Energy & Environmental Science

ROYAL SOCIETY OF CHEMISTRY

ANALYSIS

View Article Online
View Journal | View Issue

Cite this: *Energy Environ. Sci.*, 2020, **13**, 2262

Energy, economic, and environmental benefits assessment of co-optimized engines and bio-blendstocks†

Jennifer B. Dunn, *[a] Emily Newes,[b] Hao Cai,[a] Yimin Zhang,[b] Aaron Brooker,[b] Longwen Ou,[a] Nicole Mundt,[b] Arpit Bhatt, [b] Steve Peterson[c] and Mary Biddy[b]

Received 6th March 2020,
Accepted 26th May 2020

DOI: 10.1039/d0ee00716a

rsc.li/ees

Advances in fuel and engine design that improve engine efficiency could lower the total cost of vehicle ownership for consumers, support economic development, and offer environmental benefits. Two fuel properties that can enhance the efficiency of boosted spark ignition engines are research octane number and octane sensitivity. Biomass feedstocks can produce fuel blendstocks with these properties. Correspondingly, using a suite of models, we evaluated the change in energy and water consumption and greenhouse gas and air pollutant emissions in the light duty fleet from 2025 to 2050 when bio-blendstocks isopropanol, a methylfuran mixture, and ethanol are blended at 31%, 14%, and 17%, respectively, with petroleum. These blended fuels increase engine efficiency by 10% when used with a co-optimized engine. In these scenarios, we estimated that petroleum consumption would decrease by between 5–9% in 2050 alone and likely by similar levels in future years as compared to a business as usual case defined by energy information administration projections. Overall, between 2025 and 2050, we determined that, when isopropanol is the bio-blendstock, GHG emissions, water consumption, and $PM_{2.5}$ emission cumulative reductions could range from 4–7%, 3–4%, and 3%, respectively. Cumulative reductions would continue to increase beyond 2025 as the technology would gain an increasing foothold, indicating the importance of allowing time for technology penetration to achieve desired benefits. Annual jobs increased between 0.2 and 1.7 million in the case in which isopropanol was the bio-blendstock. Overall, this analysis provides a framework for evaluating the benefits of deploying co-optimized fuels and engines considering multiple energy, environmental, and economic factors.

Broader context

Engines and fuels can be co-developed so that engines are designed to exploit unique fuel properties that are exhibited by fuel molecules. In particular, fuel blendstocks derived from biomass have the potential to elevate engine efficiency in boosted spark ignition engines. As vehicles with these engines and the fuels that enable them to achieve higher efficiency enter the market, it is likely that key environmental metrics for the transportation sector, including greenhouse gas emissions, would improve. It is important to consider the influence of this technology deployment on multiple environmental metrics including water consumption and air pollutant emissions and effects on net jobs. In this paper, we use a suite of models to evaluate the energy, economic, and environmental benefits of co-optimized fuels and engines and highlight necessary advances to realize these benefits. Importantly, this analysis goes beyond considering the effects of increasing the renewable content of fuel to consider the additional benefits of engine efficiency gains.

Introduction

Worldwide, energy consumption, along with associated greenhouse gas (GHG) emissions, has increased rapidly over the past few decades[1,2] and is expected to continue growing out to 2040.[3] Transportation accounted for about 14% of the global GHG emissions in 2010, and was the largest sector for GHG emissions in the U.S. in 2017.[4] The U.S. domestic transportation CO_2 emissions increased by 23% between 1990 and 2017, an annualized increase of 0.8%. The largest sources of transportation GHG emissions in the U.S. in 2017 were passenger cars (41.2%) freight trucks (23.3%), and light-duty trucks (17.5%). Since 2014, with a steady improvement of vehicle fuel economy from about 20 miles per gallon (MPG) in 2004 to about 25 MPG in 2017, CO_2 emissions from passenger cars and light-duty trucks have declined about 8%.[4] Shares of major criteria air pollutants from

[a] Argonne National Laboratory, Argonne, IL, USA. E-mail: jdunn@anl.gov
[b] National Renewable Energy Laboratory, Golden, CO, USA
[c] Lexidyne, LLC, Colorado Springs, CO, USA

† Electronic supplementary information (ESI) available. See DOI: 10.1039/d0ee00716a

transportation out of all emission sources have steadily declined since 1990 given enforcement of more stringent emission standards. However, highway transportation remains a primary source of air pollutant emissions, especially nitrogen oxides, carbon monoxide, and volatile organic compounds in the U.S., accounting for 32%, 29%, and 10% of the total emissions in 2018.[5]

The transportation sector's energy consumption, GHG emissions, and criteria air pollutant emissions, and economic impacts, have driven major innovations in passenger cars and light-duty vehicle technologies in the U.S. and elsewhere. One example of innovation has been advancements in engine technologies, including higher compression ratios, downsizing, turbocharging, downspeeding, and hybridization for spark-ignited (SI) engines. A second example is fuel technologies such as higher octane ratings for gasoline. Both of these examples are major technologies under ongoing development to meet regulatory requirements on fuel economy, GHG emissions, and criteria pollutant emissions.[6] Most recently, several light-duty gasoline engine technology concepts, such as gasoline direct injection compression ignition, reactivity controlled compression ignition, homogeneous lean burn, and lean-burn gasoline direct injection (GDI) have the potential for 10–15% and, for some technologies, up to 30% CO_2 emission reductions relative to today's GDI engines.[7] Among these technologies, boosted and downsized SI engines have gained attention for improving fuel economy.[8] Such technologies, however, are generally limited by the anti-knock quality of the available market gasolines, commonly described in terms of the research and motor octane numbers (RON and MON, respectively).[9,10]

Prototype engines built with novel design concepts that allow for studying the impact of fuel octane number on engine performance highlighted the importance of RON in contributing to enhanced engine efficiency.[11] A more octane-responsive engine design supports larger increases in fuel efficiency than a less octane-responsive engine design,[12] highlighting the importance of engine and fuel co-design and co-optimization for possibly achieving the largest engine efficiency gain. Meanwhile, an octane-on-demand concept, an engine-fuel technology characterized by the use of two fuels with different octane quality, has been introduced and examined to address challenges associated with production and blending of high-octane fuel components such as ethanol or other octane boosters with the petroleum gasoline blendstock.[10,13–15]

Vehicles with high-efficiency engines based on improvements in fuels and engines could lower the total cost of vehicle ownership for consumers, support economic development, and offer environmental benefits. Biomass feedstocks can produce blendstocks with certain desirable fuel properties, such as high RONs[6,16,17] and high octane sensitivity, both of which increase engine efficiency. Octane sensitivity is the difference between RON and MON. In addition, some bio-blendstocks exhibit synergistic blending (with petroleum), resulting in blended fuels with RONs above the level that would be expected from the RONs of the individual blend components.[18]

Previous studies regarding the economic and environmental effects of engine-efficiency-enhancing fuels have nearly exclusively focused on high-octane fuels (HOFs), produced by blending ethanol at levels up to 40% by volume.[6,16,17,19] These studies examining HOF concluded that manufacturing petroleum-based HOF with lower ethanol blending levels (*e.g.*, E10) could consume more energy and produce more GHG emissions than manufacturing fuels with higher ethanol blending levels. The efficiency gains of high-ethanol-blend fuels also reduce per-mile-based WTW GHG emissions from vehicles.[6,16,17,19]

Table 1 Properties of the bio-blendstocks[20]

Name	RON	Motor octane number (MON)	Octane sensitivity (RON–MON)	Heat of vaporization (kJ kg^{-1})
Ethanol	109	90	19	918
Isopropanol	109	97	12	744
Furan[a]	102	87	15	330

[a] 2-Methylfuran/2,5-dimethylfuran mixture (40%/60% by weight).

This study estimates the potential economic and environmental benefits and challenges of large-scale adoption of three bio-blendstocks with engine-efficiency-enhancing fuel properties (Table 1). We assume the efficiency benefits of co-optimized fuels and engines apply to vehicles with boosted spark ignition engines and extend to vehicles with hybridized power trains. This analysis considers the influence of parameters including engine efficiency gain, incremental vehicle cost, shares of new vehicles sold, rate of biorefinery and dispensing equipment buildout, and other factors. It examines their influence on changes in current energy consumption, GHG emissions, water consumption, air pollutant emissions, and net jobs from 2025 to 2050, as compared to a business-as-usual (BAU) case, quantifying benefits and highlighting potential drawbacks.

Previously, 40 bio-blendstocks were identified that had promising properties: a RON of 98 or greater, a melting point (or cloud point) < -10 °C, and a boiling point (or T90) < 165 °C for blending into a conventional or reformulated petroleum blendstock for advanced SI engines.[20] A subset (24) of these, including alcohols, furans, alkenes, aromatics, ketones, and esters, were analysed further in a screening analysis to assess their near-term economic and environmental viability.[21] From this subset, two biomass-derived blendstocks with RONs exceeding 98 were selected that have the potential to increase engine efficiency by 10% at blending levels below 50 vol% for boosted SI engines. These thresholds were set to achieve viable levels of bio-blendstock demand. Higher blend levels (> 50%), even if they could enable higher efficiency gains, are hard to achieve in the near term when new biorefinery construction would not keep pace with demand. Isopropanol and a methylfuran mixture[21] (hereinafter referred to as furan) met these criteria and were identified as being commercially viable with favourable life-cycle GHG emissions. Ethanol produced from either corn starch or corn stover is also considered in this study. The properties of these bio-blendstocks are listed in Table 1. As part of the analysis, we consider the production of these fuels from biomass based on previous work. Previously, furan was modelled as produced *via* a hybrid of thermochemical and biochemical conversion processes from corn stover. Isopropanol has been modelled as produced biochemically from corn stover. Based on corrosivity, neither of these bio-blendstocks, nor ethanol, are generally compatible with existing petroleum fuel infrastructure. Like ethanol, the bio-blendstocks would need to be transported to point of use by truck or by rail, not *via* a pipeline.

To-date, several analyses regarding the use of bio-blendstocks have shown that elevating fuel economy could bring about economic and environmental benefits including GHG emission reduction and reduced transportation costs for consumers. Furthermore, some studies have characterized how the expansion of the bioeconomy to encompass feedstock production at scale and additional cellulosic biofuel plants could generate jobs in rural America. For example, Swenson *et al.*[22] estimated the state-wide economic benefits of blending cellulosic ethanol produced from homegrown biomass feedstocks in the state of New York at levels 5–10% greater than today's 10% blending level by 2020. Swenson *et al.* developed a hybrid input–output method, using IMPLAN-derived multipliers, to estimate the economic impacts for multiple ethanol scenarios, and assumed ethanol prices. Bailey *et al.*[23] examined potential rural development impacts (jobs, landowner income and tax revenues, in particular) that could be generated from increasing timber harvest to supply feedstock to six cellulosic ethanol biorefineries in Alabama. Recently, Rogers *et al.*[24] assessed the size and economic and environmental benefits of a Billion Ton Bioeconomy, a vision to enable a sustainable market for producing and converting a billion tons of U.S. biomass to bio-based energy, fuels, and products by 2030. A study to estimate environmental effects of potential biomass production scenarios in the United States, with an emphasis on agricultural and forest biomass, revealed that both beneficial and adverse environmental effects including changes in soil organic carbon, GHG emissions, water quality and quantity, air emissions, and biodiversity might be expected.[25] However, none of the existing studies assessed the environmental effects and net employment impact of the rollout and a potential large-scale deployment of engines that are co-optimized for use with engine-efficiency-enhancing bio-blendstocks.

This paper contributes to the existing body of research on development and deployment of co-optimized fuels and engines by offering insights into the overall economic and environmental benefits and potential challenges of large-scale adoption of bio-blendstocks with engine-efficiency-enhancing fuel properties.

Caveats, limitations, and assumptions

The scenarios with the three options for blended fuels (all cases other than BAU) were designed as bounding scenarios where each blended fuel enjoys large-scale adoption to evaluate the possible extent of associated benefits. Therefore, the biofuels industry responds to the vehicle fleet demand by achieving the necessary fuel production capacity. It is assumed that:

• The petroleum industry continues to supply the gasoline required for blending with the biofuel, and the oil price follows the Annual Energy Outlook 2017 reference case trajectory.[26]

• Conventional gasoline prices are rigid, *i.e.* reduction in demand for conventional gasoline does not result in a corresponding reduction in the price.

• The biofuels industry only produces starch ethanol, cellulosic ethanol, biodiesel, hydro-processed esters and fatty acids, isopropanol, and furan.

• Existing starch ethanol refineries have the capacity to satisfy the low-ethanol-blend demand of conventional gasoline vehicles, hybrid electric vehicles (HEVs), and plug-in hybrid electric vehicles (PHEVs) up to 56.8 billion litres per year, above which cellulosic ethanol refineries augment production.

• The low-ethanol blend composition transitions from E10 to E15 throughout the simulation, reaching 60% of the mix by 2050.

• Battery costs drop from \$500 per kW per h to \$210 per kW per h between 2020 and 2035.[27]

• Vehicles with advanced engine technology do not have significant perceived risk to the customer as compared to other vehicle options, or significant regional differences.

• The 10% improvement in engine efficiency is enjoyed by the owner of the vehicle and not shared by members of the fuel or vehicle supply chain, who would have other incentives to participate.

• Consumer purchase costs for co-optimized vehicles are limited to a \$100 price increment over the standard vehicle in the same class.

• U.S. average electricity generation mix comprising fossil and renewable sources is fixed at 2014 levels out to 2050 (see Table S5, ESI† for composition).

The following are key assumptions that were used for all the blended fuels and ethanol cases:

• Vehicle introduction year: 2028.

• The biofuel portion of blended fuels is blended with petroleum gasoline (E0 with 94 RON).

• 10% engine efficiency gain results from using blended fuel in co-optimized vehicles. We assume identical efficiency gains for vehicles with only combustion engines, HEVs, and PHEVs. Because of powertrain losses, a fuel consumption improvement of 8% is assumed. (See Bio-blendstock blending section for more details.)

• Incremental vehicle cost is assumed to be \$100; sensitivity analyses indicate that simulation results are relatively insensitive to an incremental vehicle cost of up to \$600.

• Cellulosic feedstocks enter the market on the basis of demand, price, and availability.

• The following existing policies are in place: Renewable Fuel Standard (RFS), Corporate Average Fuel Economy (CAFE) requirements, the Biomass Crop Assistance Program, and Low Carbon Fuel Standard (LCFS) in the Pacific region.

• Expansion of the use of new bio-blendstocks would require retailers to replace existing dispensers with compatible dispensers.

For this analysis, the Biomass Scenario Model (BSM) was modified to include ethanol, isopropanol, or furan to be selected as a bio-blendstock for the blended fuel. Several simplifying assumptions were made to facilitate the scenario analysis:

• Fuel retailers utilize existing equipment (*e.g.*, E85) to dispense blended fuel whenever possible to decrease needed capital investment.

• Vehicles with elevated fuel economy resulting from the combination of advanced engines and blended fuels with tailored properties (*i.e.*, "co-optimized" fuels and engines) are fuelled with regular gasoline (because premium is not differentiated in the BSM) until the new fuel that enables increased engine efficiency becomes available within a region.

• Vehicles that benefit from co-optimized fuels and engines do not experience an increase in engine efficiency until they are able to use the fuel that enables this efficiency to increase.

To gain a better understanding of potential benefits, certain modelling assumptions were made in order to explore fairly high levels of deployment. (For sensitivity analyses that explores the influence of assumptions on results, please see the ESI.†)

Integrated modelling framework

To carry out this analysis, a suite of modelling tools is used (Fig. 1). The Automotive Deployment Options Projection (ADOPT) model[28] estimates vehicles sales by type. The National Renewable Energy Laboratory (NREL), with support from the DOE Vehicle Technologies Office, Fuel Cell Technologies Office, and Bioenergy Technologies Office, has developed ADOPT to explore the impact of vehicle technology improvements, including co-optimized fuels and engines, on vehicle sales and efficiency.[28–31] ADOPT estimates sales based on the most consumer-valued attributes, including price, fuel cost, acceleration, range, and size, while considering the influence of existing policies including the Corporate Average Fuel Economy (CAFE) standards, GHG emission standards, and federal electric vehicle tax incentives. The results have been extensively validated by comparing ADOPT's estimated sales to historical data to provide confidence in the results.

ADOPT simulations begin with all currently existing LDV options at the make and model level, extending to the trim level for engine size variations, for a realistic market representation. These vehicle options evolve over time with market conditions. They are adjusted for technology improvements such as lightweighting, engine efficiency improvements, and battery cost reductions.

Three triggers instigate the creation of new vehicle options. One trigger creates new variations of a vehicle when it sells exceptionally well for its price. Another trigger creates additional options for several years when a new powertrain is introduced. A third creates new options for the best-selling powertrain. Poorly selling options are dropped.

New vehicle options are created by swapping high-selling powertrains into other platforms and optimizing the component sizing to achieve the best-selling combination of vehicle attributes. The best-selling combination of vehicle attributes changes for each of the disaggregated income groups, where higher income groups are less sensitive to cost and thus place more emphasis on size, acceleration and range. For example, when creating a new battery electric vehicle (BEV) option for the high-income group, ADOPT will optimize to a larger battery that provides longer range and better acceleration at a higher price.

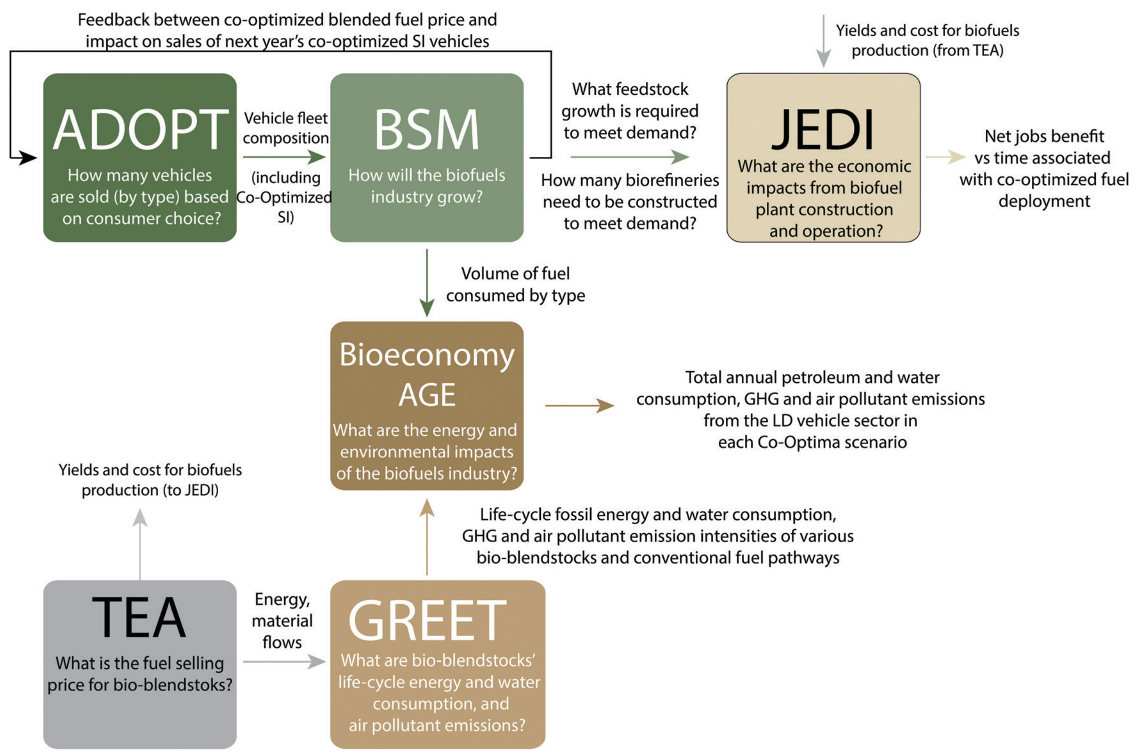

Fig. 1 Integrated modeling for economic and environmental benefit analysis of large-scale deployment of co-optimized fuel and engine technologies. ADOPT: Automotive Deployment Options Projection Tool, BSM: Biomass Scenario Model; JEDI: Jobs and Economic Development Impact, AGE: Air and Greenhouse Gas Emissions; TEA: Techno-Economic Analysis, GREET: Greenhouse gases, Regulated Emissions and Energy use in Transportation.

ADOPT's framework provides flexibility for capturing co-optimized vehicle sales and efficiency estimates in several ways. The new powertrain trigger initiates the creation of many different options of vehicles with co-optimized technology for several years, reflecting past trends of new powertrain introductions. Since co-optimized engines can be used in conventional vehicles, HEVs, and PHEVs, ADOPT creates options for each of those combinations. Finally, the trigger that creates more powertrain options for the best-selling powertrain can quickly expand the co-optimized options and sales. For this analysis, ADOPT assumed that co-optimized vehicles did not have significant perceived risk compared to other vehicle options, or significant regional differences.

ADOPT is integrated with the BSM, which the DOE Bioenergy Technologies Office and NREL have developed to explore possible evolution trajectories for biofuels within the United States.[32] The model, geographically stratified in accordance with the ten U.S. Department of Agriculture farm production regions, uses commercial system dynamics modelling software[33] to represent interactions along the biofuel supply chain, focusing on feedstock production and logistics, feedstock conversion, and downstream elements including fuel inventories, dispensing stations, and fuel demand driven by the fleet of LDVs in the United States. The model captures shifts in agricultural production, investment in new technologies, competition from petroleum fuels, and vehicle demand for biofuels. The system dynamics approach has long been used to analyse the behaviour of feedback-rich social, economic, and environmental systems, and it can facilitate investigation of system bottlenecks, analysis of policies, and diagnosis of unintended consequences.[34] Extensive analyses have been performed utilizing the model to address the critical role played by system bottlenecks, gasoline pricing, industrial learning, and financing in the development of the biofuel industry.[35–40] The ESI† contains additional details about ADOPT and the BSM.

The BSM and ADOPT models are interlinked in an annual time step.[29] ADOPT calculates sales and efficiency information and sends it to the BSM. The BSM estimates and returns fuel prices. BSM output consists of yearly fuel consumption, fleet travel demand in terms of total vehicle miles travelled by vehicle technology, and fleet average fuel economy by vehicle technology. This output, together with BAU scenario data from the 2017 Annual Energy Outlook,[26] was used as the input for the calculation of changes in energy consumption, GHG emissions, and $PM_{2.5}$ emissions. These calculations were performed in a model called Bioeconomy Air and Greenhouse Gas Emissions (Bioeconomy AGE), which is a derivative of Argonne National Laboratory's Greenhouse gases, Regulated Emissions and Energy use in Transportation (GREET™) model.

GREET has been under development at Argonne since 1995, is publicly available, and has over 30 000 users worldwide. It models many different advanced fuel and vehicle technologies consistently, and contains life-cycle, energy, and environmental results for over 100 vehicle-fuel pathways. The most critical GREET pathways for the present analysis include corn, grain, and cellulosic ethanol production, as well as the production of isopropanol, furan mixture, and conventional gasoline. Recently, petroleum pathways in GREET have been updated to reflect new results for Canadian oil sands[41] and shale oil[42,43] as feedstocks in U.S. refineries. Documentation describing the development of other pathways in GREET is publicly available.[44]

In this study, GREET was used to generate life-cycle petroleum consumption, GHG emissions, water consumption, and $PM_{2.5}$ emissions of bio-blendstock pathways including isopropanol, furan, and ethanol, as well as of conventional fuels including gasoline, diesel, compressed natural gas (CNG), electricity, and hydrogen on a yearly basis from 2025 to 2050. These results were then built into Bioeconomy AGE. Bioeconomy AGE has been developed and used to estimate the environmental benefits of large-scale development of a bioeconomy in the United States.[24] It allows users to specify feedstock-to-fuel combinations over time to meet transportation fuel sector demand and examine impacts on petroleum consumption, GHG emissions, water consumption, and $PM_{2.5}$ emissions. The total yearly life-cycle petroleum consumption, GHG emissions, water consumption, and $PM_{2.5}$ emissions of the LDV sector were estimated in each scenario using Bioeconomy AGE. The model's input is fuel consumption by type (*e.g.*, E10, diesel, isopropanol, furan, ethanol, electricity, hydrogen, and CNG) from BSM/ADOPT simulations.

BSM/ADOPT simulation results along with cost estimates from TEA are also used to inform economic impact analysis with the Jobs and Economic Development Impact (JEDI) model.[45] Economic impact analysis is often used to estimate changes in employment, income, and tax revenues that could result from new economic activities. The fundamental rationale behind economic impact analysis is that changes in economic activity are multiplied through the entire economy because of the inter-industry linkages of industrial sectors. A change in expenditure on goods and services made by one industry results in a change in demand for goods and services from other industries. Input–output analysis, originally developed to trace supply linkages in the economy, is one of the commonly used approaches to tracking the ripple effects of changes in economic activity throughout an economy.

Because the production of isopropanol and cellulosic ethanol has not been fully commercialized, no off-the-shelf input–output model includes these bio-blendstocks. To estimate the employment impacts of these new bio-blendstocks, NREL developed pathway-specific JEDI models by leveraging the most up-to-date cost data along with feedstock production and logistics data from BSM outputs to represent the supply chain and relevant expenditures associated with each bio-blendstock examined in this analysis.

Each JEDI model uses the same basic input–output approach (a commonly-used method in economic impact analysis such as Swenson *et al.*[22]) to estimate the economic effects, including new jobs created, from the expenditures made by biorefineries during their construction and operation phases. Input–output analysis requires a detailed accounting of expenditures and proper allocation of each expenditure to the impacted sectors within an economy. The economic sectors affected by each expenditure are identified by matching the description of each expenditure (*e.g.*, type of equipment purchased and installed) with the North American Industry Classification System (NAICS), a standard used by federal statistical agencies to classify business establishments for the purpose of collecting and analysing statistical data related to the U.S. economy.

In addition to quantifying the new jobs that would be created by the growth in the biofuel industry, the employment change in the mature petroleum industry resulting from the change in petroleum consumption (estimated by ADOPT/BSM) is also taken into account. To estimate the potential employment change in the petroleum industry due to the introduction of new bio-blendstocks, a model is developed that estimates how a change in domestic petroleum consumption affects employment in the U.S. petroleum sector. A two-step approach is utilized that first links U.S. gasoline consumption to domestic petroleum production, and then links petroleum production to employment in the U.S. petroleum industry. Details on how the model is developed and validated against available literature are presented in the ESI.†

As suggested in Fig. 1, the JEDI simulations are informed by inputs to and outputs from the BSM/ADOPT runs and TEA. For example, feedstock cost, fixed capital investment for biorefinery construction, and fixed and variable operations & maintenance (O&M) costs for biorefinery operation used in the JEDI modelling are identical to those used in the BSM/ADOPT runs and TEA. Outputs from the BSM/ADOPT simulations such as the number of new biorefineries required to be built to produce bioblendstocks to meet demand, and projected market penetration of various biofuel blendstocks (*e.g.*, biofuel actual output) under the BAU and biofuel scenarios, are also used as model inputs to the JEDI analysis. In addition, data on U.S. gasoline consumption and projected petroleum prices over time are provided by BSM/ADOPT outputs.

We estimate incremental employment impact, defined as the difference in the number of annual full-time equivalent jobs under the three biofuel scenarios in Table 1 in compared to the BAU scenario, taking into account the employment effect in the relevant biofuel and petroleum sectors. Given that the BSM/ADOPT simulation results for biofuels are aggregated to the U.S. Department of Agriculture (USDA) region level, the biofuel-related employment effect is first estimated for each USDA region and then summed up for the contiguous United States. On the other hand, BSM/ADOPT reports petroleum consumption on a national level. As such, the job effect for the petroleum industry is estimated for the contiguous United States. Sensitivity analysis is performed for biofuel scenarios to provide insights into how incremental employment impact varies by criteria, which define the biofuel scenarios.

Bio-blendstock blending levels

A merit function for stoichiometric SI engines operating in conventional flame propagation combustion modes was developed in previous work.[46] This function estimates the effects of key fuel properties such as RON, MON, octane sensitivity, heat of vaporization, particulate matter index, and flame speed, among others, on engine efficiency. This merit function calculated blend levels for different bio-blendstocks that would achieve a 10% engine efficiency gain at blending levels (with petroleum gasoline, E0, that has a 94 RON) below 50% relative to conventional SI vehicles using E10. (Higher blending levels would require longer times for realization because the additional volume needed would require more capacity growth.) It was determined that two blended fuels that meet the blending-level criterion are a 31% blend of isopropanol with E0 and a 14% blend of furan with E0. E17 (a 17% blend of ethanol with 94 RON petroleum gasoline) also meets this criterion and was included as a scenario as ethanol production is currently at scale from starch. (E17 was modelled as produced from corn starch (97% of demand by volume) and from agricultural residues (3% of demand).) These three cases were evaluated individually in our modelling.

Large-scale bio-blendstock deployment and business-as-usual scenarios

The BAU scenario is defined, against which the blended fuel cases would be evaluated, on the basis of the reference case of the 2017 Annual Energy Outlook.[26] This scenario does not include any furan- or isopropanol-blended fuels and is described in more detail in the ESI.†

Base cases for the two non-ethanol blended fuels (one with isopropanol, one with furan) and an E17 case were simulated to examine the growing use of co-optimized vehicles and fuels over time. For these simulations, it is assumed that biorefineries would be built to satisfy demand regardless of internal rate of return (IRR) in order to explore the potential benefits of co-optimized fuels and engines for the vehicle trajectories. Biorefinery construction is, however, subject to constraints related to relative fuel price of the bio-blendstock in comparison with E10–15, feedstock availability, and construction limitations. In base simulations, it is also assumed that fuel dispenser replacement is incentivized such that fuel station owners install new dispensers as needed to accommodate new fuels. These assumptions are then relaxed individually to run cases where (1) biorefineries are subject to IRR constraints and therefore not built to meet demand (but dispensing is available) and where (2) fuel station owners decide whether to invest in dispensing equipment with no incentives available (but biorefineries are built to meet demand). Table 2 summarizes the key assumptions of these cases.

It should be noted that this analysis estimates potential changes in fuel consumption by type that result in different environmental and cost outcomes from the BAU scenario. The results are estimates that stem from the parametric assumptions and modelling choices and are viewed as informing potential benefits and challenges of large-scale deployment of bio-blendstocks that increase engine efficiency. They are not intended as definitive predictions.

Table 2 Key assumptions in base cases

Scenario name	Co-optimized vehicle introduction	Blending level, vol%	Biomass feedstock	Bio-refinery investment	Dispensing equipment investment
Ethanol	2028	16.7%	Corn and cellulosic feedstocks enter the market on the basis of demand, price, and availability	NPV (net present value)-based investment logic	No constraint
Furan, base	2028	14.5%	Cellulosic feedstocks enter the market on the basis of demand, price, and availability	Investment to meet expected demand	No constraint
Furan, supply–demand balance				NPV-based investment logic	No constraint
Furan, supply–demand balance				Investment to meet expected demand	NPV-based investment logic
Isopropanol, base	2028	30.7%		Investment to meet expected demand	No constraint
Isopropanol, supply–demand balance				NPV-based investment logic	No constraint
Isopropanol, supply–demand balance				Investment to meet expected demand	NPV-based investment logic

Results and discussion

This section begins by discussing ADOPT-based estimates of vehicle sales in the BAU and co-optimized scenarios. In the BAU scenario, PHEVs are about half the market by 2050 and continue expanding because of incentives related to CAFE and GHG standards and lower fuel costs. Please see ESI† for more details on how the vehicle fleet evolves in the BAU case.

In the co-optimized scenarios, co-optimized vehicles become the best-selling vehicle after 2035 because they combine better acceleration and lower fuel cost per mile compared to the best-selling conventional gasoline and gasoline PHEV vehicles. Gasoline PHEVs expand in the market rapidly after 2026, as in the BAU scenario. The co-optimized technology is introduced in 2028, and begins gaining market share in conventional, hybrid electric, and plug-in hybrid electric powertrains because of their higher efficiency, low incremental cost, and growing vehicle options through 2034.

In 2035, a co-optimized PHEV option is created that becomes best-selling and triggers a faster model option creation rate that leads to much faster market adoption. The best-selling co-optimized PHEV's manufacturer's suggested retail price (MSRP) is a few hundred dollars higher than that of the gasoline PHEV because of a slightly larger battery (resulting from ADOPT's component sizing optimization) and additional co-optimized vehicle cost. However, the MSRP disadvantage is outweighed by the lower fuel cost from better efficiency, greater incentives from vehicle manufacturers to help meet regulations, reflected in the sales price, and the slightly better acceleration due to the larger battery. The co-optimized PHEV sales expansion continues to the end of the simulation (see Fig. 2).

With the high penetration of co-optimized vehicles, there will be a high corresponding demand for the fuel that enables the elevated fuel economy. For these simulations, it is assumed that biorefineries will be built to satisfy the projected bio-blendstock demand (to assess potential benefits of the blended fuels in each scenario); however, the ability to meet the demand will be limited by high bio-blendstock prices, shortages of dispensing facilities, and shortages of fuel owing to biorefinery construction limits and feedstock scarcity.[29] In addition, it is assumed that fuel-compatible dispensing tankage and equipment will be installed at the same rate as co-optimized fuel demand growth. As a result of these assumptions, the growth in bio-blendstock production in the base cases (Fig. 3) could be considered aggressive. While the isopropanol and furan cases experience delays in meeting demand, the ethanol case shows very little gap between supply and demand because the existing starch ethanol industry provides a buffer for the developing cellulosic ethanol industry. As a result, cumulatively in the three scenarios, 568, 569, and 583 billion liters of blended fuels (with bio-blendstock blending levels of 30.7%, 14.5%, and 16.7% in the isopropanol, furan, and ethanol cases, respectively) would be consumed during 2025–2050, which accounts for about 4% of the total transportation energy demand, and reduces E10–15 fuel consumption by about 6% in these three base cases (Fig. 4).

Energy benefits assessment

Fig. 5 illustrates the yearly petroleum fuel consumption from 2025 to 2050 in the isopropanol, furan, ethanol, and BAU scenarios. In the BAU case, the petroleum fuel consumption decreases mostly because of improved fleet fuel economy and replacement of E10–15 conventional vehicles by more efficient HEVs and PHEVs. In the isopropanol, furan, and ethanol scenarios, petroleum fuel consumptionis reduced primarily driven by the overall reduction in E10–15 fuel consumption as a result of fleet replacement by more efficient co-optimized vehicles. With about 111, 85.6, and 85.4 million co-optimized vehicles sold to the market, about 85.0, 68.3, and 68.1 million co-optimized vehicles in the LDV fleet remain in service in 2050 in the three cases, and these more efficient vehicles meet about 31% of the total LDV travel demand in all three cases. In the isopropanol case, about 371 billion liters of petroleum gasoline blendstock and 102 billion liters of ethanol are displaced by about 202 billion liters of isopropanol blended into the co-optimized fuel at 31%. As a result, E17, furan, and isopropanol co-optimized vehicles could reduce life-cycle petroleum consumption in the

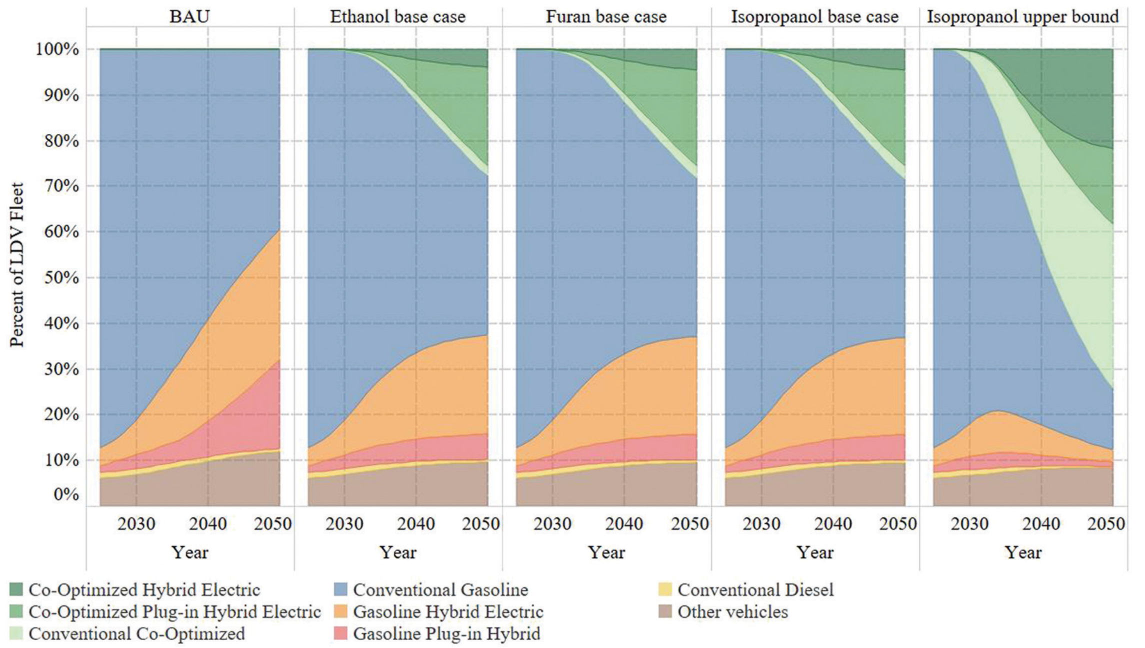

Fig. 2 Percent of LDV fleet by vehicle type under the BAU, ethanol, furan, and isopropanol base cases, in addition to the isopropanol upper-bound case, 2025–2050.

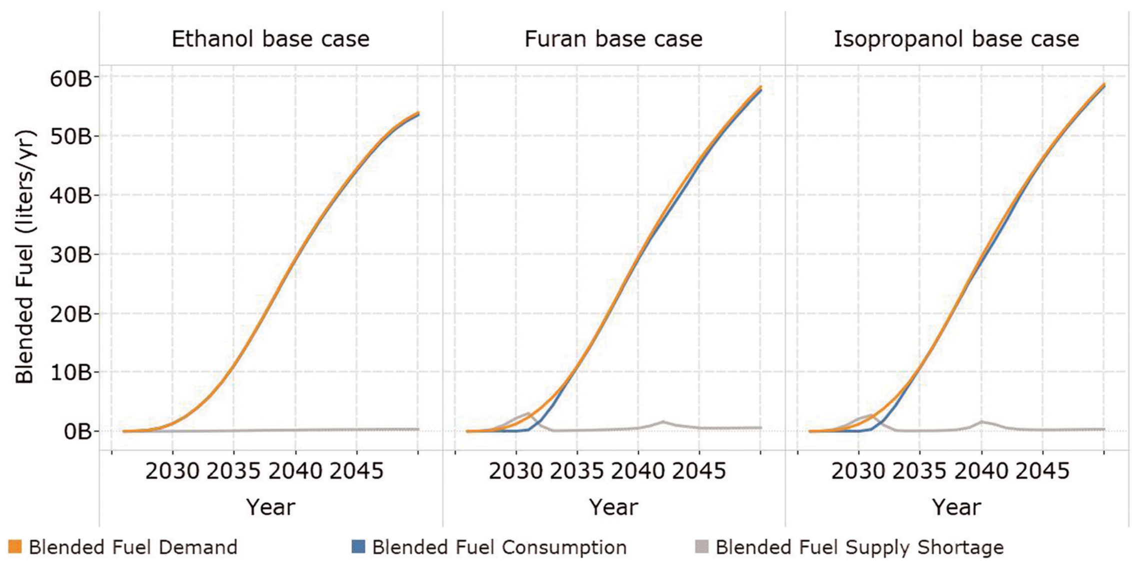

Fig. 3 Total Co-Optima fuel demand *versus* consumption and blended fuel supply shortage by scenario, 2028–2050.

LDV sector by 9%, 5%, and 8%, respectively, in such scenarios in 2050 itself and likely by similar levels in future years. The difference in the petroleum reduction benefits among the three cases reflects the differences in blending levels and the LHVs of the bio-blendstocks. The LHVs of isopropanol, furan, and ethanol are 24, 27, and 21 MJ per litre, respectively.

Environmental benefits assessment

This section shows results for GHG emissions, water consumption, and $PM_{2.5}$ emissions in three cases in which isopropanol is the bio-blendstock. Results are compared to the BAU case. The results for furan and ethanol cases would be similar, given the similar fleet turnovers and the resulting reduction in petroleum fuel consumption when these co-optimized fuels are deployed. For the isopropanol case, a base case is considered in which fleet evolution is market-driven in addition to an upper-bound case in which new vehicle adoption is not reliant on market factors, but is completely co-optimized vehicles within ten years ("Upper Bound Case").

Fig. 6(a) illustrates the yearly light-duty transportation sector GHG emissions from 2025 to 2050 in the isopropanol scenarios alongside the BAU case. In the BAU case, GHG emissions start

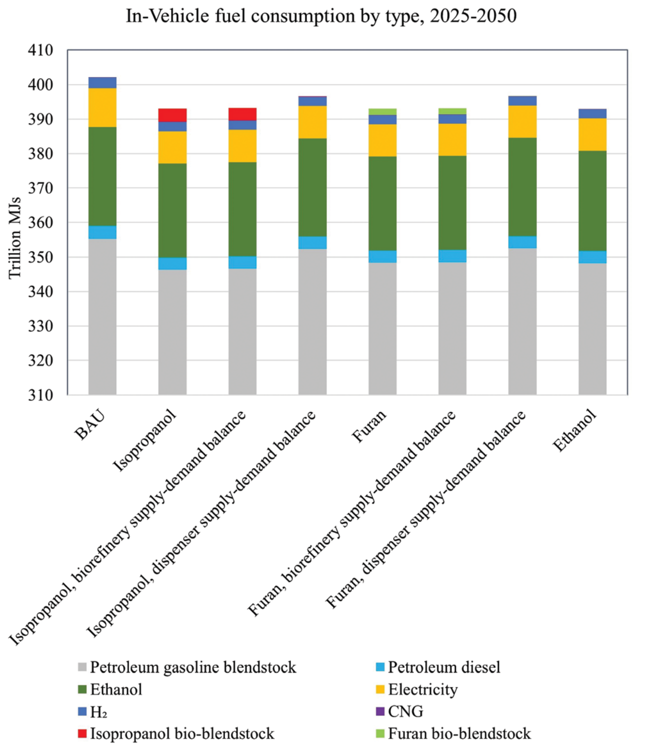

Fig. 4 Vehicle-phase fuel consumption by type for 2025–2050 of Co-Optima scenarios, in comparison to the BAU case.

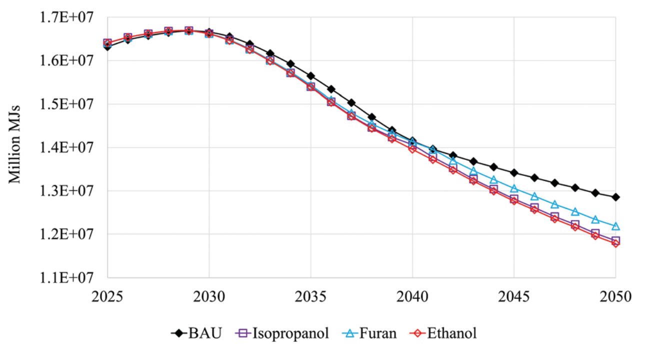

Fig. 5 Petroleum fuel consumption, in million Btus, of isopropanol, furan, and ethanol cases, in comparison to the BAU case.

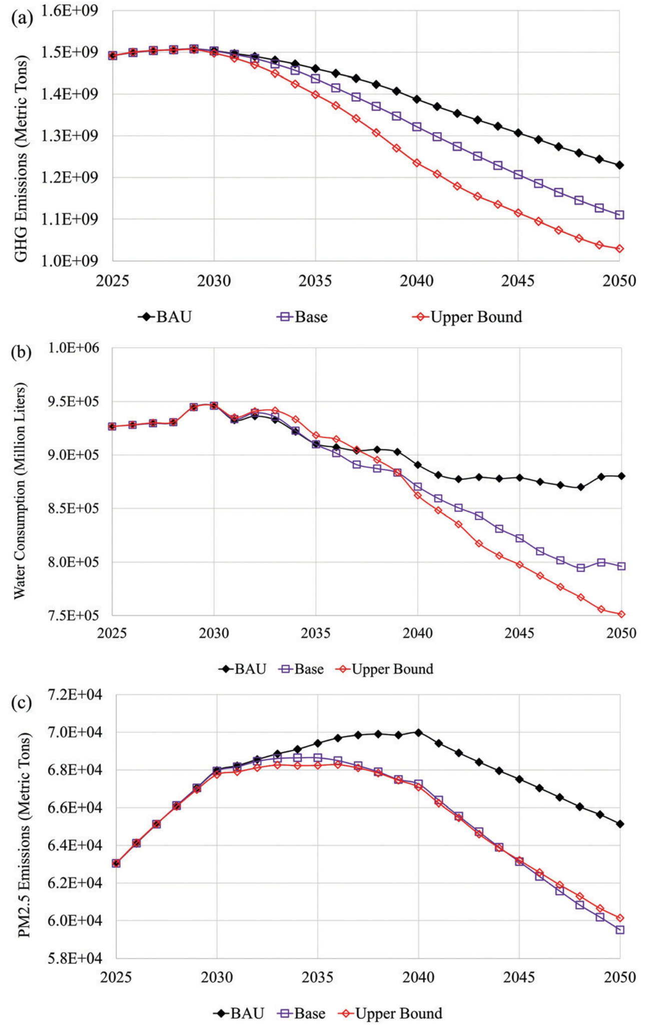

Fig. 6 (a) GHG emissions, in metric tons; (b) water consumption, in million liters; and (c) $PM_{2.5}$ emissions, in metric tons, of isopropanol base and upper bound cases, in comparison to the BAU case.

to decline in 2029 after a short period of emission increase driven by increased total fleet mileage. Emissions then continue to decline until 2050 in the BAU case. The CAFE and GHG regulations and falling battery prices drive reductions in E10–15 fuel consumption and the emissions associated with it in the BAU case. Battery costs are assumed to drop from \$500 per kW per h to \$210 per kW per h between 2020 and 2035,[27] leading to more electrified-vehicle sales. About 23% of the E10–15 conventional LDV fleet is replaced by more efficient PHEVs (19%) and HEVs (4%). This trend cuts E10–15 fuel consumption and thus emissions. To a lesser extent battery electric vehicles (BEVs) and hydrogen fuel cell electric vehicles (FCEVs) also gain market share. These gains contribute to lower fleet GHG emissions because BEVs and FCEVs are more efficient and less GHG-intensive than conventional vehicles on a per-mile basis (see Fig. S4 in ESI†).

Compared to the BAU case, the isopropanol base and upper-bound cases offer GHG emission reduction benefits in the 2025–2050 period, representing 1311 and 2661 million metric tons of GHG emissions reduction, or a cumulative 3.6% and 7.3% reduction, respectively. These emission reductions are driven by the 10% engine efficiency gain and 26% lower GHG emission intensities of the Co-Optima fuel with 31% isopropanol by volume relative to the displaced petroleum gasoline (E0). The neat isopropanol bio-blendstock reduces GHG emissions by 56% relative to E0.[21] The small cumulative emissions reductions are reflective of the relatively small share of the vehicle population and fuel consumption of co-optimized vehicles and fuels in the time period considered. For example, between 2025 and 2050, about 202 billion and 903 billion liters of isopropanol bio-blendstocks, or about 657 billion and 2944 billion liters of blended fuel-economy enhancing fuels, are consumed in the base and upper-bound cases, respectively, compared to about 12.3 trillion liters of E10–15 petroleum gasoline fuel in the BAU case. With the highest blending level and the lowest life-cycle GHG emission intensity among the three bio-blendstocks, the isopropanol case offers slightly better GHG emission reductions compared to the other cases (results not shown). On the other hand, in 2050, the isopropanol base and upper-bound cases reduce GHG emissions by 10% and 16%, respectively, with the continuous and scaled-up deployment of co-optimized vehicles over time. In that year, the co-optimized technology has gained a foothold and if the analysis window were extended, cumulative gains over the BAU scenario would be greater.

In the BAU case, water consumption (Fig. 6b) goes up in the late 2020s owing to increased E10–15 fuel consumption, consistent with Annual Energy Outlook 2017[26] projections, and then decreases until the early 2040s because of reduced E10–15 fuel consumption, as well as reduced consumption of petroleum diesel and CNG fuels. Water consumption starts to increase again in the late 2040s as a result of increased market penetration of BEVs and FCEVs. BEVs consume electricity (the U.S. average generation mix) that is more water-intensive to produce compared to the E10–15 fuel[47] (see Fig. S5 in ESI†). In the isopropanol base and upper-bound cases, water consumption decreases by about 2.4 and 3.2 trillion liters, or 3% and 4%, respectively, in the 2025–2050 period. The fuel displacement effects of isopropanol co-optimized vehicle deployment reduce consumption of E10/E15, as well as electricity due to fleet turnover from conventional PHEVs to co-optimized PHEVs, which outweighs the somewhat more water-intensive isopropanol-based Co-Optima fuel than those of conventional E10/E15 fuels (see Fig. S5 in ESI†), resulting in a net reduction in water consumption by about 318 and 488 billion liters in 2050 in the base and upper-bound cases, respectively. Similar trends that drive down water consumption are found in the furan and ethanol cases (results not shown). The major difference in the furan case is that the life-cycle water intensity of the furan bio-blendstock is about 60% lower than that of isopropanol, which contributes to an even larger water-consumption reduction benefit.

In the BAU case, the $PM_{2.5}$ emissions show an increasing trend until 2030 (Fig. 6c), which is driven by increased E10 gasoline fuel usage during the period. The $PM_{2.5}$ emissions start to decline in 2040 as a result of reduced fuel consumption by various vehicle types, including E10 vehicles, diesel vehicles, and CNG vehicles, which largely takes place because of increased market shares of PHEVs, BEVs, HEVs, and FCEVs in the fleet that exhibit higher vehicle fuel economy to meet the CAFE regulations. Despite the $\sim$20–35% higher life-cycle $PM_{2.5}$ emission factors of isopropanol, furan, and ethanol-based blended fuels relative to that of the E10 fuel (see Fig. S6 in ESI†), E10–15 fuel consumption by the fleet is reduced by about 20%, because a significant portion of the fleet has been replaced by more efficient co-optimized PHEVs (see Fig. 2). Fleet turnover from conventional E10–15 vehicles to BEVs contributes to additional $PM_{2.5}$ emission reduction because per-mile life-cycle $PM_{2.5}$ emissions for BEVs are about 35% lower than for conventional counterparts.[44] Over the 2025–2050 period, a reduction of about 56 000 and 57 000 metric tons of $PM_{2.5}$ emissions in the isopropanol base and upper-bound cases, respectively, represents a reduction by 3.2% in both the base and upper-bound cases. Particularly in 2050, the $PM_{2.5}$ emission reduction amounts to about 9% and 8% in the isopropanol base and upper-bound cases, respectively.

Economic benefits assessment

This section reports the net job-growth benefits of the two isopropanol cases (*i.e.*, market-based turnover with all vehicles and assuming full sales turnover with all vehicles – "Upper Bound Case"), in comparison with the BAU case. The incremental employment effects are reported for two distinct economic activities, construction of biorefineries (note that no new petroleum refinery is expected to be built under the bio-blendstock and BAU scenarios) and operation of refineries (both biorefineries and petroleum refineries), respectively. The number of jobs reported here represents annual jobs, which is defined as a full-time equivalent job for one year. Under each scenario, the number of construction-related jobs is dependent on the number of each type of biorefinery (isopropanol, cellulosic ethanol) to be constructed and its associated capital investment requirement. Capital investments not only support on-site construction workers, who develop the site, construct the office and warehouse, and install equipment, among other structures, but also generate supply-chain-related jobs through procurement of goods and services (*e.g.*, equipment, construction materials, insurance, permits) from other sectors. Over the simulation period (2025 to 2050), the incremental construction-related jobs fluctuate, peaking at 60 000 annual jobs under the market-based turn over case and 128 000 annual jobs under the full fleet-turn over case. Cumulatively, over the entire simulation period from 2025 to 2050, the market-based turnover case could support 278 000 more annual jobs owing to the required capital investment to build out new biofuel facilities, whereas the construction under the full-fleet turnover case could support 1 740 000 more annual jobs compared to the BAU case. The full fleet-turnover case is estimated to yield many more construction-related jobs compared to the market-based turnover case because the former scenario requires 570 more new biorefineries (isopropanol and cellulosic ethanol biorefineries combined) to meet the increased biofuel demand as compared to the latter scenario. The required total capital investment in new biorefineries in the full-fleet-turnover case is approximately 242 billion dollars higher than that required for the market-based-turnover case (339 *vs.* 97 billion dollars). This differential explains the large difference in incremental construction-job increases supported by these two cases.

The incremental operation-related job increases take into account jobs supported by the production of biofuel blendstocks as well as jobs displaced in the petroleum sector as a result of reduced consumption of petroleum gasoline. Key factors that influence the number of operation-related jobs include biofuel output (production volume), fixed O&M cost, feedstock requirement, and non-feedstock O&M cost. Over the simulation period (2025 to 2050), the incremental operation-related jobs fluctuate, peaking at 123 000 annual jobs under the market-based turn over case and 374 000 under the full fleet-turn over case (see Table S4 in ESI†). Summing up operation-related jobs across the entire period from 2025 to 2050, the incremental growth in operation-related jobs is estimated at 1.1 and 4.3 million cumulative annual jobs, respectively, for the isopropanol market-based and full-fleet-turnover cases relative to the BAU. A breakdown of jobs by sector indicates that the increased production of biofuels could benefit the rural economy. Our results show that the agricultural sector alone accounts for 39% and 40% of the incremental gain in operation-related jobs, respectively, for the market-based-and full-fleet-turnover cases, resulting primarily from the economic activities associated with feedstock production and logistics. Combining construction and operation jobs, the adoption of co-optimized biofuel blendstocks could create 1.4 and 6.0 million more cumulative annual jobs over the 25 year simulation period for the market-based and full-fleet turnover cases, respectively, compared to the BAU scenario. Fig. S7 and S8 (ESI†) show the yearly variation of incremental job changes (construction and operation jobs, respectively) for the two co-optimized isopropanol cases, compared to the BAU scenario. Our analysis also suggests that the employment displacement effect is minimal in the petroleum industry (see ESI† for details).

Sensitivity analysis

Sensitivity analyses were performed with isopropanol as the bio-blendstock to understand the extent to which limiting biorefinery construction or dispensing capacity might affect fuel production. Fig. S9 (ESI†) shows the yearly petroleum consumption for two isopropanol sensitivity cases, compared to the BAU and base cases. In the isopropanol cases, the absence of the assumption that biorefineries will be built to meet demand has little impact on petroleum consumption relative to the isopropanol base case. Assumptions regarding dispensing equipment do, however, have a large impact. Without sufficient dispensing capacities, the demand for co-optimized bio-based blended fuels could be suppressed significantly. When dispenser costs are borne in full by fuelling station owners, impacts on results are much larger than when biorefinery expansion must meet return on investment criteria rather than to meet demand. The influence of assumptions about dispensing equipment costs is large because dispensing stations make very low margins on fuel sold. Without an incentive (*e.g.*, capital investment grant) to offset the high capital cost of installing additional equipment, stations in the BSM simulations make extremely limited investments.

In addition to these sensitivities, variations in other parameters in the BSM for isopropanol were explored: expected rate of return on biorefinery investment, consumer blended fuel price sensitivity, and carbon taxes (including the LCFS). (See ESI† for information on additional sensitivities.)

Conclusions and future work

Cellulosic-derived ethanol, isopropanol, and furan diversify the fuel resource base, create a resilient and reliable supply of bio-blendstocks, and improve engine efficiency. These bio-blendstocks can be mixed with petroleum-based BOBs with a 94 RON to make low- and medium-blend fuels that could achieve a 10% engine efficiency gain relative to E10 conventional fuel, according to the merit function.

Our modelling results indicate that blended fuel production could reach over 61 billion litres by 2050. Even with the assumption that biorefineries will be built and dispensing stations installed to meet bio-blendstock demand, a gap between supply and demand sometimes exists owing to combinations of high blended fuel prices, biorefinery construction delays, and feedstock availability. In model simulations, dispensing-station availability tends to be a more limiting factor than biorefinery construction. Blended fuel production is decreased by over 60% in 2050 without sufficient dispensing capacities (see Fig. S2, ESI†), compared to the base case without this limitation.

Petroleum consumption, GHG emissions, water consumption, and $PM_{2.5}$ emissions are all reduced when co-optimized fuels and engines emerge. Given the short period of time considered in this analysis (2025 to 2050), cumulative benefits are relatively small. Over time, much greater annual energy and environmental benefits could be expected as co-optimized fuel and vehicle technologies gain a foothold. For example, beginning in 2050, GHG emission reductions in the range of 7–9% could be realized. Given the cost and performance advantages of co-optimized PHEVs and their contribution to the quantified benefits, future research and development of PHEV co-optimization technology might be a key area for realizing the potential environmental benefits of co-optimized LDVs.

Furthermore, job growth in areas of feedstock and bio-blendstock production upon deployment of co-optimized fuels and engines could be significant. On the basis of modelling results, the petroleum sector would be minimally influenced by the expansion of bio-blendstock production.

This study has highlighted some of the key barriers to increased use of co-optimized vehicles and biomass-derived fuels, including speed of vehicle adoption, lagging feedstock supply, and construction capacity for new biorefineries. It has also highlighted the need for time to allow the benefits from these technologies to unfold as the industry develops. While the technology to produce the bio-blendstocks should be available in the relatively near term, economic requirements for biorefinery investment and deployment costs of infrastructure are likely to impede the adoption and delay the associated benefits of the increased use of these fuels. Future work would explore these barriers more closely, in addition to taking into account potential compatibility issues. Another area of future focus is the potential dynamic interaction between the biofuels and petroleum sectors.

Conflicts of interest

There are no conflicts to declare.

Acknowledgements

The research reported in this paper was sponsored by the U.S. Department of Energy (DOE), Bioenergy Technologies Office

(BETO) and Vehicle Technologies Office (VTO), under the DOE Co-Optimization of Fuels and Engines Initiative. The authors gratefully acknowledge the support and guidance of Alicia Lindauer at BETO, Kevin Stork at VTO, and the Co-Optima project leadership team. This work was supported by DOE contracts DE-AC02-06CH11357 at Argonne National Laboratory and DEAC36-08GO28308 at the National Renewable Energy Laboratory. This work was authored in part by Alliance for Sustainable Energy, LLC, the manager and operator of the National Renewable Energy Laboratory for the DOE under Contract No. DE-AC36-08GO28308. Funding was provided by the DOE Office of Energy Efficiency and Renewable Energy, Bioenergy Technologies Office. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

References

1 U.S. Environmental Protection Agency, Global Greenhouse Gas Emissions Data, https://www.epa.gov/ghgemissions/global-greenhouse-gas-emissions-data, accessed August 28, 2019.
2 Enerdata, World Energy Consumption Statistics, https://yearbook.enerdata.net/total-energy/world-consumption-statistics.html, accessed August 28, 2019.
3 U.S. Energy Information Administration, International Energy Outlook 2018, https://www.eia.gov/outlooks/ieo/executive_summary.php, accessed August 28, 2019.
4 U.S. Environmental Protection Agency, Inventory of U.S. Greenhouse Gas Emissions and Sinks, https://www.epa.gov/ghgemissions/inventory-us-greenhouse-gas-emissions-and-sinks, accessed August 28, 2019.
5 U.S. Environmental Protection Agency, Air Pollutant Emissions Trends Data, https://www.epa.gov/air-emissions-inventories/air-pollutant-emissions-trends-data, accessed August 28, 2019.
6 T. G. Leone, J. E. Anderson, R. S. Davis, A. Iqbal, R. A. Reese, M. H. Shelby and W. M. Studzinski, *Environ. Sci. Technol.*, 2015, **49**, 10778–10789.
7 T. Johnson and A. Joshi, *SAE Int. J. Engines*, 2018, **11**, 1307–1330.
8 M. Kassai, C. Aksu, T. Shiraishi, R. Cracknell and M. Shibuya, SAE Technical Paper 2019-01-0035, 2019, DOI: 10.4271/2019-01-0035.
9 E. Kasseris, J. B. Heywood, S. Seitz and R. Kolakaluri, SAE Technical Paper 2018-01-0879, 2018, DOI: 10.4271/2018-01-0879.
10 A. Khan, K. Morganti, M. Sendi, M. Almansour and E. Hamad, *Energy*, 2019, **169**, 1079–1089.
11 A. Prakash, J.-H. Redmann, K. Giles, R. Cracknell, N. Turner, A. A. Aradi, A. Lewis and S. Akehurst, SAE Technical Paper 2018-01-0269, 2018, DOI: 10.4271/2018-01-0269.
12 N. Yokoo, K. Nakata, B. Chapman, D. Joseph, N. Sabio, J. Farenback-Brateman, C. Goheen and A. Sahnoune, SAE Technical Paper 2019-01-0629, 2019, DOI: 10.4271/2019-01-0629.
13 J. Chang, Y. Viollet, A. Alzubail, A. F. N. Abdul-Manan and A. Al Arfaj, SAE Technical Paper 2015-01-1264, 2015, DOI: 10.4271/2015-01-1264.
14 K. Grubel, W. Chouyyok, D. J. Heldebrant, J. C. Linehan and J. T. Bays, *Energy Fuels*, 2019, **33**, 1869–1881.
15 Y. Viollet, M. Abdullah, A. Alhajhouje and J. Chang, SAE Technical Paper 2015-01-1265, 2015, DOI: 10.4271/2015-01-1265.
16 J. Han, A. Elgowainy, M. Wang and V. Divita, Well-to-Wheels Greenhouse Gas Emissions Analysis of High-Octane Fuels with Various Market Shares and Ethanol Blending Levels, Argonne National Laboratory Technical Report ANL/ESD-15/10, Argonne National Lab. (ANL), Argonne, IL, United States, 2015.
17 T. G. Leone, E. D. Olin, J. E. Anderson, H. H. Jung, M. H. Shelby and R. A. Stein, *SAE Int. J. Fuels Lubr.*, 2014, **7**, 9–28.
18 E. Monroe, J. Gladden, K. O. Albrecht, J. T. Bays, R. McCormick, R. W. Davis and A. George, *Fuel*, 2019, **239**, 1143–1148.
19 J. Han, M. Wang, A. Elgowainy and V. DiVita, Well-to-Wheels Greenhouse Gas Emission Analysis of High-Octane Fuels with Ethanol Blending: Phase II Analysis with Refinery Investment Options, Argonne National Laboratory Technical Report ANL/ESD-16/9, Argonne National Lab. (ANL), Argonne, IL, United States, 2016.
20 R. L. McCormick, G. Fioroni, L. Fouts, E. Christensen, J. Yanowitz, E. Polikarpov, K. Albrecht, D. J. Gaspar, J. Gladden and A. George, *SAE Int. J. Fuels Lubr.*, 2017, **10**, 442–460.
21 J. B. Dunn, M. Biddy, S. Jones, H. Cai, P. T. Benavides, J. Markham, L. Tao, E. Tan, C. Kinchin, R. Davis, A. Dutta, M. Bearden, C. Clayton, S. Phillips, K. Rappé and P. Lamers, *ACS Sustainable Chem. Eng.*, 2018, **6**, 561–569.
22 D. Swenson, Renewable Fuels Roadmap, APPENDIX I: Biofuel Industry Economic Impacts and Analysis, NYSERDA Report 10-05, 2010.
23 C. Bailey, J. F. Dyer and L. Teeter, *Biomass Bioenergy*, 2011, **35**, 1408–1417.
24 J. N. Rogers, B. Stokes, J. Dunn, H. Cai, M. Wu, Z. Haq and H. Baumes, *Biofuels, Bioprod. Biorefin.*, 2017, **11**, 110–128.
25 R. A. Efroymson, M. H. Langholtz, K. Johnson, B. Stokes, C. C. Brandt, M. R. Davis, C. Hellwinckel, K. L. Kline, L. M. Eaton and J. Dunn, 2016 Billion-ton report: advancing domestic resources for a thriving bioeconomy, volume 2: environmental sustainability effects of select scenarios from volume 1, Oak Ridge National Lab. (ORNL), Oak Ridge, TN, United States, 2017.
26 US Energy Information Administration, Annual Energy Outlook 2017 with Projections to 2050, 2017.
27 E. Islam, A. Moawad, N. Kim and A. Rousseau, An Extensive Study on Sizing, Energy Consumption, and Cost of Advanced Vehicle Technologies, ANL/ESD-17/17, Argonne National Lab. (ANL), Argonne, IL United States, 2017.
28 A. Brooker, J. Gonder, S. Lopp and J. Ward, SAE Technical Paper 2015-01-0974, 2015, DOI: 10.4271/2015-01-0974.
29 C. Johnson, E. Newes, A. Brooker, R. McCormick, S. Peterson, P. Leiby, R. U. Martinez, G. Oladosu and

M. L. Brown, High-Octane Mid-Level Ethanol Blend Market Assessment, National Renewable Energy Lab. (NREL), Golden, CO, United States, 2015.

30 E. Kontou, M. W. Melaina and A. D. Brooker, Light-Duty Vehicle Attribute Projections (Years 2015–2030), National Renewable Energy Lab. (NREL), Golden, CO, United States, 2018.

31 A. H. C. Yip, J. J. Michalek and K. S. Whitefoot, *Transportation Research Part B: Methodological*, 2018, **116**, 163–188.

32 E. Newes, Systems Analysis and Modeling – Biomass Scenario Model, National Renewable Energy Laboratory, 2017.

33 isee systems, Stella Professional, https://www.iseesystems.com/store/products/stella-professional.aspx, accessed September 24, 2018.

34 MIT OpenCourseWare, System Dynamics for Business Policy, https://dspace.mit.edu/bitstream/handle/1721.1/91162/15-874-fall-2003/contents/index.htm, accessed September 24, 2018.

35 L. J. Vimmerstedt, E. S. Warner and D. Stright, Effects of Deployment Investment on the Growth of the Biofuels Industry. 2016 Update, National Renewable Energy Lab. (NREL), Golden, CO, United States, 2016.

36 L. J. Vimmerstedt, B. W. Bush, D. D. Hsu, D. Inman and S. O. Peterson, *Biofuels, Bioprod. Biorefin.*, 2015, **9**, 158–176.

37 L. J. Vimmerstedt, B. Bush and S. Peterson, *PLoS One*, 2012, **7**, e35082.

38 E. K. Newes, B. W. Bush, C. T. Peck and S. O. Peterson, *Biofuels*, 2015, **6**, 21–29.

39 E. Newes, D. Inman and B. Bush, in *Economic Effects of Biofuel Production*, ed. M. A. D. S. Bernardes, IntechOpen, 2011, DOI: 10.5772/17090.

40 C. M. Clark, Y. Lin, B. G. Bierwagen, L. M. Eaton, M. H. Langholtz, P. E. Morefield, C. E. Ridley, L. Vimmerstedt, S. Peterson and B. W. Bush, *Environ. Res. Lett.*, 2013, **8**, 025016.

41 H. Cai, A. R. Brandt, S. Yeh, J. G. Englander, J. Han, A. Elgowainy and M. Q. Wang, *Environ. Sci. Technol.*, 2015, **49**, 8219–8227.

42 S. Yeh, A. Ghandi, B. R. Scanlon, A. R. Brandt, H. Cai, M. Q. Wang, K. Vafi and R. C. Reedy, *Energy Fuels*, 2017, **31**, 1440–1449.

43 A. R. Brandt, T. Yeskoo, M. S. McNally, K. Vafi, S. Yeh, H. Cai and M. Q. Wang, *Energy Fuels*, 2016, **30**, 9613–9621.

44 Argonne National Laboratory, The Greenhouse gases, Regulated Emissions, and Energy use in Transportation Model, https://greet.es.anl.gov/, accessed August 28, 2019.

45 National Renewable Energy Laboratory, JEDI: Jobs & Economic Development Impact Models, https://www.nrel.gov/analysis/jedi, accessed August 28, 2019.

46 P. Miles, Efficiency Merit Function for Spark-ignition Engines: Revision and Improvements Based on FY16-17 Research, US Department of Energy, Office of Energy Efficiency & Renewable Energy, 2018.

47 D. J. Lampert, H. Cai and A. Elgowainy, *Energy Environ. Sci.*, 2016, **9**, 787–802.

