineries unable to sell finished gasoline. Integrating bio-blendstocks with superior fuel properties may help less advantaged refineries remain competitive despite changing market demands and increasingly stringent fuel quality specifications.

Co-Optima researchers have evaluated several bio-blendstocks based on their fuel properties, scalability, and compatibility with existing infrastructure [14–17]. Candidates for the BSI combustion mode were systematically screened to down select promising candidates which encompass a range of functional groups [18]. An empirical relationship was developed to estimate the theoretical gains in engine efficiency as a function of bio-blendstock properties such as octane number, sensitivity (defined as the difference between research octane number (RON) and motor octane number (MON)), and heating value, among others [7]. Promising bio-blendstocks which met the fuel performance and efficiency improvement criteria were further evaluated to estimate their production costs using techno-economic principles as well as environmental impact and domestic job market growth metrics [7,17–19].

Of the top bio-blendstocks that were identified, seven of those: ethanol (ETC), isopropanol (IPR), *n*propanol (NPR), isobutanol (IBU), diisobutylene (DII), cyclopentanone (CYC), and a furans mixture (FUR) are investigated in this study, because of the availability of blending data of these bio-blendstocks with hydrocarbon blendstocks for oxygenated blending (BOBs) in Co-Optima research [6,20]. Previous research, from Co-Optima and other projects, has also focused on cost-benefit analysis and scalability of bio-blendstock production, but none so far have explored the economic potential for market adoption of biofuels from a full refinery operations perspective [17,21,22]. An in-depth literature search indicated that such analysis is not comprehensively discussed in scientific literature, and when discussed, is largely limited to valuing new fossil feedstocks [22,23]. This work proposes an innovative modeling framework that inlcudes all refinery operations (instead of only a blending terminal) to estimate the potential benefits to the refiner. Analysis efforts predicated upon these refinery-wide models have two key outcomes of interest. First, value propositions to refiners and biofuel producers from blending performance advantaged fuels into gasoline are identified. Understanding the impact of favorable biofuel properties such as octane, sensitivity, or Reid Vapor Pressure (RVP) on refinery economics can help generate market pull for new bio-blendstocks from refiners. Second, coupling refinery models with life cycle assessment (LCA) can identify the environmental benefits and tradeoffs of Co-Optima fuel blending (this will be the subject of an upcoming publication).

With the aforementioned interests in mind, the economic opportunity of blending the most promising Co-Optima BSI blendstocks into the gasoline pool is explored in the following three sections: (1) method development for benchmarking and analysis, (2) key results and implications, and subsequently, (3) discussion regarding limitations and future outlook. The methods section outlines the assumptions for establishing a model baseline with an emphasis on the development of refinery pricing structures. Other key underpinnings of the analysis included in the modeling approach such as gasoline specifications, fuel demand projections, and blending properties of bio-blendstocks are also described (Section 2). Further, the results section dives into the specific quantification of the bio-blendstock value to refineries, particularly as a function of its fuel properties at different blending ratios and different crude oil prices (Section 3), while the discussion section highlights some of the challenges and shortcomings of this analysis approach (Section 4). Overall, the objective of this analysis is to evaluate the value of unique and high performing bio-blendstocks within the economics of a traditional petroleum refinery.

2. Methods

AspenTech' s Process Industry Modeling System (PIMS) software [24] was used to develop and optimize three different refinery configuration models using the "Gulf-Coast" (belonging to the Petroleum Administration for Defense District 3, PADD3) example as a starting point. Differentiations between the three refinery configurations included varying complexities, production rate targets, and crude slates. These are labeled as PADD3-Large, PADD3-Medium, and PADD3-Small intending to represent refineries of decreasing conversion capacity and complexity, all located within the U.S. Gulf-Coast PADD3 region.

Information on the crude oils available to PADD3 region refineries can be retrieved from Ref. [25]. The properties of these crudes were sourced from conventional crude assays and were embedded in the example PIMS model. Primary petroleum processing units and their corresponding capacities shown in Table A2 along with typical yield compositions are also built into the model [26]. Ideas to expand the scope of the model are presented after results in the model customization section.

The objective function in PIMS advanced optimization mode aims to maximize the refinery model's gross margin subject to constraints on crude availability, limitations on process unit capacities and operating conditions, and specifications on finished fuels. The mass and energy balances are consistently maintained in all operations. The refinery

models considered here produce two grades of gasoline (a) regular and (b) premium for two blend types - conventional and reformulated - as well as a high-efficiency co-optimized BSI gasoline (similar in specs to reformulated premium) containing one of the several candidate bio-blendstocks. Notably, the co-optimized BSI gasoline blend enacts constraints on two gasoline features to improve efficiency and performance: (i) a novel minimum sensitivity of 10, and (ii) a minimum RON of 98. Table A3 displays the finished fuel specifications applied in the analysis.

The following subsections highlight all components incorporated into the refinery models including the following: (2.1) refinery configuration and capacity data, (2.2) product demand projections (from EIA, OPIS and ADOPT), (2.3) pricing structure, (2.4) bio-blendstock properties for blending, and (2.5) break-even value calculation. These bases derived from other Co-Optima projects, published literature, and experimental data provide a comprehensive framework to assess refinery impacts and valuation results for the BSI bio-blendstocks.

2.1. Refinery configuration and capacity data

Table A2 summarizes the process unit capacities of the refinery models employed in this study. These configurations were developed based on U.S. Energy Information Administration (EIA) data on the US refining infrastructure by each Petroleum Administration for Defense Districts (PADD) [26]. The goal was to develop sets of refinery models that span a wide range of refinery configurations and complexities as indicated by the calculated Nelson Complexity Index values in Table 2 [27]. Our analysis focuses on the PADD3-Large refinery configuration and PADD3-Small configuration which are intended to serve as book-ends for minimum to maximum biofuel value estimation.

2.2. Product demand projections from EIA, OPIS and ADOPT

Demand for gasoline range fuels for light duty vehicles is expected to decline over the next 30 years. To isolate the economic impact of biofuels blending, time-based scenarios are considered between years 2020 to 2050 to represent changing market demands. Fig. 1 presents the basis for the refinery operating scenarios with projections for the major refinery product categories such as liquified petroleum gas (LPG), gasoline, jet, distillate, and residual fuels. EIA projections from the Annual Energy Outlook (AEO) provide a complete basis for all product groupings [28]. In addition to the EIA gasoline BOBs projection, a second gasoline projection is also considered in the refinery scenarios from the Automotive Deployment Options Projection Tool (ADOPT) [29]. ADOPT is a consumer choice vehicle model developed by the National Renewable Energy Laboratory (NREL) taking parameters like vehicle price, fuel cost, and range into account, which in turn predicts the fuel demand. The ADOPT results predict a sharper decline in gasoline demand owing to a higher level of projected electrification in light-duty vehicles. Product demand projections in terms of volumes can be found in Table A6.

In addition to the projections for overall market demands, scenarios also consider a projection for the market share of premium gasoline relative to total gasoline products (Second Y axis, Fig. 1). Premium gasoline demand is important within the context of the analysis because Co-Optima gasoline is categorized within the premium gasolines grouping. Fig. 1 shows the premium market share interpolation between 2020 and 2050 based on data reported by OPIS [11].

2.3. Pricing structure

Crude oil and product pricing models were developed to model the impact of dynamic petroleum markets on bio-blendstock values. To simplify the number of economic inputs feeding the analysis, prices entering the model were correlated to a benchmark crude oil price, namely West-Texas Intermediate (WTI). WTI was chosen because of its longstanding position as the economic benchmark for crude oil pricing in U.S., its prevalence in the PADD3 district being the context for the analysis, and the availability of historical pricing data. Examples for each pricing calculation introduced in this section can be found in the SI.

2.3.1. Crude oil Correlation: Quality and price determination

Historically, different crude oil prices are correlated but not equal due to differences in quality, production costs, or transportation costs. Any crude oil historical pricing data that could be found in timestep with WTI was aggregated from multiple data sources and used to linearly regress the crude's price as a function of WTI price. After regression, a given crude oil's price could be modelled using equation (1):

$$P_{crude,\$} = m_c P_{WTI,\$} + b_c \quad (1)$$

where slope (m_c) and intercept (b_c) were fitted parameters yielded from linear regression. An example of a crude oil pricing calculation is shown in Example A in the **SI.** Various pricing data sources were utilized including the Energy Information Administration (EIA), Oil Price Information Service (OPIS), Bloomberg Terminal, and Baker & O'Brien's database to dilute any bias coming from an individual source. Modeling crude oil prices as a linear function of WTI price was the preferred crude oil pricing method because of the high-quality correlations typically observed.

When there was an insufficient amount of historical crude oil pricing data, a backup method for obtaining crude oil price as a function of

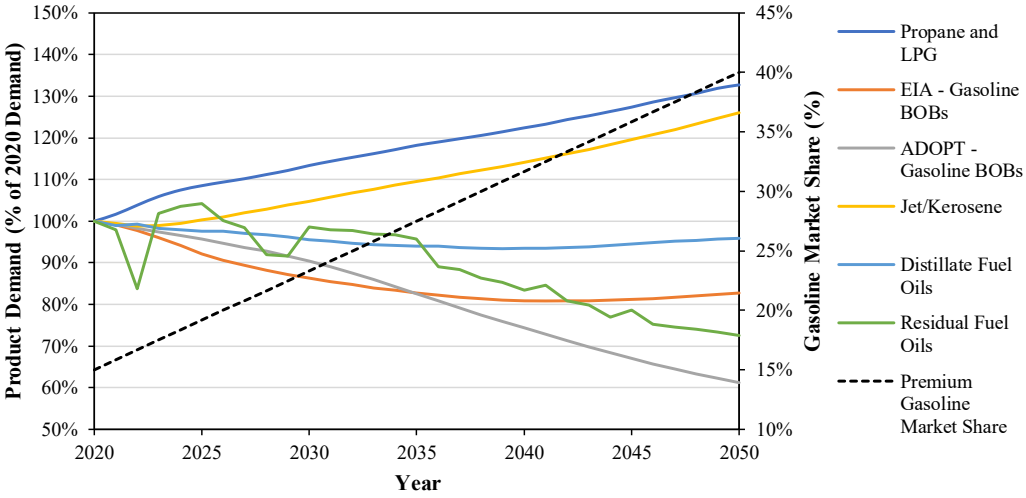

Fig 1. Projected product demands for refinery product (left Y axis) categories from EIA [28] and ADOPT model [29] alongside projected market share of premium gasoline fuels as a percentage of total gasoline fuels (shown by the dotted line linked to the right Y axis) [11]. Note: the demand projections were scaled to total 400,000 barrels/day (BPD) and 45,000 BPD for the PADD3-L and PADD3-S models, respectively, to set the maximum sale quantities for each product category in the refinery models. Capping the sales of each product depending on the year and demand projection source (EIA or ADOPT) simulated the dynamic economic conditions between 2020 and 2050.

crude qualities was developed. The variables in the pricing model include: the American Petroleum Institute (API) gravity measure, sulfur content (weight %), Total Acid Number (TAN), and WTI benchmark price [30]. API gravity is a commonly reported index of crude oil density and generally reflects the degree of conversion necessary to make high value products such as gasoline and diesel fuel. Sulfur content and TAN were measures intended to reflect the level of impurities in the crude oil and the corresponding level of treatment needed to make finished fuels. The WTI benchmark price was included to give the model a reference point and gave the model identical inputs when compared with the other pricing correlation models being utilized.

A multiple linear regression model performed well in capturing the crude oil pricing variability as a function of the four independent variables described above. Consequentially, crude oil prices determined by equation (2) supplanted pricing data determined by equation (1) when historical data limitations were encountered:

$$P_{crude,\$} = m_1(API) + m_2(Sulfur_{wt\%}) + m_3(TAN) + m_4\left(P_{WTI,\$}\right) + b \tag{2}$$

An example calculation using the crude quality model can be found in Example B in the **SI**.

2.3.2. Product price determination

Crude oil purchases are proportionally the largest cost associated with refinery operations leading to a high degree of correlation between the prices of crude oils and refinery products. Consequentially, product pricing model development with simple linear correlations was similarly enabled, when compared to the crude oil pricing models, as depicted in equation (3).

$$P_{product,\$} = m_p P_{WTI,\$} + b_p \tag{3}$$

Gaseous products such as natural gas or propane are less correlated to crude oil because they aren't exclusively sourced from crude oil production. However, the lower value of these products ultimately served to dampen the effects of pricing uncertainty on the model's profitability. Refinery intermediates were also priced to allow the PIMS-model to sell all molecules in case certain finished product specifications could not be satisfied. The same set of diverse sources used for crude oil pricing were again used to lessen the effects of bias from any one data source. An example calculation of gasoline price given a benchmark WTI crude price can be found in Example C in the **SI**.

2.3.3. Octane pricing correlation

The proposed performance-enhancing qualities of co-optimized fuels for BSI engines are twofold including 1) increased octane which is historically priced by the market through a spread between premium and regular gasolines and 2) increased sensitivity which has not been traditionally priced by the market. In an attempt to reliably and conservatively price co-optimized fuels with otherwise unknown values, an octane pricing model was developed with reference to regular gasoline. The pricing model is conservative due to its lack of accountability for increased sensitivity in the value of the co-optimized fuel. Increased engine efficiencies from higher sensitivity fuels will certainly increase value to end-users so not accounting for sensitivity effectively underprices co-optimized gasolines and the corresponding value bio-blending brings to refiners.

A single layer neural network model was fitted to historical data to predict octane value in terms of $/octane-gallon. Therefore, the model's output (Y) could be utilized in equation (4) to determine a price for co-optimized gasoline.

$$P_{co-op,\$} = Y\left(\frac{\$}{oct \bullet gal}\right)\left(AKI_{co-op} - AKI_{reg}\right)(oct) + P_{reg,\$}\left(\frac{\$}{gal}\right) \tag{4}$$

where octane value was multiplied by the difference in anti-knock index (AKI – calculated as the average of RON and MON) of the co-optimized gasoline and regular, conventional gasoline.

The neural network model inputs included a baseline regular gasoline price, total U.S. octane demand, and the differentials of benzene, toluene, and xylene commodity prices to regular gasoline price. The baseline regular gasoline price was included as a predictor to reflect the overall supply-and-demand equilibration constantly induced in the U.S. gasoline market. Total U.S. octane demand was calculated as the sum-product of regular and premium gasoline demands, respectively, and their corresponding octane numbers. This predictor was included to account for any octane-barrel supply constraints the U.S. refining industry may have faced historically that would have induced higher prices. Price differentials between commodity benzene, toluene, and xylene (BTXs) were also included because aromatics are common high-octane blendstocks refiners use to upgrade their regular gasoline pool. The price differences between regular gasoline and the constituents that are commonly added to form premium blends quantifies the value of octane to refiners to some degree. Predictors were highly correlated, so they were grouped into two principled components using principled component analysis (PCA) prior to fitting the non-linear neural network. The model was trained on 249 samples yielding a testing set R^2 of 0.97 on 62 samples with tenfold cross-validation. Fig. A1 shows a parity plot of the model's predictions and historically realized premium spreads.

2.4. Bio-Blendstock properties for blending

Blended properties were measured for each bio-blendstock in other Co-Optima projects using ASTM standard test methods (see [31] and references therein) with results stored in NREL's Fuel Properties Database [20]. The evaluated properties included RVP (ASTM D323), sulfur content (ASTM D1266/2622), distillation curve (ASTM D86), RON (ASTM D2699) and MON (ASTM D2700).

All bio-blendstocks considered in this analysis demonstrated a significant boost in final octane relative to the impact predicted by linear volumetric blending alone. To reflect the impacts of non-linear blending, effective blending properties were calculated for each blendstock at each blend level. The concept of blending octane number has been the subject of numerous studies [21] and can be summarized by the relationship shown in Equation (5) where RON_i represents the blending research octane number of a given bio-blendstock.

$$RON_{blend} = v_{BOB} RON_{BOB} + v_i RON_i \tag{5}$$

$$RON_i = \frac{RON_{blend} - v_{BOB} RON_{BOB}}{v_i}$$

Here, v_{BOB} and v_i represent the volume fractions of BOB and biofuel respectively, RON_{blend} is the measured RON of the final bio-blendstock/gasoline blend, and RON_{BOB} is the measured RON of gasoline BOB. Effective blending RONs, MONs, Sensitivities, and RVPs were calculated for each bio-blendstock, as exemplified in Equation (5), and are displayed in Fig. 2 and tabularized in Table A4.

Blending properties were used as inputs to the refinery model according to the bio-blendstock and blend level specified in each case. As a result, the refinery model would calculate the BSI gasoline's blended properties linearly, but the bio-blendstocks overwritten blending properties would cause non-linear shifts equal to those observed experimentally. The blended BSI gasoline was constrained to the specifications shown in Table A3 where equivalent specifications are shown for the traditional gasoline blends for reference.

2.5. Bio-Blendstock breakeven value (BEV) characterization

The break-even value (BEV) for a bio-blendstock, or any other refinery input, is defined as the calculated maximum purchasing cost that would preserve an equivalent gross margin under the same conditions without the purchase. The use of this calculation for valuation is consistent with industry practices for decisions like crude purchases as well as other bio-blendstock research [21]. The BEV calculation

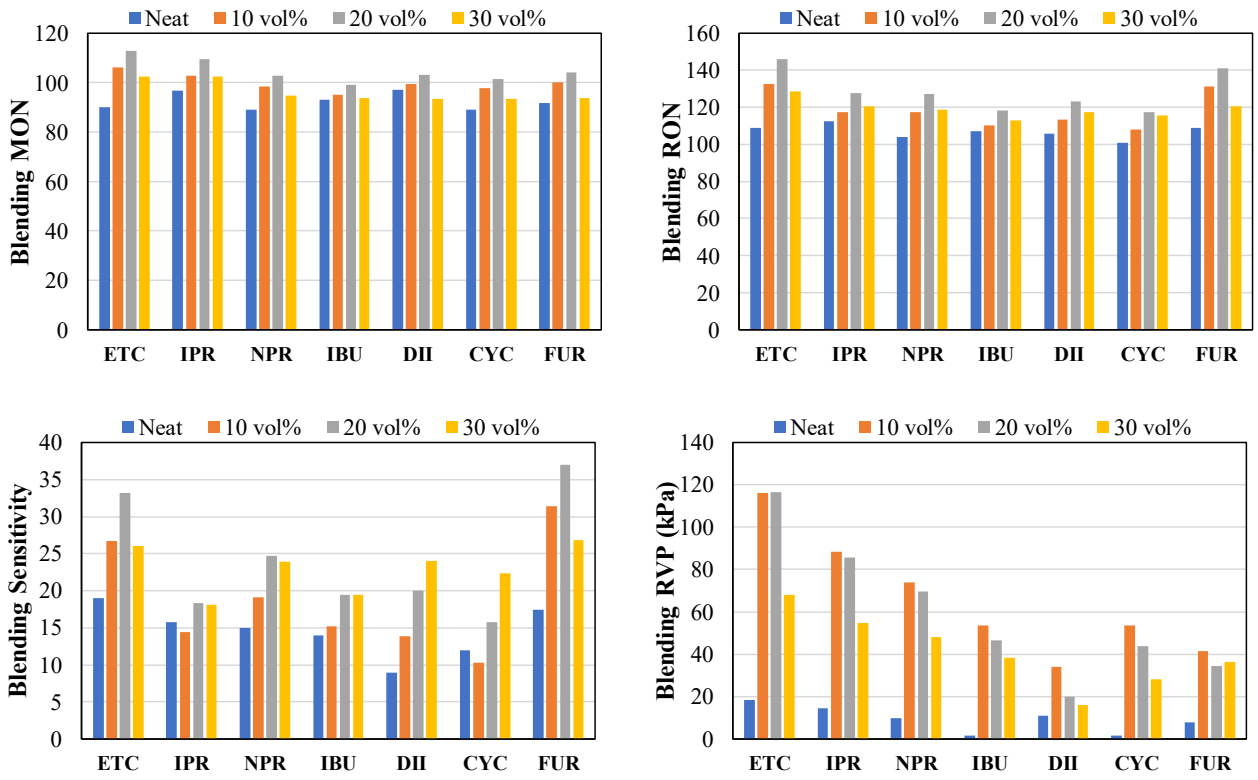

Fig 2. Graphical summary of blending properties applied in this analysis for Co-Optima BSI bio-blendstocks which show nonlinear effect on octane number, RVP, and other properties when combined with petroleum BOBs. Abbreviations are CYC: cyclopentanone, DII: diisobutylene, ETC: ethanol, FUR: furans mixture, IBU: isobutanol, IPR: isopropanol, NPR: *n*-propanol. The numerical values are described in **SI** Table A4.

procedure in this analysis was as follows: 1) fix model inputs including benchmark WTI price, year, demand projection source, bio-blendstock candidate, and blending level 2) optimize refinery model with no bio-blendstock purchasing and Co-Optima gasoline production allowed to find a baseline ($Profit_{Base}$) 3) re-optimize the PIMS refinery model with bio-blendstock prices set to zero and Co-Optima gasoline production allowed ($Profit_{BBS}$) 4) divide the difference between observed profits by the volume of bio-blendstock purchased (Vol_{BBS}) in the Co-Optima scenario as shown in Equation (6). The units for the BEV are US$ per volumetric unit of bio-blendstock (denoted by BBS below), typically calculated in barrels or gallons.

$$BEV_{BBS} = \frac{Profit_{BBS} - Profit_{Base}}{Vol_{BBS}} \tag{6}$$

The bio-blendstock BEVs are ultimately a function of product demands, crude and product prices, refinery configurations, refinery process unit capacities and constraints, blendstock properties, and finished fuel specifications. All of these elements were considered in the refinery model when optimizing refinery operating scenarios.

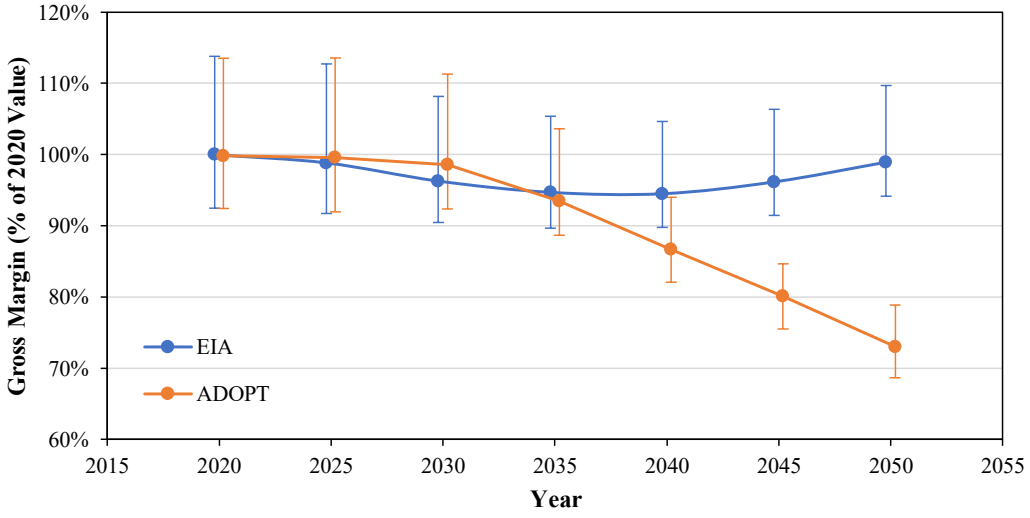

Fig 3. PADD3-Large refinery gross margins normalized to 2020 values given demand projections from both the EIA's Annual Energy Outlook (2019) and ADOPT consumer choice model.

3. Results

3.1. Establishing baseline refinery gross margin

A discussion on prospective refining strategies must consider the major market changes refiners are expected to endure over the next 30 years. As projected in EIA's Annual Energy Outlook and other industry perspectives, the refinery product slate is expected to undergo substantial transformation with the demand for gasoline in the light duty transportation sector declining while long haul transportation fuel demand is poised to increase [28,32]. Fig. 3 depicts the PADD3-L model's projected refinery gross margin extending to 2050 under both demand projections given by EIA and ADOPT, respectively. Gross margin values are given as percentages of 2020 gross margin. Whiskers represent the range of values observed over WTI benchmark crude prices varied from $20–100/bbl.

U.S. refineries are typically geared towards gasoline production (45 %–50 % of output volume), with diesel production accounting for approximately 25 % [28]. Thus, the higher level of electric vehicle market penetration predicted by the ADOPT model has a substantial effect on refinery profitability going out to 2050. The assumptions made in the EIA and ADOPT models may be considered bookends with ADOPT being the least favorable projection for the refining industry.

This work leveraged the expected trends in fuel demands to benchmark the change in refinery profitability with the assumption that the refining sector does not reconfigure. While this is an unlikely scenario, in the absence of any verifiable data, this assumption served as a basis to understand the value of bio- blendstock integration into the gasoline market.

3.2. Estimating bio-blendstock break even values

Fig. 4 depicts each bio-blendstocks' break-even value when blended at 10, 20, and 30 vol% with a WTI benchmark crude price of $60/bbl in year 2050 under EIA demand projections. This scenario was treated as a baseline as it represents a middle range WTI price during a fully developed Co-Optima gasoline market in 2050. Bio-blendstocks without a bar corresponding to the 10 vol% blending level did not have a high enough sensitivity to meet the minimum Co-Optima gasoline sensitivity specification of 10.

3.3. Determining bio-blendstock value and the role of sensitivity parameter

Traditionally, refineries provide value to gasoline consumers by increasing octane to prevent knocking in higher performance engines. Co-optimized gasolines leverage increased sensitivity alongside octane to further increase engine performance over modern high compression engines [6,33]. Common gasoline blendstocks typically have low sensitivities when compared to BSI bio-blendstocks sensitives (see Tables A4-A5). Gasoline upgrading units (i.e., reforming, isomerization, alkylation, etc.) focus on increasing octane and provide little to no operational levers to adjust blendstock sensitivities. By blending varying levels of bio-blendstocks, which feature relatively high sensitivities and low levels of impurities, and do not interfere with other gasoline specifications, could provide a control mechanism for refineries to adjust sensitivity.

Fig. 5 shows break-even values (BEVs), averaged over WTI benchmark prices of 20–100 $/bbl, of the seven bio-blendstocks under consideration at blending levels of 10, 20, and 30 vol%. Adjoining whiskers represent minimums and maximums, respectively, observed in the 20–100 $/bbl WTI benchmark range. Fig. 5**A** plots BEVs against blending octanes, accounting for variable octane boosting at different blending levels. A positive correlation is observed between the break-even values and increasing octanes. Fig. 5**B** similarly plots break-even values but juxtaposes them against the different bio-blendstock sensitivities taken as the difference between blending RONs and MONs. A slighly stronger correlation between blendstock value and sensitivity is observed when compared to Fig. 5**A** (determined by the R-squared value). Fig. A2 plots the same data but shows three individual regression lines for 10, 20, and 30 blending vol% data and shows the bulk of the correlation can be attributed to the 10 vol% data.

The data indicates that although bringing high octane bio-blendstocks to the refinery is valuable, incremental improvements in sensitivity are marginally more valuable if co-optimized engines create a market demand for high sensitivity fuel. Refineries don't necessarily need outsourced blendstocks to meet higher octane specifications or to fill excess demand since gasoline demand is projected to remain stable if not decline steadily. The true value proposition bio-blending seems to bring to refineries is the capability of producing specialty fuels with property considerations other than octane. These fuels could become additional value chains for refineries and could supplant lost revenues resulting from decreasing gasoline demands.

3.4. Determining optimal blending volumes

Fig. 6**A** also plots break even value averages for PADD3-L, with minimums and maximums observed across the 20–100 ($/bbl) WTI price range again represented as whiskers. Each bio-blendstock has a clear optimal blending level, most consistently around the 20 vol% mark except for the furan mixture. The majority of the blendstocks having an optimal value indicates that beyond a certain level, the added sensitivity brought through bio-blending no longer has a marginal benefit to the refinery. As shown in Fig. 2, furans have an octane sensitivity significantly higher than other bio-blendstocks, and therefore a lower blend level is preferred.

Fig. 6**B** relates each bio-blendstocks' optimal blending volume to its pure sensitivity and depicts a clear inverse relationship. Optimal blending volumes were determined by finding the maximums of quadratic functions fit to the data presented in Fig. 6**A**. The furans mixture is excluded because additional runs below the 10 % blending level would be required to find an optimal blending volume. With

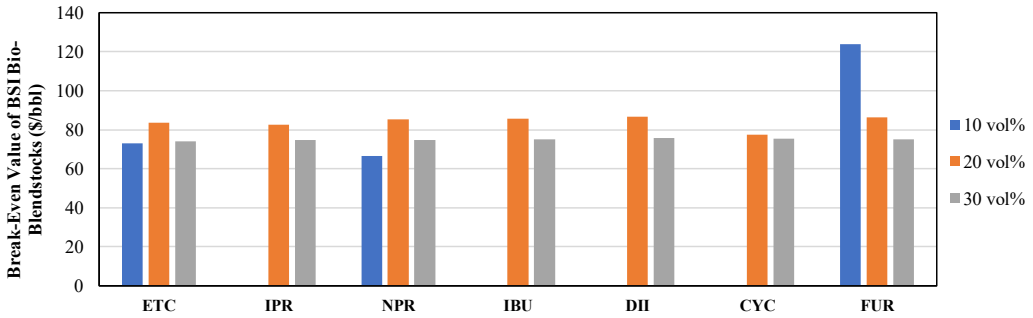

Fig. 4. BSI Bio-Blendstock break-even values ($/bbl) for the following scenario: $60/bbl WTI benchmark crude price, year 2050, and EIA demand assumptions.

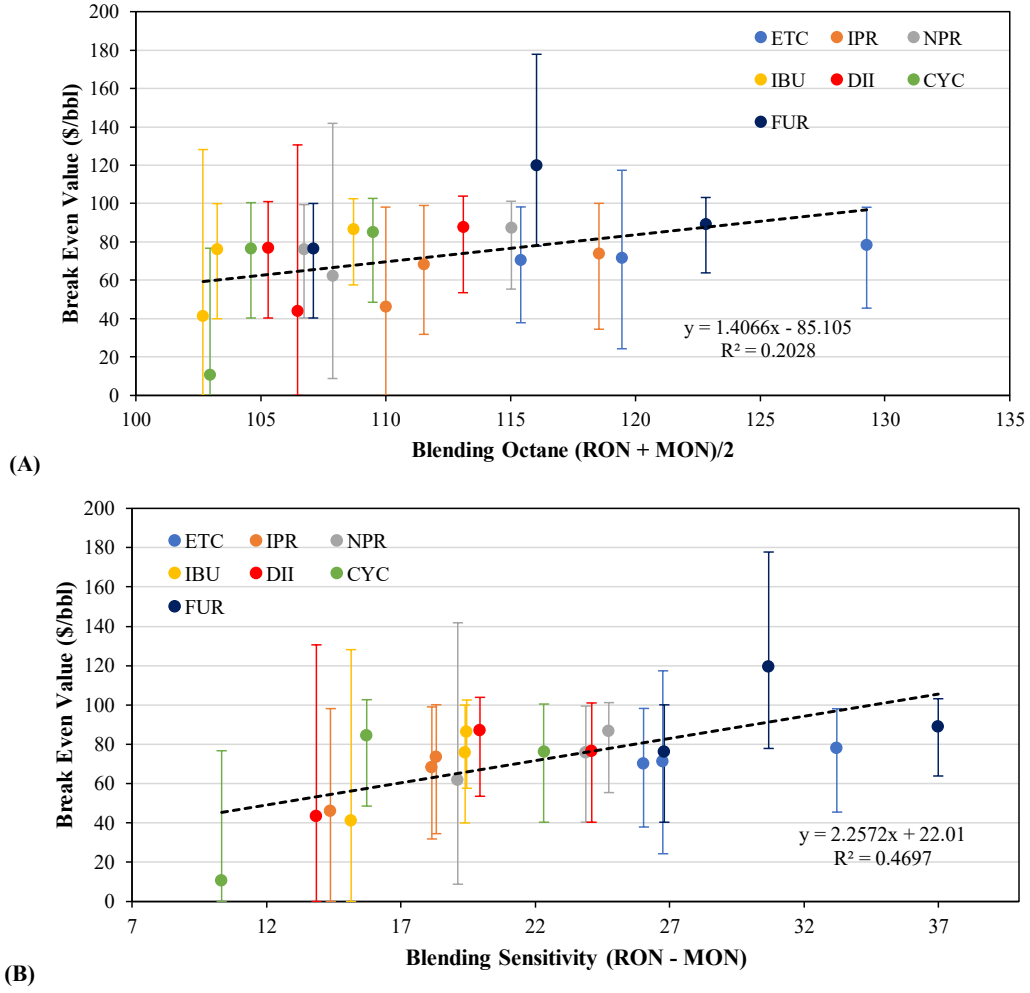

Fig. 5. Break even values for seven candidate BSI bio-blendstocks, at 10%, 20%, and 30% blending levels plotted against corresponding **(A)** blending octanes and **(B)** sensitivities. CYC: cyclopentanone, DII: diisobutylene, ETC: ethanol, FUR: furans mixture, IBU: isobutanol, IPR: isopropanol, NPR: *n*-propanol.

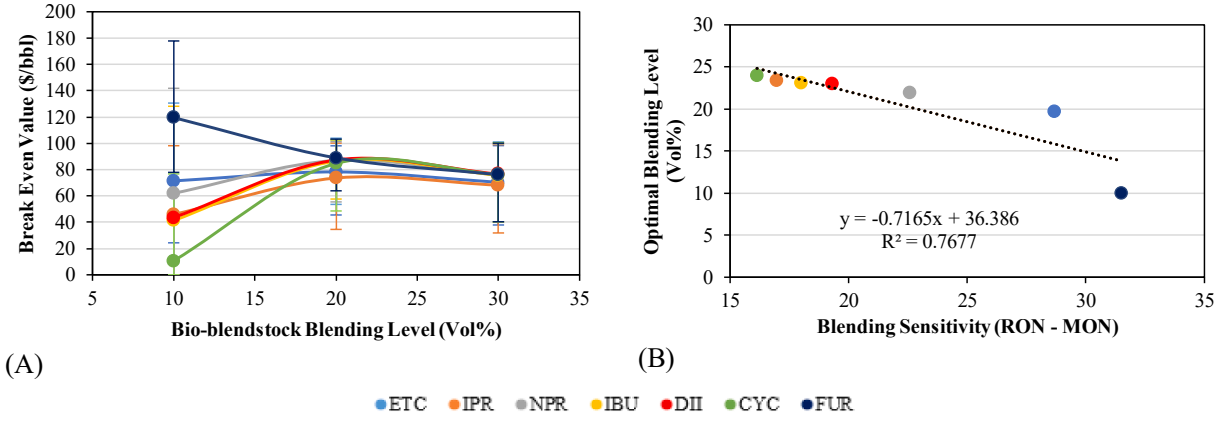

Fig. 6. (A) Bio-blendstock break even values, averaged over 20–100 $/bbl WTI benchmark prices and EIA/ADOPT projections from 2020 to 2050, plotted against blending level in co-optimized gasoline. **(B)** Optimal blending level plotted against pure bio-blendstock sensitivity. CYC: cyclopentanone, DII: diisobutylene, ETC: ethanol, FUR: furans mixture, IBU: isobutanol, IPR: isopropanol, NPR: *n*-propanol.

increasing sensitivity, less bio-blendstock is required to meet the co-optimized gasoline pools sensitivity specification.

3.5. Bio-Blendstock integration value over time

Integrating bio-blendstock can give refiners access to novel value-chains with the potential to replace expected lossses in revenue stemming from declining gasoline demand. Fig. A.4. depicts the average break-even value for PADD3-L across all bio-blendstocks and 20–100 ($/bbl) WTI benchmark price levels with observed minimums and maximums as whiskers. Using the specific methods described in this analysis, the value of bio-blending to refiners does not appear to be

agnostic to the gasoline market's projected contraction. The aggregate break-even values appear to correlate with the decreasing refinery gross-margin depicted in Fig. 3 with a more severe decline under ADOPT gasoline demand projections. More notably, the average break-even values remain steadily high during the anticipated gasoline market contraction from 2030 to 2050 indicating consistent value to refiners through unfavorable market conditions. Blending co-optimized fuels could combat decreasing gasoline sales by adding new value chains to the gasoline market while diversifying feedstock sourcing with the displacement of traditional fossil feedstocks with bio-derived feedstocks.

3.6. Bio-Blendstock value to Low-Conversion refinery

Although sensitivity has been identified as the key value driver for refineries to integrate Co-Optima bio-blendstocks, the supplemental octane boost can be an additional attraction for certain refineries facing conversion or octane constraints. Lower complexity refineries with less conversion capacity have inherently less flexibility in their blending operations and can often be octane constrained. The value proposition of bio-blending to conversion constrained refineries was studied using the PADD3-Small refinery model. The main changes from the PADD3-Large model included reducing the capacity from 400,000 bbl/day to 43,500 bbl/day and removing the gasoil hydrotreating, catalytic cracking, hydrocracking, and delayed-coking units.

Without bio-blending, the PADD3-Small model could not produce enough high-octane gasoline blendstocks to sell premium gasoline. As shown in Fig. 7, integrating BSI bio-blendstocks induced a step change in profitability for the small refinery because the bio-blendstocks' high octane compensated for the refineries lack of octane-barrels. A portion of the refinery's lower-quality gasoline blendstocks could be diluted by the high-quality bio-blendstocks in the co-optimized gasoline pool, featuring a large pricing premium over regular gasoline. At the 10 % blending level, there was not enough high-octane bio-blendstock purchasable by the model to compensate for the low-quality gasoline blendstocks, so no co-optimized fuel could be sold. For this reason, Fig. 7 only compares the 20 % and 30 % blending level scenarios observed for the PADD3-Small and PADD3-Large models.

Results in Fig. 7 show that bio-blending is more valuable to lower complexity refineries, at an average of 26 %, because it not only brings in capabilities to produce specialty, high-value fuels, but also introduces high octane-barrels into their otherwise constrained blending operations. Moreover, smaller refineries could take advantage of the low to non-existent sulfur content of bio-blendstocks to either dilute or lower the hydrotreating severity needed for fossil blendstocks. Additionally, these refineries could potentially buy more lower quality (sour)/cheaper crudes because of alleviated desulfurization requirements. Since this added value is directly derived from the incorporation of the bio-blendstock, the greater the blending level, the larger the benefits for the refinery.

4. Discussion

4.1. Model customization and improvement

This work demonstrates an approach to assess the value of a biofuel based on its fuel characteristics. Though this analysis focuses on Co-Optimized BSI gasoline and demonstrates high sensitivity and RON as fuel properties driving value to refiners, other products can be put into focus such as diesel as shown in Ref [5]. The modeling framework presented herin could be more generally regarded as a biofuel valuation tool which can be applied to any biofuel and any refinery product pool. Studying other products could help identify more biofuel property value propositions with refinery marketability that could also guide future biofuels research. Moreover, each refinery is unique in its location, design, crude/product slate, operational constraints, and product specifications. The model could be regionalized to value Co-Optima bio-blendstocks more accurately if a specific refinery region or configuration of interest is identified.

One shortcoming of the model was that the blending models were constructed using blending data from only 3 summer BOBs (combination of conventional and reformulated) to obtain blending properties, which was a small sample size. Higher resolution blending data could improve the non-linear blending model's accuracy. Also, previous research has shown that the determination of specific BOB characteristics (PIONA, RVP, etc.) would allow for a more specific blending octane number and a higher degree of accuracy rather than a generic calculation for blending octane numbers [34–37]. The same applies for RVP [38–40]. More specific determinations of blending properties (RON, S, RVP) can enable more accurate calculations and can be tailored for specific refinery outputs and characteristics.

Another notable aspect is the impact on ease of vaporization or the distillation profile (D86 curve), which influences drivability [38,41,42]. In this analysis, the focus was on accurately modeling the non-linearities of regulatory specifications such as RVP and octane. However, including D86 data could be an additional step that can be taken to make the blending models more comprehensive.

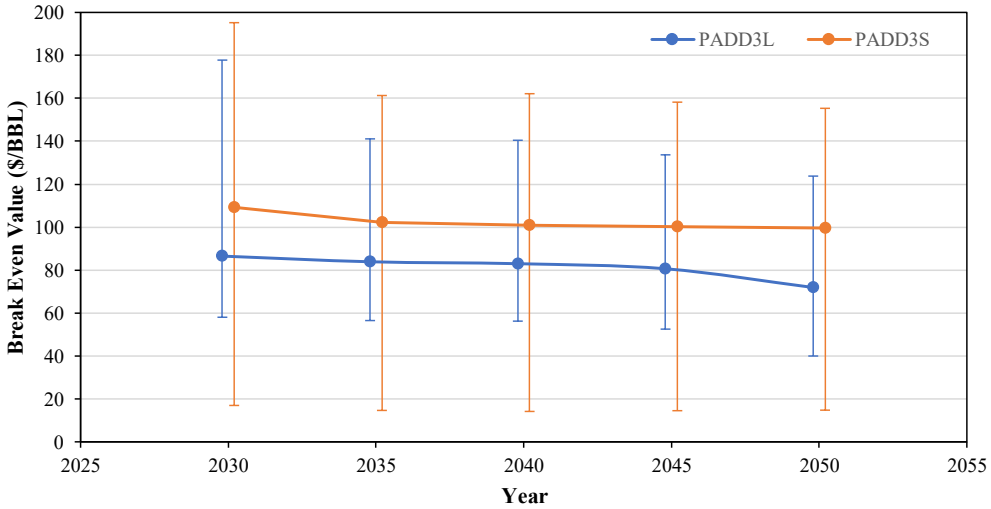

Fig. 7. Break even values averaged over the six candidate BSI bio-blendstocks, 20–100 $/bbl WTI benchmark prices, and 20% and 30% blend levels with comparison between the PADD3-Large and PADD3-Small refinery models.

Further, BSI specifications presented here resemble reformulated summer gasoline specifications, which are more stringent in terms of RVP, as opposed to winter, which has a higher RVP minimum [43]. For instance, the high-octane blendstocks which hit the maximum RVP constraint of summer gasoline could potentially still be valuable for winter gasoline when cheaper naphtha streams and butane are available for blending. This would allow refiners to still create finished gasoline with higher biofuel blending levels specifically in situations where the constraining criteria is seasonal.

Another limitation stems from the lack of wide scale adoption, i.e., second generation biofuel, from feedstocks such as herbaceous biomass or woody feedstocks, that are not currently available in sufficient volumes and that lack sufficient infrastructure for production, transportation, and distribution [19,44]. With the limited availability of bio-blendstocks, their prices might be constrained by the supply and demand which can potentially impact refinery economics. In this analysis, it is assumed that sufficient biofuel is available for all refineries to meet their demand, but it would be dictated by supply and demand factors. Some of these aspects are discussed in an upcoming publication.

4.2. Outlook and next steps

The refinery models detailed here could serve as the basis for even more comprehensive models. Potential modifications could range from PIMS sub-model alterations, the addition of new bio-blendstocks/products, to simple backend calculations using the material and cash flows produced by the PIMS models. More specific ideas to build upon the analysis presented here are discussed below:

1. *Shared value between biofuel producers and refiners:* A more complete understanding of each bio-blendstock's economic feasibility could be obtained by taking the difference between its BEV and minimum selling price (MSP), derived from pathway techno-economic analysis (TEA). These differences would represent the potential shared benefits between the bio-blendstock producer and petroleum refiner. Alternatively, calculating the price premiums, over a benchmark gasoline, needed to incentivize the refinery to purchase bio-blendstocks at their TEA derived MSPs, combined with the anticipated efficiency gains expected from Co-Optima engines, would yield an even more comprehensive picture of each bio-blendstock's market potential.
2. *Integration with Sustainable Aviation Fuels/Heavy-Duty Fuels/Petrochemical Plants*: The most intriguing aspect of this work lies in the potential for integrating drop-in biofuels not just for the gasoline pool but adopting the same approach for the entire product slate at a refinery. This methodology can be applied for sustainable aviation fuels (SAFs) as well as heavy duty (HD) fuels [5], which can alternatively route more fossil derived streams to petrochemicals plants such as BTX or other high value chemicals, ultimately leading to increased profitability and sustainability at a refinery.
3. *GHG Emissions Reduction:* Future work will consider the life cycle greenhouse gas benefits of blending biofuels into the gasoline and diesel-range fuel pools, by coupling Aspen PIMS refinery simulation with life cycle analysis (LCA). This novel perspective accounts for energy use and emissions in the refinery complex foreground, such as utility requirements, process energy use, and emissions across individual refinery processing trains, as well as background changes in the supply chains of refinery inputs over time (e.g., changes in the carbon intensity of purchased electricity, crude oil supply, etc.). Life cycle impacts can be aggregated refinery-wide, or shown for individual refinery products, and benchmarked against a reference refinery case to contextualize the potential emissions benefits. Further, this approach can track environmental impacts over time and across a wide array of sustainability and climate metrics, and thus provides a broad-based understanding of the impact of key parameters such as changes in demand for refinery products, crude oil price, biofuel blending level, etc. on the environmental sustainability of refinery operations.
4. *Co-processing as an avenue for more opportunities:* A more direct optimization with the objective of lowering the carbon footprint as well as maximizing the profitability of the refinery can be accomplished. The work presented here addressed direct biofuels blending alone, but coprocessing with pyrolysis oil or algal/terrestrial hydrothermal liquefaction oil could be other strategies for bringing bio-derived intermediates into a refinery and upgrading them into finished fuels. The California Air Resources Board is actively looking into methods by which they can quantify the biogenic content of the finished fuel from coprocessing, creating markets for new low carbon fuels.
5. *Policy Factors for Adoption:* Policy incentives whether from low carbon fuel standard (LCFS) in California or federal RIN credits could initiate a Co-Optima biofuels market and incentivize faster growth. California's policies have been very effective in creating a renewable diesel market. Other countries, such as those in the EU, have also instituted policies that have effectively promoted biofuels adoption.

5. Conclusion

This work demonstrates a framework and methodology to estimate the value of low carbon bio-blendstocks for the refining industry which estimates the break-even value of biofuels to vary from $10-$120/bbl, depending on the market conditions (such as benchmark crude oil) and biofuel properties (such as octane ratings). While all refinery and terminal blending operations are unique due to regional market and fuel specifications, a novel and generalizable modeling framework for biofuel valuation has been designed and demonstrated. Sensitivity was found to be the dominant property providing value to refiners by enabling the production of novel, high-performance fuels that extend value to consumers. A consistent optimal BSI bio-blendstock blending level of 20 vol% was identified. Declines in gasoline demand were demonstrated to significanlty decrease refinery profitability over the next 30 years which sets the stage for investment in BSI gasolines to potentially help compensate losses. Finally, smaller refiners, with low conversion and octane capacity may find biofuels more valuable, at an average of 26 %, since their integration allows them to produce specialty, high-value fuels despite their otherwise constrained blending operations. Moreover, this analysis is one example of the framework to evaluate the value propositions of integrating biofuels (in other fuel sectors as well) and that refiners facing dynamic economic and market conditions can produce specialty, high-value fuels to stay competitive.

6. Data Availability

For any data requests, please reach out: Nicholas.Carlson@nrel.gov.

CRediT authorship contribution statement

Nicholas A. Carlson: Data curation, Formal analysis, Methodology, Visualization, Writing – original draft, Writing – review & editing. **Avantika Singh:** Conceptualization, Formal analysis, Funding acquisition, Investigation, Project administration, Writing – original draft, Writing – review & editing. **Michael S. Talmadge:** Conceptualization, Formal analysis, Investigation, Writing – original draft. **Yuan Jiang:** Conceptualization, Validation, Writing – review & editing. **George G. Zaimes:** Writing – review & editing. **Shuyun Li:** Validation, Writing – review & editing. **Troy R. Hawkins:** Conceptualization, Project administration, Supervision, Writing – review & editing. **Lauren Sittler:** Resources. **Aaron Brooker:** Resources. **Daniel J. Gaspar:** Supervision. **Robert L. McCormick:** Funding acquisition, Resources. **M.M. Ramirez-Corredores:** Investigation, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

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