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Energy, economic, and environmental impacts assessment of co-optimized on-road heavy-duty engines and bio-blendstocks†

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Abundant domestic biomass and waste resources can be converted to a number of liquid transportation fuels, including those for aviation, marine, and diesel-fueled vehicles. For example, diesel-range renewable blendstocks with favorable properties such as high-cetane number, low sulfur, and oxygenation can be produced for heavy-duty (HD), mixing controlled compression ignition (MCCI) engine vehicles. Renewable MCCI fuels and a ducted fuel injection technology could reduce engine-out soot and nitrogen oxide emissions, leading to reduced total cost of vehicle ownership and a potential to penetrate the market at scale. We employed a suite of integrated models to evaluate different MCCI fuels (polyoxymethylene dimethyl ether from forest residues; alkoxy alkanoate ester ether from corn stover; renewable diesel from fats, oils, and greases (FOG), wastewater sludge, and swine manure) that are potentially technically viable, and scalable. We assessed how MCCI fuels could be produced and deployed over time in potential deployment scenarios, considering their impact on consumer vehicle choices, market availability and build-out of biomass- or waste-derived MCCI fuels and biorefineries, and the effects of a hypothetical U.S. carbon tax. In the absence of a carbon tax, co-optimized MCCI vehicles account for 9–325 thousand TJ per yr of renewable fuels to supply 4–9% of heavy-duty vehicle (HDV) stock in 2050 across all scenarios. Consequently, we estimated that the life-cycle petroleum consumption would decrease by 2–15%, life-cycle greenhouse gas (GHG) emissions would decrease by 2–11%, and net jobs would increase by 4600–25 400, compared to a business-as-usual (BAU) scenario defined by energy information administration projections. With a carbon tax, co-optimized MCCI vehicles account for 175–338 thousand TJ per yr of renewable fuels to supply 7–35% of HDV vehicle stock in 2050. Consequently, we estimated that the life-cycle petroleum consumption would decrease by 8–16%, the life-cycle GHG emissions would decrease by 7–11%, and net jobs would increase by 3000–29 000. With a carbon tax and a nationwide renewable diesel policy framework, even greater benefits would be expected when additional renewable diesel fuels are produced and used by co-optimized MCCI vehicles. Ultimately, we put forward a framework to evaluate the energy, environmental and economic impacts associated with deployments of co-optimized MCCI fuels and engines in class 8 long-haul trucks.

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Introduction

The United States has set a societal decarbonization goal to reach carbon neutrality by 2050. The transportation sector is the largest sources of GHG emissions in the U.S., contributing over 27% of U.S. emissions in year 2020. As such, large-scale decarbonization of the transportation sector is critical for meeting U.S. climate targets, and can be achieved through the adoption of advanced vehicle technologies, low-carbon fuels, and fuel-efficient vehicles.[1] Medium- and heavy-duty vehicles (MHDVs) contributed 26% of the total GHG emissions in the U.S. transportation sector in 2020, which is more than the combined contributions of aircraft, rail, and ships.[1] Additionally, MHDVs

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are one of the major sources of hazardous emissions such as oxides of nitrogen (NO_x) and particulate matter (PM). Heavy-duty diesel vehicles accounted for 23% of NO_x and 23% of PM_{10} emissions from all the mobile sources in the United States in 2017.[2] Though MHDVs account for just 5% of on-road vehicles, they consume 31% of all road vehicle energy.[3] In 2021, the U.S. Environmental Protection Agency and the U.S. Department of Transportation's National Highway Traffic Safety Administration jointly finalized standards for MHDVs that aim to improve fuel efficiency and reduce GHG emissions by promoting a new generation of cleaner, more fuel-efficient trucks. The standards encourage the development and deployment of new, advanced, cost-effective technologies, such as aerodynamic designs that reduce drag, engine technologies that reduce friction, advanced fuel injection systems that improve engine efficiency, and improved tires and tire pressure monitoring to improve vehicle energy efficiency, and other measures.

In addition to improving technology for existing powertrains, research programs have also focused on developing alternative fuels and engines for MHDVs. Co-Optimization of fuels & engines (Co-Optima) is a Consortium of the U.S. Department of Energy (DOE) that brings together nine national laboratories and more than 20 university and industrial partners. Co-Optima explores how simultaneous innovations in fuels and engines can improve vehicle performance and fuel economy while reducing emissions. In order to identify biomass and renewable carbon-derived fuel blendstocks (bio-blendstocks) that meet a set of specified characteristics for a specific combustion mode, Co-Optima uses a tiered screening approach. Promising performance-enhancing bio-blendstocks for boosted, spark-ignited (BSI) engines for light-duty vehicles have been identified in the literature.[4–6] Dunn *et al.* determined that GHG emissions could be reduced by 7–9% beginning in 2050 with cellulosic-derived ethanol, isopropanol, and furan.[7] These fuels both boost the boosted spark ignition (BSI) engine efficiency to reduce overall fuel consumption and replace higher emitting petroleum fuels. Recently, research within Co-Optima has focused on the heavy-duty market, specifically identifying promising mixing-controlled compression ignition (MCCI) bio-blendstock candidates that provide favorable environmental and cost performance relative to petroleum diesel fuels.[8–10] From a fuel-properties standpoint, these MCCI bio-blendstocks meet requirements for conventional petroleum diesel fuels and possess favorable fuel properties such as high octane number and/or oxygenation that could reduce engine-out soot and NO_x emissions when they are used in tandem with a ducted-fuel injection (DFI) technology.

It has been shown that DFI reduces diesel engine-out soot emissions. In addition, it simultaneously attenuates soot and NO_x emissions with increasing dilutions, thus breaking the tradeoff between the two emissions.[11,12] DFI could be effective for NO_x control at cold-start and light-load operating conditions because more dilution can be used without running into problems with excessive soot. The Co-Optima team has demonstrated that, over a test cycle with today's DFI technology and a single-cylinder optical engine, both soot and NO_x could be reduced by approximately 80% without significant increases in hydrocarbon or carbon monoxide emissions or efficiency loss.[13] The combination of co-optimized MCCI fuel with DFI could reduce engine-out soot and NO_x emissions even further, enabling reduced life-time costs of the aftertreatment systems. The lower emission-control cost is mainly realized by (1) reduced urea consumption by a selective catalytic reduction device for control of engine-out NO_x emissions and (2) lower fuel consumption for active regeneration of diesel particulate filters that are used to control engine-out soot emissions. Ou *et al.* estimated that an MCCI vehicle could reduce the manufacturing and operating costs of such redesigned emission after-treatment systems by over \$4000.[14]

This paper analyzes how different co-optimized MCCI fuels could deploy over time, given vehicle choice and biofuel market considerations. Market potential and the associated environmental and economic benefits of transitioning the heavy-duty vehicle (HDV) fleet to technologies with lower emissions profiles have been explored in various studies. Julio *et al.* explore potential biodiesel, conventional diesel, and renewable diesel (RD) production in Brazil. They conclude that deployment of RD for the heavy-duty trucks would be the most effective in terms of economics and emissions to meet environmental goals and suggest that national policy should be employed to make RD pathways more competitive.[15] Alonso-Villar *et al.* perform a case study analysis of HDVs in Iceland and find that electric vehicles would be most economically and environmentally attractive for delivery trucks, while compressed natural gas and hydrogen could be effective for regional routes if cost and feedstock availability are addressed. Finally, RD is a satisfactory option when considering cost of ownership, environmental attributes, energy security, and technical feasibility.[16] In Sweden, Soam and Börjesson show that using logging residues as a feedstock for fuel used in heavy-duty transportation could displace 50–100% of current conventional diesel use with up to a 94% GHG emission reduction.[17] The United States has specific regions where particular feedstocks would naturally play a larger role in biofuel production. Therefore, it is important to consider a variety of feedstocks when considering national deployment. Witcover reflects that in the United States, biofuels (including RD) will be needed for decarbonization of the heavy-duty sector, especially in the short run. However, these fuels will be feedstock-limited since other sectors would also be competing for that same biomass resource.[18]

The United States has supported domestic biofuel production through volumetric mandates and tax credits *via* regulation frameworks such as the renewable fuel standard (RFS) and state-level low carbon fuel standards (LCFS). In 2019, the U.S. Environmental Protection Agency issued a regulation permitting the sale of E15 year-round with availability at more than 1800 retail fuel stations across 31 states in the United States.[19] The number of E15 stations has since increased, with more than 2150 stations across the United States.[20] In addition, policy targeting vehicles in coordination with biofuel incentives have pushed the consumption of additional biofuel. Flex-fuel vehicles (FFVs) that operate most efficiently with E85 as fuel became popular in the 1990s in response to the alternative motor fuels act. In response, the number of E85 stations across the United States increased from 113 to 5050 between 2012 and 2020, accompanied by an increase in the volume of E85 sold, potentially because of incentives programs as well as national and state low carbon fuel standards.[20] Previous work showed that the impact of the RFS ethanol mandate on GHG emissions ranges from −0.5% to −5% relative to the status quo and is reduced when tax credit accompanies the mandate.[21] Huang *et al.* found that when a carbon price is imposed along with the RFS and LCFS policy, fuel conservation is primarily induced and GHG emissions are reduced in greater depth than under other policy scenarios. Even with offsetting market-mediated effects, greater reductions in GHG emissions are achieved. Because they improve the terms of trade for the United States, these policies result in higher net economic benefits for the transportation and agricultural sectors than a no-policy baseline.[22] Meanwhile, Chen *et al.* found that mandates, like the RFS, for corn and cellulosic biofuels have multiple impacts on the environment, including altered land use, nitrogen leakage, and GHG emissions.[23] Carbon intensity standards (CI) for transportation fuels have been in effect in California and British Columbia since 2011, and in Oregon since 2016. In California, Oregon, and British Columbia, respectively, the share of energy generated by lower-carbon alternative fuels in transport rose to about 11%, 8%, and 7% by 2019, according to a University of California Davis study.[24] As of 2019, RD generated significant compliance credits in both jurisdictions, contributing more than 16% by volume of California's liquid diesel pool and approximately 30% of British Columbia's alternative fuel credits. In California, the growth of cost-effective diesel substitutes led to over-compliance with the diesel pool standard (a 25% CI reduction in 2020), more than offsetting under-compliance in the gasoline pool (a 3% CI reduction). To a lesser extent, this is also true in Oregon and British Columbia.

In addition to generating environmental and energy benefits, increased biofuel production using domestic feedstock in the last decades supported a growing number of jobs sustained by these industries. In 2019, the ethanol industry contributed 349 000 jobs and $43 billion to the GDP (0.2%).[25] In the case of biodiesel, a study from Ditzel *et al.* estimated 62 000 jobs and $6.5 billion GDP contribution in 2017.[26] As a comparison, PricewaterhouseCoopers estimated that 11.3 million jobs and 7.9% of the U.S. gross domestic product (GDP) in 2019 were sustained by the operation and investments from the oil and natural gas industry.[27] Avelino *et al.* showed that jobs sustained by corn ethanol (dry-mills) and soybean biodiesel grew more than tenfold between 2002 and 2017, while their share of GDP increased more than eightfold.[28] This reflects the fact that biofuels require relatively more labor-intensive processes than conventional petroleum fuels, a more mature technology. For example, Lamers *et al.* estimated net positive economic gains (8500 additional jobs and 0.06% increase in GDP) in replacing 2.6% of conventional gasoline by 5 billion gallons of cellulosic ethanol.[29] In a previous study for co-optimized fuel blendstock for light-duty vehicle applications, Dunn *et al.* estimated that 123 000 incremental operation-related jobs can be supported under a market-based turnover case and 374 000 incremental operation-related jobs can be supported under a full fleet turnover case when isopropanol is used as a bio-blendstock.[7]

In this paper, we build upon work previously published for BSI fuels and engines for light-duty vehicles.[7] Here, we evaluate co-optimized MCCI fuels that could be produced from biomass and waste feedstocks and low-emission engine technologies (*e.g.*, DFI) in terms of their potential economic and environmental benefits, along with barriers to rapid large-scale adoption. Through detailed integrated modeling and analysis, the study targets near-term solutions with the potential to improve diesel fuels and engines in the marketplace, as well as revolutionary longer-term contributions to low-carbon transportation systems. First, we address methodology and scenario design, including brief descriptions of the models employed. Then we discuss the potential benefits of co-optimized MCCI fuels and engines (for class 8 long-haul trucks) and the implications for large-scale deployment. Finally, we highlight major conclusions and recommendations for future work.

Integrated modeling framework

This study applies an integrated modeling framework, as shown in Fig. 1. It employs four models: the Automotive Deployment Options Projection Tool (ADOPT), the Biomass Scenario Model (BSM), the Bioeconomy Air emissions, Greenhouse gas emissions, and Energy consumption (Bioeconomy AGE) model, and the Bio-based circular carbon economy Environmentally-extended Input–Output Model (BEIOM), which address unique but connected research questions around biomass supply for MCCI fuel production, adoption of co-optimized MCCI vehicles and fuels, and resulting energy, environmental, and economic impacts relative to a business-as-usual (BAU) scenario.

Several model enhancements and modifications were made across the modeling suite to support analysis of MCCI fuels and vehicles. For BSM and ADOPT, class 8 long-haul trucks and renewable MCCI diesel fuel options were added to the existing model architecture. For Bioeconomy AGE, the model was expanded to address heavy-duty powertrain technologies and fuel technologies considered in the Co-Optima MCCI research and development portfolio,[8–10] as well as those in the U.S. Energy Information Administration's (EIA) Annual Energy Outlook (AEO) scenarios.[30] Bioeconomy AGE was also updated with lifecycle profiles for new fuel production pathways and HDV technologies,[31,32] and it was enhanced with automated data flows and results visualization to enable more reliable modeling of multiple scenarios as well as quick interpretation of results. To estimate the employment impacts resulting from the adoption of new MCCI bio-blendstocks, the original BEIOM model was expanded with new pathway-specific sectors (*e.g.*, AAEE diesel fuel manufacturing, corn stover collection, collection and rendering of used cooking oil) (data and model details are available in the ESI†).

ADOPT is a consumer choice model used to estimate vehicle sales. It was first developed for the U.S. light-duty market.[33] As stated by Brooker *et al.*[33] "ADOPT uses techniques from the

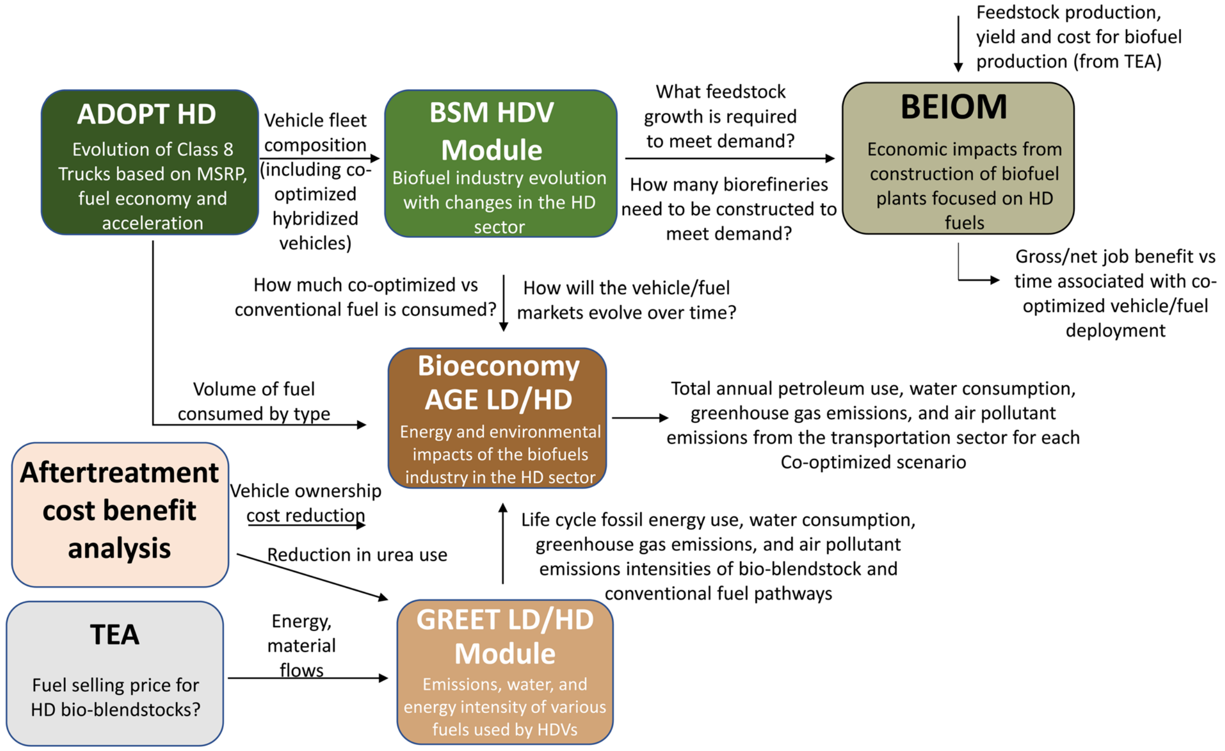

Fig. 1 Integrated modeling framework.

multinomial logit method and the mixed logit method to estimate vehicle sales."

ADOPT sales simulations begin in 2015. A database of existing vehicle make model options is entered into ADOPT to represent all of the vehicle options available at the beginning of the simulation. Scenario inputs, including fuel prices, regulations, the distribution of vehicle miles traveled, battery costs, fuel cell technology costs, and engine efficiency improvements are specified prior to running the model. ADOPT calculates a "weighted value of key attributes including vehicle price, fuel cost, acceleration, range and useable volume"[33] for each vehicle option, and uses the weighted value to rank vehicles in terms of estimated number of sales. All vehicle options in the model are updated over time to account for changes in component costs and performance, such as improvements in engine efficiency and reductions in battery cost. ADOPT creates options for each engine type that uses compression ignition, *e.g.*, those that can be co-optimized (see the ESI† for detail). See the ESI† for battery electric and fuel cell technology cost estimates. Other analyses performed after this analysis assume greater cost decreases, which result in higher penetrations for these vehicles.[34]

New vehicle models are also created in ADOPT to represent market evolution over time using the Future Automotive Systems Technology Simulator (FASTSim).[35] The new vehicle options created are based on the best-selling options from the previous year. The outputs of ADOPT are the number of sales for each vehicle make model by year. For powertrains that are not available in the beginning year, ADOPT introduces them to the market in the year specified by the user. In this analysis, only diesel powertrains were included in the initial vehicle database. Hybrid, electric, and fuel cell powertrains are introduced to the market in simulation year 2025. Co-optimized hybrid and diesel powertrains are introduced to the market in simulation year 2027.

The heavy-duty ADOPT model was developed by adapting the light-duty version of the ADOPT model. Input datasets for vehicle sales, driving patterns, technology costs, vehicle survival, and other categories were updated to reflect the conditions of the heavy-duty market. The heavy-duty model simulated sales for class 8 tractors only (including conventional diesel internal combustion engine, conventional diesel hybrid, hydrogen fuel cell, and battery electric vehicles). As a category, class 8 tractors are responsible for the largest percentage of transportation emissions of any class, largely because they log many more annual miles than any other vehicle type.[36] For this reason, the emissions reduction potential for the class 8 tractor trailers category should constitute a large percentage of the potential benefits in the entire heavy-duty market.

Consumers in the HD market are segmented by annual vehicle miles traveled (VMT). In the model, annual VMT affects a purchaser's sensitivity to specific attributes, namely, range and fuel costs. HDV purchasers aim to minimize total costs. The cost value of some attributes, such as manufacturer's suggested retail price (MSRP), are straightforward. The value of others, such as range, are quantified through penalties. Key ADOPT modeling assumptions used in this analysis are summarized in

Table 1 Key modeling assumptions of the ADOPT, BSM, and Bioeconomy AGE models in each scenario

		Scenario 1			Scenario 2		Scenario 3
MCCI bio-blendstock		POME	AAEE	Renewable diesel *via* sludge HTL	FOG *via* HEFA[a]	Swine manure HTL[b]	All 5 pathways
ADOPT key variables	Blend fraction	20%	20%	20%	20%	20%	20%
	Co-optimized engine efficiency improvement	1%	0%	0%	0%	0%	Varies
	Co-optimized vehicles' year to enter market	2027	2027	2027	2027	2027	2027
	Incremental cost of adding DFI	\$100	\$100	\$100	\$100	\$100	\$100
	After treatment cost reduction	−\$4563	−\$4563	−\$4563	−\$4563	−\$4563	−\$4563
	Tech targets	Baseline goals (no program)			Baseline goals (no program)		Baseline goals (no program)
	Price of co-optimized fuel assumption	Equivalent to diesel on a \$/gal basis			Equivalent to diesel on a \$/gal basis		Equivalent to diesel on a \$/gal basis
	Prices of conventional fuels	Based on Fig. A4 in the ESI			Based on Fig. A4 in the ESI		Based on Fig. A4 in the ESI
BSM key variables	Policy effects	RFS RINs[c], LCFS[d] credits: base, PTC[e]: base			RFS RINs, LCFS credits: base, PTC: base		RFS RINs, LCFS credits: high, PTC: high
	Biorefineries are built to meet demand	Yes			Yes		Yes
	Consumer price sensitivity	Consistent with Dunn *et al.*[5]			Consistent with Dunn *et al.*[7]		Consistent with Dunn *et al.*[7]
	Capital cost of refineries	Consistent with Bartling *et al.*[9]			Consistent with Bartling *et al.*[9]		Consistent with Bartling *et al.*[9]
	Maximum number of biorefineries built per year	25			25		25
	Oil feedstock availability[f]	Amount available limited to 30% (soy), 50% (FOG), 60% (DCO) of total available			Amount available limited to 30% (soy), 50% (FOG), 60% (DCO) of total available		Amount available limited to 80% of total available
	Rate of return required from biorefinery investors	10% for n^{th} plant			10% for n^{th} plant		10% for n^{th} plant
Bioeconomy AGE key variables	Feedstock types	Forest residues	Corn stover	Wastewater sludge	FOG	Swine manure	Varies
	Life-cycle GHG emissions (g CO_2e per MJ)	17.1	32.5	24.1	11.2	−31.5	Varies

[a] Near-term co-optimized bio-blendstock. [b] A long-term co-optimized bio-blendstock. [c] Renewable identification numbers (RINs) under the renewable fuel standard (RFS) set at \$1.70/RIN. [d] Low carbon fuel standard based on 5 year average of the California LCFS credit applied to pacific region (base) and on 5 year maximum credit applied to the entire continental United States (high). [e] Historic production tax credit (PTC) levels (base) or an additional \$2/gal applied to low-TRL technologies (high). [f] Fats, oils, and greases (FOG); distillers corn oil (DCO).

Table 1. Technology assumptions and fuel prices have been added to the ESI.†

The vehicle sales results from ADOPT are an input to the BSM, which the DOE Bioenergy Technologies Office and the National Renewable Energy Laboratory (NREL) have developed and used to look at how biofuels could be deployed within the United States under different scenarios. The model uses the system dynamics methodology to explore the biofuel supply chain (feedstock supply/logistics, conversion to biofuels, and downstream sectors) interactions, including biofuel industry growth driven by the HDV fleet in the United States. The ten U.S. Department of Agriculture farm production regions are used for geospatial disaggregation. The model can follow agricultural production changes, new technology adoption, petroleum liquid fuels competition, and biofuel demand related to the vehicle sector. The system dynamics modeling methodology has a history of being applied to behavioral questions, focusing on the feedback-rich social, economic, and environmental systems; it allows for robust analysis of system bottlenecks, potential policy impacts, and potential unintended consequences.[37] Specifically, the BSM explores how the systems that comprise the biofuels supply chain could evolve over time, given different input parameters. As one example, the feedstock system may not develop exactly in coordination with the conversion system, given that supply may not always meet demand. However, pricing mechanisms in the model moderate the gap between supply and demand, raising price when supply is not meeting demand. The BSM is a mature model, with extensive published analyses, including the exploration of potential of different fuel technologies, industrial learning, facility investment characteristics, and policies in the development of the biofuel industry.[7,38–42] For this analysis, the BSM was expanded to include the HDV fleet and additional waste feedstocks with data from Badgett *et al.*[43]

BSM/ADOPT simulations provide the trajectory of biorefinery buildout, production of MCCI and other fuels, and fleet turnovers and market penetration of powertrain technologies and fuel options in the HDV sector. Key variables from BSM/ADOPT are passed to Bioeconomy AGE, a scenario-based spreadsheet model integrated with the GREET™ model, to calculate the changes in sector-wide life cycle energy consumption and GHG emissions. The Argonne National Laboratory's GREET™ (greenhouse gases, regulated emissions, and energy use in technologies) model is a tool that examines the life-cycle impacts of vehicle technologies, fuels, products, and energy systems. The GREET model was used to estimate the life-cycle profiles of various MCCI bio-blenstocks/other biofuels and conventional–fuel pathways.[31] These results were then built into Bioeconomy AGE to assess the environmental and energy impacts of each scenario. Argonne's Bioeconomy AGE model has been used in past works to support cross-sectoral analysis and assessment of co-optimized fuels and light-duty engines.[7,44,45] For this study, Bioeconomy AGE was expanded to include analysis of class 8 HDVs, which allows users to track sector-wide environmental impacts of MCCI fuel and vehicle deployment across a suite of environmental metrics, including life-cycle petroleum energy consumption, GHG emissions, water consumption, and NO_x emissions. Bioeconomy AGE accounts for changes to the U.S. electric power sector and variations to the transportation fuel mix over time by coupling EIA's AEO forecasts for the bulk U.S. energy system with environmental analysis in GREET to enable temporally resolved life cycle profiles for material, energy, and fuel pathways.[30]

In addition to environmental benefits, we assessed associated economic benefits using BEIOM. As illustrated in Fig. 2, BEIOM uses external information generated from BSM/ADOPT to simulate technology deployment, fuel substitution, and production levels each year. The BEIOM module incorporated all biofuels and conventional petroleum fuels covered in the BSM model and simulated biofuel and conventional fuel as separate industries. Construction impacts are estimated based on the number of new biorefineries projected (by BSM) to be built in given years to produce bio-blendstocks to meet demand. Construction costs and itemization are technology-specific (*i.e.*, by MCCI bio-blendstock pathway) and are scaled from an n^{th} size plant according to the actual size provided by BSM. The average yield of the biorefineries portfolio in each year is used to scale the variable costs of biorefineries in BEIOM. Total fuel production informs the required biorefinery output for each year. Demand is then allocated between final demand and sectors according to the consumption structure of 2012 for diesel, and any substitution effect is done on an energy basis (a detailed description of the model, data, and assumptions is provided in the ESI†).

BEIOM estimates net employment impacts, defined as the difference in the number of annual full-time equivalent jobs under each scenario compared to the BAU, considering the employment effect in the relevant biofuel and petroleum sectors. Job effects account for both construction and operation in each year and are estimated at the national level. Net effects reflect reduced employment from conventional diesel production and the positive effect from the deployment and expansion of MCCI bio-blendstocks. Production volumes for each type of fuel and construction schedules are provided by BSM.

Scenario design

The ADOPT model estimates sales for diesel trucks as well as several alternative powertrains that have recently entered, or will soon enter, the market. In this analysis, battery electric trucks, fuel cell trucks, and hybrid electric trucks are introduced to the market in 2025. In the co-optimized scenarios, co-optimized trucks are introduced to the market in 2027.

Inputs to the ADOPT model for the co-optimized MCCI scenarios are shown in Table 1. The co-optimized cases were compared to a BAU case, in which co-optimized vehicles are not deployed to the market. Other advanced powertrains such as hybrid diesels, fuel cells, and battery electric vehicles (BEVs) are still deployed in the BAU case. In the BAU case, technology component price projections for battery costs and hydrogen storage costs were extrapolated from historical trends. These technology prices are referred to as the "low tech" assumptions. The "low tech" assumptions are used both in the BAU and the baseline co-optimized cases. In some of the sensitivity cases,

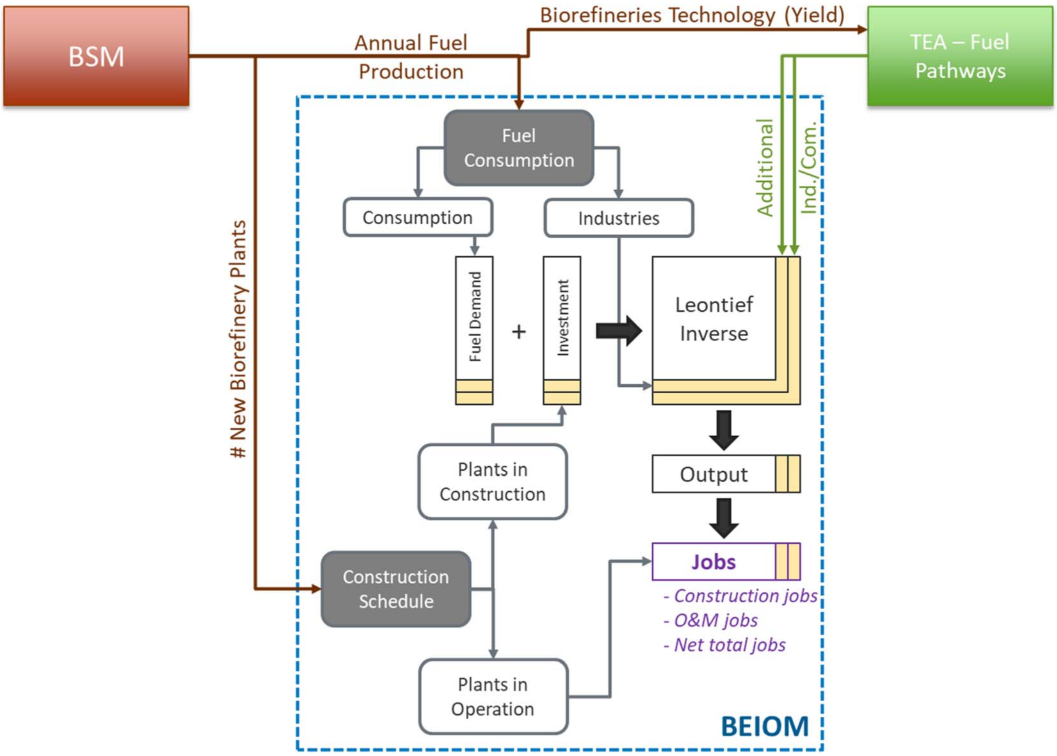

Fig. 2 Overview of BEIOM-BSM integration.

more optimistic price forecasts (referred to as the "tech success" assumptions) were assumed for these technology costs. The "tech success" assumptions represent faster declines in fuel cell and battery technology costs than have been achieved historically. Our assumptions on vehicle technologies and adoption decisions are in line with DOE estimates and methodologies available at the time the analysis was run, though we note that these have since been updated (See the ESI† for more information).[34]

The diesel fuel price projections used in this analysis were from the AEO reference case.[30] Due to uncertainty in the future prices of the co-optimized bio-blendstocks, we assumed that all bio-blendstocks were priced at the same rate as diesel on a $/gallon basis. This price parity could be achieved through the application of subsidies or, eventually, through economies of scale, or perhaps due to rises in diesel prices.[46] This paper does not focus on the market mechanisms that determine fuel prices. The incremental vehicle costs (costs over non-co-optimized vehicles) were assumed to be $100 to account for adding the DFI component. An incremental engine efficiency gain of 1% was applied for the polyoxymethylene dimethyl ether (POME) bio-blendstock cases only.[8,47] That is, engines powered by POME blends were assumed to see an incremental increase of 1% in engine efficiency over the engine efficiency of diesel engines. Engine efficiency gains for the other bio-blendstocks were assumed to be 0%, as estimates did not show a significant increase in engine efficiency for the remaining bio-blendstocks. Research conducted as part of the Co-Optima Consortium found that fuel changes had little or no impact on MCCI engine efficiency, except for improvement of emissions or operability, which were enabled by changes in fuel properties and composition.[8] POME, as an oxygenated bio-blendstock however shows a consistent engine efficiency gain of 1% relative to the baseline diesel engine.[8,43] POME has an extremely low-soot formation potential, which helps heat release into the later part of the expansion stroke in the engine, resulting in higher efficiency.

Using the BSM, we estimated the potential co-optimized fuel production levels, given the co-optimized vehicle fleet, techno-economic assumptions for biorefineries, and other assumptions and constraints in the model.

• Oil price is based on the reference case from the annual energy outlook,[30] and conventional diesel is supplied by the existing petroleum industry.[48]

• Conventional diesel prices do not respond to other market factors (*e.g.*, increase in biofuel production), since co-optimized fuel does not have a large share of the diesel market. Other market factors are usually regional and difficult to predict.

• Biorefineries only produce starch ethanol, cellulosic ethanol, biodiesel, hydro-processed esters, fatty acids, and the co-optimized bio-blendstock.

• The bio-blendstock is combined with petroleum diesel; excess supply is consumed by conventional diesel vehicles.

• Cellulosic feedstocks are supplied on the basis of demand, price, and availability.

• Initial feedstock prices are from the POLYSYS model;[49] prices change over time due to supply *versus* demand dynamics.

• Co-optimized vehicles are fuelled with regular diesel until the new MCCI fuel becomes available within a region.

A set of scenarios was developed to evaluate five different MCCI bio-blendstocks under various market conditions. These five bio-blendstocks were chosen from a list of screened MCCI bio-blendstocks that hold promise for being technically viable, cost-effective, environmentally advantageous, and potentially scalable.[9] We analyzed the potential deployment and benefits of oxygenated fuels, including polyoxymethylene dimethyl ether (POME) and alkoxy alkanoate ester ether (AAEE), which offer higher energy densities than fuels such as cellulosic ethanol. We also addressed non-oxygenated, renewable diesel blendstocks made through the hydroprocessed esters and fatty acids (HEFA) or hydrothermal liquefaction (HTL) processes, produced from forest residues, corn stover, swine manure, wastewater sludge, and fats, oils, and greases (FOG). These fuels represent a range of fuel properties such as energy content, oxygen content, and octane number as well as different production pathways that could ramp up the fuel production with a diversity of feedstocks and conversion technologies. Our scenarios consider the influence of factors that affect both vehicle purchasers and fuel producers. We explored variations in parameters related to MCCI fuel production, biorefinery buildout, vehicle cost of ownership, vehicle performance, taxes, policies, and market conditions. To examine the effects of these variables, we tracked model outputs of vehicle adoption, fuel production, energy consumption, GHG emissions, and net job creation from 2025 to 2050. We compare the results of individual scenarios to corresponding BAU cases that do not include co-optimized MCCI fuel and engine technologies.

We considered three deployment scenarios of co-optimized MCCI fuels and vehicles.

(1) We looked at less-mature fuel conversion technologies (POME, AAEE, and HTL) with promising characteristics.

(2) We considered a deployment scenario where an MCCI bio-blendstock at a higher technology readiness level (TRL) could be introduced to the market in the near term before transitioning to another MCCI bio-blendstock at a lower TRL in the longer term (after 5 years – HEFA transitioning to HTL). In this scenario, we could expect a possible expansion of production and market penetration of MCCI fuels and vehicles in earlier years of the simulation (currently, the ADOPT HD model does not include the capability to switch the co-optimized fuel source during the simulation, and so for these Scenario 2 runs, vehicle sales projections from the higher TRL fuel were used for all years).

(3) We considered how a nationwide policy framework that promotes the production and adoption of low-carbon RD fuels *via* offering national carbon credits (similar to California's LCFS) could further stimulate the adoption and deployment of co-optimized MCCI fuels.

Table 1 summarizes key assumptions about co-optimized vehicles, fuels, and policy in the three deployment scenarios and associated cases. Note that co-optimized vehicles are assumed to consume a blend fraction of 80% diesel fuel and 20% bio-blendstock. The blend fraction of bio-blendstock is limited to 20% to ensure a level of blending that the biomass available could support. Overall, this level of blending could lead to meaningful benefits without causing significant challenges to quickly ramping up infrastructure, biorefinery build-out, *etc.*, which is otherwise required. For details on the economic and emissions information associated with the production of various MCCI bio-blendstocks based on the feedstocks and conversion technologies used, refer to Gaspar *et al.*,[8] Bartling *et al.*,[9] and Ou *et al.*[10]

In each scenario, we consider a pessimistic case and an optimistic case as bounding cases where we vary certain assumptions and model as sensitivity cases (Table A3 in ESI†). In the pessimistic case, we lower the blending level of the MCCI bio-blendstock to 10%. We consider a higher incremental cost of adopting the co-optimized fuel and vehicle technologies, a 10% higher co-optimized fuel price relative to that of the incumbent diesel fuels, no carbon credits for the MCCI bio-blendstocks, a maximum number of 25 biorefineries to build each year without a guarantee to meet fuel demand, and a higher rate of return of biorefinery operations. We also consider greater success and progress in conventional vehicle technologies relative to the MCCI vehicles. In the optimistic case, we consider a blending level of 30%, greater reduction in after-treatment cost, 10% cheaper MCCI fuel price than petroleum diesel fuels, lower capital cost, and lower rate of return of biorefineries that could be built out without a limitation per year.

The aforementioned scenarios and associated cases do not consider a carbon tax. In addition to these cases, we consider an alternative set of cases where a carbon tax is levied. The taxes imposed are based on the vehicles' tailpipe diesel fuel emissions.

The tax level was set at a rate that would promote a smooth sales curve of co-optimized vehicles for some bio-blendstock scenarios (see the ESI†). The actual dollar amounts to achieve this goal are dependent on all other assumptions in the analysis, especially fuel price forecasts. It was not the intention to design policy, but rather to model a case under which co-optimized vehicles could be price competitive with conventional vehicles. The tax was applied as a price penalty—a dollar amount per ton of CO_2 emitted from the combustion of diesel fuel. Tailpipe emissions from the combustion of bio-blendstock fuels were not considered. Similarly, no penalty was applied for the consumption of hydrogen or electricity. A tax on diesel fuel alone promotes the consumption of fuel alternatives: alternatives that carry the potential to become lower emitting than conventional fuels over time.

Results and analysis

Co-optimized vehicle deployment assessment

Key variables in the ADOPT modeling that had a large effect on sales were the fuel cost projections used, the energy densities of fuels, the incremental vehicle cost, the engine efficiency gain, and the technology component costs. After running the baseline scenarios for the first time, under the assumption that a gallon of co-optimized fuel would be priced equally to a gallon of diesel in all years, we saw limited sales of co-optimized vehicles (Fig. 3). In the HD ADOPT model, fuel costs are quite influential to vehicle choice. Because all co-optimized bio-blendstocks

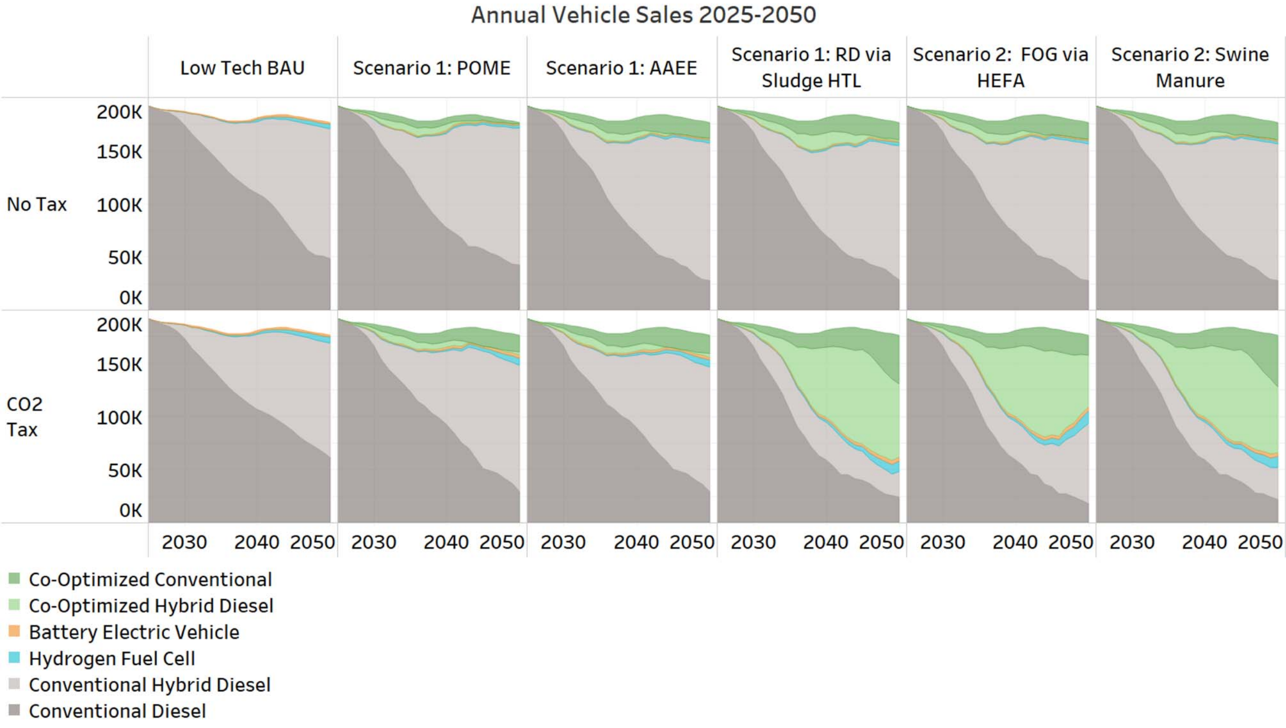

Fig. 3 New vehicle sales in the no carbon tax case and in the carbon tax case, 2025–2050.

considered have a lower energy density than diesel, lifetime fuel costs were higher for co-optimized vehicles than for non-co-optimized vehicles. A lower energy content per gallon at an equal price per gallon leads to a higher cost per unit of energy. The higher fuel costs could have been offset by aftertreatment cost savings, if those cost savings had been high enough. We found that the aftertreatment cost savings considered in this analysis, which ranged from \$4563 to \$4932, were not high enough to offset the higher fuel costs.

Scenarios for the higher energy density bio-blendstocks (HEFA and HTL) show higher co-optimized vehicle sales than those with lower energy densities, but overall market penetration was still low in all scenarios without the carbon tax. Knowing that fuel cost was the main barrier to the adoption of co-optimized vehicles, we ran an additional set of scenarios in which we penalized petroleum fuel usage by adding a carbon tax to diesel fuel prices.

We retained the assumption of price parity with diesel on a volumetric basis and implemented a carbon tax on diesel fuel. We chose to only place the carbon tax on diesel fuel, with the goal of reducing heavy-duty tailpipe emissions to show how such a policy could impact both vehicle adoption and biofuel production. If a holistic national carbon policy were implemented, it could also include a carbon tax on electric generators, impacting the fuel price for BEVs. The effect of this policy was to increase the sales prices of diesel fuel, allowing some co-optimized fuels to be price competitive with diesel on a \$/BTU basis, and incentivizing the sales of alternative-fueled vehicles.

The carbon tax on diesel fuel emissions promotes co-optimized vehicle sales in all cases, but the impact of the carbon tax is relative to the energy density of the bio-blendstock (Fig. 3). The greatest adoption benefit is seen for the fuels at the higher energy density range: RD *via* sludge HTL, HEFA *via* FOG, and RD *via* swine manure HTL. In these cases, the higher price of diesel fuel offsets the slight energy density loss from the bio-blendstock fraction of the fuel. Co-optimized vehicles are assumed to consume a blend fraction of 80% diesel fuel and 20% bio-blendstock. In the carbon tax scenarios, the 80% diesel blend fraction of the fuel is still taxed, but the 20% of co-optimized fuel consumption is not taxed, giving these vehicles an advantage over powertrains that consume 100% diesel fuel. An even greater benefit could be achieved for co-optimized fuels if the blend fraction of the bio-blendstock could be increased.

The carbon tax helps co-optimized vehicles compete with diesel powertrains only. BEVs and fuel cell vehicles (powertrains that consume no diesel fuel) are not affected by this carbon tax. Under the price and blend fraction assumptions in this analysis, for some of the lower energy density fuels there is no tax level at which co-optimized vehicles can outcompete both diesel and other alternative powertrains. If the tax level is set high enough to price-advantage co-optimized vehicles over 100% diesel vehicles, then it is also set too high for co-optimized vehicles to compete with BEVs and fuel cells (although a holistic carbon policy would also impact fuel prices for BEVs and fuel cells, depending on grid mix). In order to drive sales of vehicles powered by POME and AAEE, the prices of these fuels would need to be reduced to compensate for energy density differences, or the blend fraction would need to be increased and a carbon tax imposed at a high enough level.

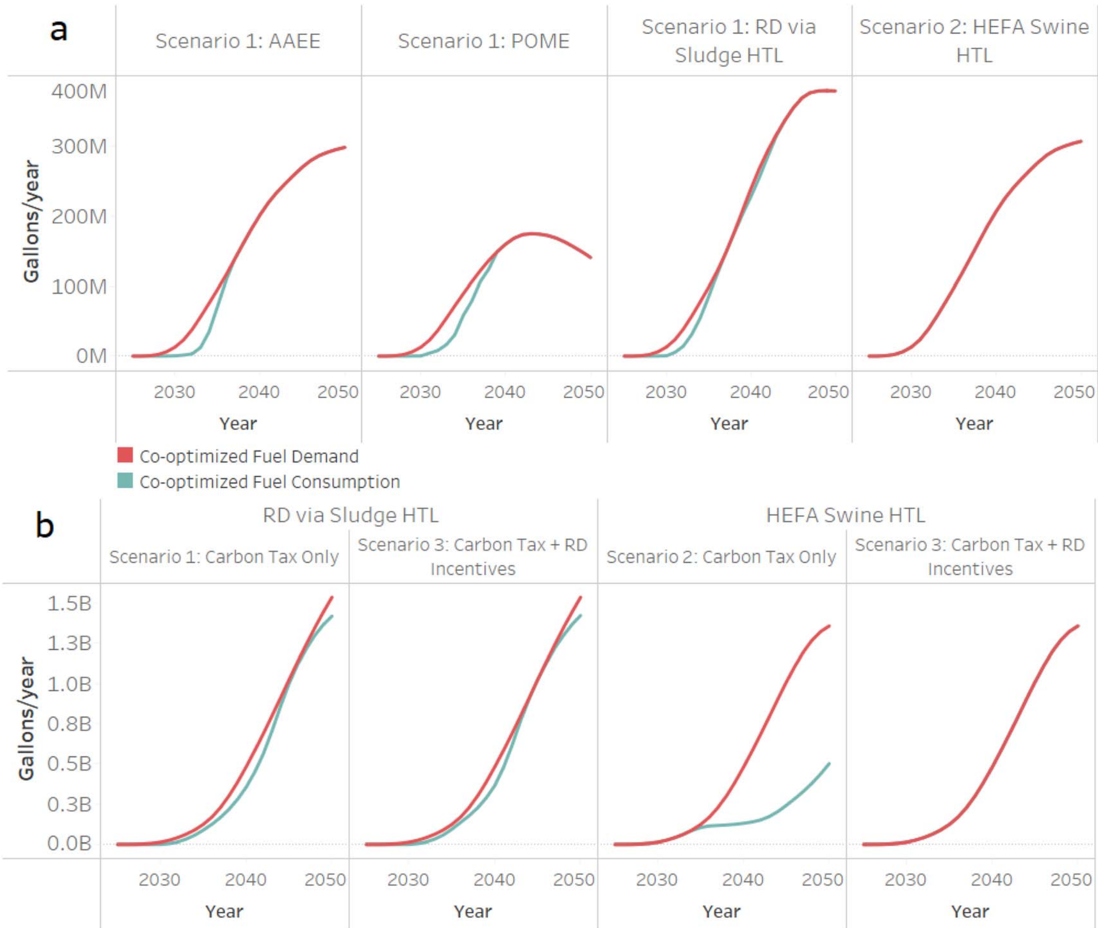

Fig. 4 Co-optimized fuel demand *versus* consumption (gallons per year) by co-optimized vehicles in the no carbon tax case (panel a) and in the carbon tax case, with and without additional renewable diesel incentives (panel b), 2020–2050. Note that HEFA swine HTL refers to HEFA transitioning to HTL.

Co-optimized fuel deployment assessment

With different levels of co-optimized vehicle adoption, there are corresponding relative levels of co-optimized fuel use. For BSM simulations, biorefineries are constructed to fill co-optimized HDV demand regardless of desired investment return to explore the potential benefits of co-optimized fuels and engines associated with ADOPT vehicle outputs. However, supply may not always equal demand due to high bio-blendstock prices, annual biorefinery construction limits, and lack of feedstock. In the cases where the bio-blendstock is produced using cellulosic feedstocks (POME and AAEE), there is an initial gap between co-optimized fuel demand and supply while the feedstock market is ramping up to meet the biofuel demand (Fig. 4a).

The initial gap is not as apparent or prolonged in the HEFA/swine HTL and HTL sludge cases, respectively, since these feedstocks already exist. As was discussed in the vehicle adoption results, cases with the HTL technology saw greater co-optimized vehicle deployment when there was a carbon tax applied. Fig. 4b shows these cases with and without availability of additional renewable diesel incentives. Co-optimized fuel production benefits from using a more mature technology in the early years. Since manure-to-HTL is a yet unproven technology, and dewatering costs have been estimated to be quite high, biorefineries are not built to meet demand unless there are additional incentives for the investors.[50] Sludge-to-HTL is also a nascent technology, so there is a lag in supply in the initial years, waiting for the economics to become more attractive through industrial learning. For POME and AAEE fuels, the additional incentives for renewable diesel decrease the risk of investing in these technologies, as the price for the fuel is competitive with conventional diesel; therefore, more biorefineries are built in the model, and there is additional production above what is needed as the bio-blendstock for the co-optimized fuel (Fig. 5). Once fuel demand for co-optimized vehicles is met, we assume this "extra" fuel is used by conventional vehicles, since the fuel would be compatible with existing diesel engines. Renewable diesel made through the HEFA process, for example is already being used in conventional diesel vehicles.

Environmental benefits assessment

Annual life-cycle petroleum consumption and GHG emissions for the HDV sector are tracked across several MCCI technology

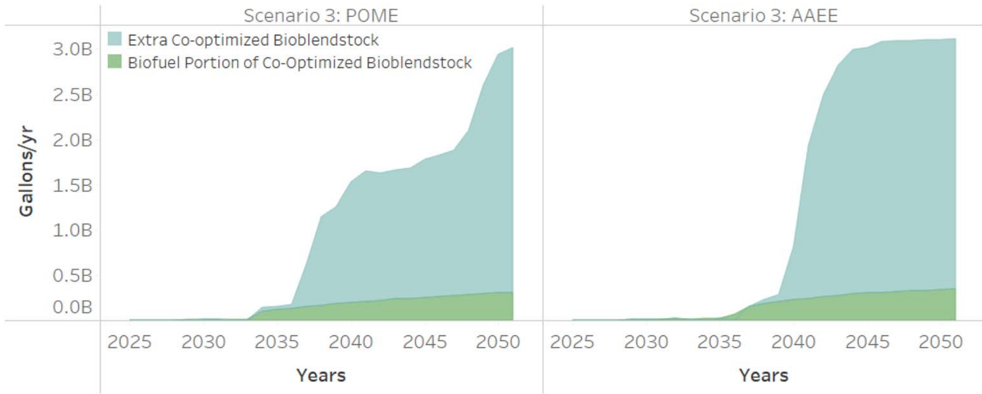

Fig. 5 Biofuel production (gallons per year) in the carbon tax case, with additional renewable diesel incentives representing both the bio-blendstock for co-optimized fuel and excess production, 2020–2050.

adoption scenarios, representing various future market conditions, technological adoption scenarios, MCCI bio-blendstocks, and other key variables. These scenarios are benchmarked against a hypothetical BAU case, derived from ADOPT/BSM, which forecast the evolution of the HDV sector absent the introduction of co-optimized fuels and technologies. This perspective contextualizes the relative environmental impacts and benefits of co-optimized MCCI fuels and vehicles and provides a broad-based understanding of the sustainability value-proposition of co-optimized heavy-duty technology.

Energy benefits assessment. We estimate the energy and environmental benefits for the deployment scenarios (see Table 1) of co-optimized MCCI fuels and vehicles. As stated earlier, the FOG HEFA transitioning to swine manure HTL will be referred to as HEFA swine HTL. Scenarios account for the decarbonizing grid for the simulation period as defined in the GREET model.[30]

No carbon tax case. Fig. 6 shows the annual sector-wide life-cycle petroleum energy consumption between the BAU and the four co-optimized MCCI fuels. The reduction in the life-cycle petroleum energy consumption over time in the BAU case can be attributed to increased vehicle fuel economy of conventional HDVs and the replacement of conventional diesel vehicles with more efficient hybrid electric vehicles (HEVs) and, to a lesser extent, with battery electric vehicles (BEVs) and fuel cell vehicles (FCVs). In the AAEE, HEFA swine HTL, and sludge HTL cases, life-cycle petroleum fuel consumption is reduced primarily by reducing diesel fuel consumption as the fleet turns over to co-optimized vehicles. Co-optimized vehicles account for 4–9% of HDV vehicle stock and 4–11% of HDV travel demand in 2050 across all cases, resulting in a 325 693 TJ reduction in the life-cycle petroleum energy consumption in the AAEE case relative to the BAU case (see Table 2). As shown earlier in Fig. 5, the POME and AAEE cases see excess production of MCCI fuels above the demand from co-optimized vehicles. This excess production of MCCI fuels is assumed to be consumed by conventional diesel vehicles and to displace conventional petroleum fuel. The excess production is, however, more profound in the AAEE case compared to POME (Table 2). In the HEFA swine HTL case, the small petroleum energy reductions reflect the insignificant market penetration of the co-optimized MCCI fuel in 2050.

With carbon tax case. In the carbon tax case, a proxy for optimistic adoption of co-optimized vehicles and fuels, introducing a carbon tax (on fossil CO_2 emissions) results in a slight increase in the adoption of BEVs and FCVs in the BAU and the co-optimized scenarios (most notably in the HEFA swine and sludge

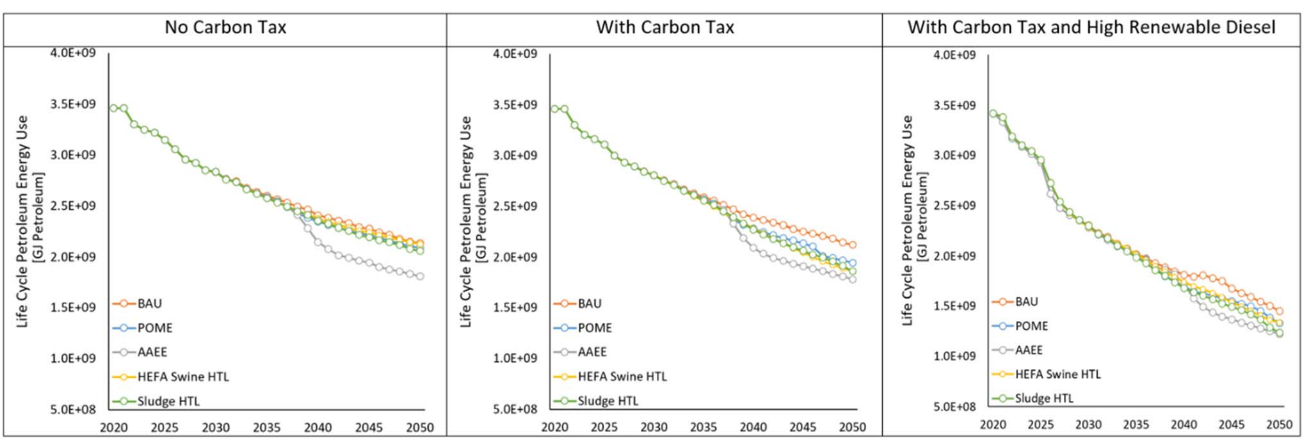

Fig. 6 Life-cycle petroleum energy consumption of BAU and co-optimized scenarios.

Table 2 Reduction in life-cycle petroleum energy consumption across all cases in 2050

Cases	No carbon tax: Co-optimized share of HDV stock in 2050 (%)	No carbon tax: Co-optimized share of HDV travel demand in 2050 (%)	No carbon tax: Reduction in life cycle petroleum energy consumption (TJ)	With carbon tax: Co-optimized share of HDV stock in 2050 (%)	With carbon tax: Co-optimized share of HDV travel demand in 2050 (%)	With carbon tax: Reduction in life cycle petroleum energy consumption (TJ)	With carbon tax and high RD: Co-optimized share of HDV stock in 2050 (%)	With carbon tax and high RD: Co-optimized share of HDV travel demand in 2050 (%)	With carbon tax and high RD: Reduction in life cycle petroleum energy consumption (TJ)
BAU	—	—	—	—	—	—	—	—	667 486 (due to RD)
POME	4	4	50 243	7	8	174 726	7	8	121 125
AAEE	7	8	325 693	8	9	338 088	8	9	231 019
HEFA swine HTL	8	9	8639	31	38	257 250	31	38	119 974
Sludge HTL	9	11	76 193	35	45	255 590	35	45	216 045

HTL scenarios). The share of co-optimized vehicles in the HDV vehicle stock also increased. With co-optimized vehicles accounting for 8–45% of total HDV travel in 2050, the reduction in the life-cycle petroleum energy consumption increased across all scenarios (as shown in Table 2). In all the MCCI fuel cases, the increased fleet turnover to co-optimized conventional and co-optimized HEVs reduced the sales of conventional diesel vehicles; however, this effect was more significant in the HEFA swine and sludge HTL cases. In addition, as the blend level is held constant (20% by volume) across cases, differences in the level of co-optimized vehicle adoption for POME, AAEE, HEFA swine, and sludge HTL is attributed to variations in the fuel energy density relative to diesel. POME and AAEE have 38% and 15% lower energy densities, respectively, than diesel; while the energy densities of swine and sludge HTL are 3% and 2% lower than diesel, respectively. HEFA swine and sludge HTL waste fuels have energy densities that are more comparable to diesel. As a result, a carbon tax can compensate for the higher fuel cost due to extra fuel purchased for miles traveled. However, POME and AAEE-fueled powertrains require a higher carbon tax on diesel emissions to compete with conventional diesel powertrains due to their low energy densities. These results suggest that policies such as a carbon tax could help sell waste-derived fuels that are energy-dense. Nevertheless, surplus POME/AAEE production above what is needed by the co-optimized vehicles drives the significant reduction in the life-cycle petroleum energy consumption despite low adoption of co-optimized vehicles in the POME/AAEE scenarios because of their more attractive nth-plant economics.

With carbon tax and high RD case. In addition to the carbon tax, both the BAU and the Co-Optima scenarios experienced high penetration of renewable diesel with the introduction of RD-focused incentives (as shown in Table 1). These scenarios were completed in the BSM using the carbon tax case from ADOPT. The high penetration of RD reduced the life-cycle petroleum energy consumption in the BAU by 667 486 TJ (31%) compared to the level with carbon tax only. In the POME and AAEE cases, the life-cycle petroleum energy consumption decreased by 121 125 TJ and 231 019 TJ compared to BAU with carbon tax and high RD in 2050 due to high penetration of POME/AAEE. In the HEFA swine HTL and sludge HTL cases, the life-cycle petroleum energy consumption decreased by ~8% (119 974 TJ) and 15% (216 045 TJ), respectively. These reductions can be attributed to decreased diesel fuel consumption as a result of an increased market share of co-optimized vehicles/fuels. Co-optimized fuels make up ~8% of 2050 energy demand in the swine manure HTL and Sludge HTL cases (Table 3). In general, when RD incentives come into play, the overall larger penetration of biofuels onto the market pushes the life cycle petroleum energy use down.

Life-cycle GHG emissions benefits assessment

No carbon tax case. Fig. 7 shows the life-cycle GHG emissions for the BAU and the co-optimized scenarios in the MCCI adoption cases. In the absence of a carbon tax, BAU GHG emissions decline from 2020 to 2050. Increased sales of more

Table 3 Fuel share by fuel type (energy basis) in 2050

	No carbon tax					With carbon tax					With carbon tax and high RD				
	BAU (%)	POME (%)	AAEE (%)	HEFA swine HTL (%)	Sludge HTL (%)	BAU (%)	POME (%)	AAEE (%)	HEFA swine HTL (%)	Sludge HTL (%)	BAU (%)	POME (%)	AAEE (%)	HEFA swine HTL (%)	Sludge HTL (%)
Diesel blendstock	81.3	79.2	68.3	81.1	78.7	80.9	74.2	67.7	72.2	72.2	55.9	50.6	46.3	51.8	48.1
Biodiesel	10.2	10.7	10.4	10.3	10.3	11.8	12	11.9	15.8	12.3	16.7	16.9	16.5	15.2	17.5
RD	7.8	6.7	7.1	6.6	7.9	6.5	5.4	5.3	7.7	6.4	26.7	21.5	21.7	24.2	25.3
Electricity	0.4	0.3	0.3	0.3	0.3	0.5	0.52	0.51	0.7	0.7	0.5	0.5	0.5	0.8	0.7
Hydrogen	0.2	0.2	0.2	0.2	0.2	0.3	0.3	0.3	0.5	0.42	0.3	0.3	0.3	0.5	0.42
POME		3.0					7.6					10			
AAEE			13.8					14.2					14.7		
Swine manure HTL				1.6					3.1					7.5	
Sludge HTL					2.6					7.9					8.1

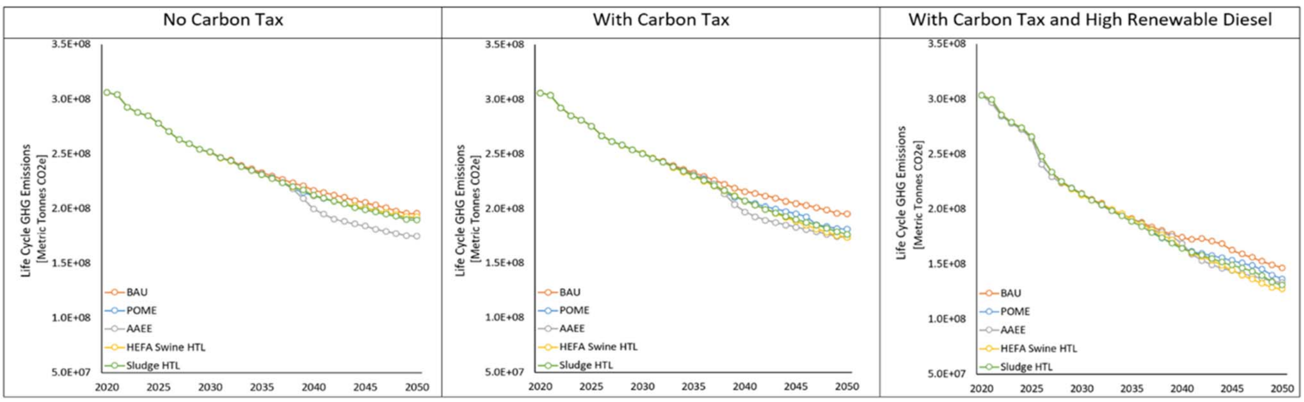

Fig. 7 Life-cycle GHG emissions of BAU and co-optimized scenarios.

efficient diesel HEVs, BEVs, and FCVs underline this trend. About 35% of conventional diesel trucks are replaced by more efficient HEVs (33%), BEVs (1%), and FCEVs (1%) in 2050. The adoption of these efficient vehicles cuts diesel consumption and the associated emissions. Compared to the BAU, the POME, AAEE, HEFA swine HTL, and sludge HTL cases show emissions reduction of 4.2, 21, 3.2 and 6.1 million metric tons, representing ∼2%, ∼11%, ∼2%, and 3% GHG emissions reduction in 2050, respectively. The small GHG emissions reduction across most of the cases is tied to the relatively low adoption of co-optimized powertrains and fuels. POME only accounts for 3% (energy basis), swine HTL 1.6%, and sludge HTL 2.6% of the HDV fuel market in 2050 (Table 3). In the AAEE scenario, however, the displacement of petroleum diesel consumed by conventional vehicles with excess AAEE produced drives the higher reduction in emissions. Investment and proliferation of AAEE fuel drive down costs of producing the fuel and makes it economically viable to have excess production to displace some of the conventional diesel demand.

With carbon tax case. The emissions reduction in the BAU with carbon tax case follows the same trend as in the no carbon tax case. In the co-optimized scenarios, the carbon tax increased the adoption of co-optimized HEV significantly with waste-derived fuels (swine manure HTL and sludge HTL) but not for POME or AAEE despite their significant emission reductions relative to petroleum diesel per MJ of the fuel. Although the addition of a carbon tax produces no significant impact on the adoption of co-optimized vehicles in the POME and AAEE cases, the excess production of POME/AAEE consumed by the conventional vehicles results in 7.2% (14 million metric tons) and 11% (22 million metric tons) emission reductions, relative to the BAU with carbon tax. Emissions reduction reaches about 21 million metric tons in the HEFA swine HTL case (11% reduction relative to the BAU with carbon tax) and 19 million metric tons in the sludge HTL case (10% reduction relative to the BAU with carbon tax) in 2050. However, only 4.4% of the benefit in the HEFA swine HTL case can be ascribed to co-optimized fuels (given 3.1% market penetration on an energy basis in 2050 and >100% lower GHG intensity relative to diesel). The remaining benefit can be attributed to the increased biodiesel and RD consumption and partly to increased fuel cell and BEV adoption, as reflected in Table 3. Biodiesel and RD play a larger role in this case due to the carbon tax placed on diesel. In addition, 2% of this benefit is associated with the difference

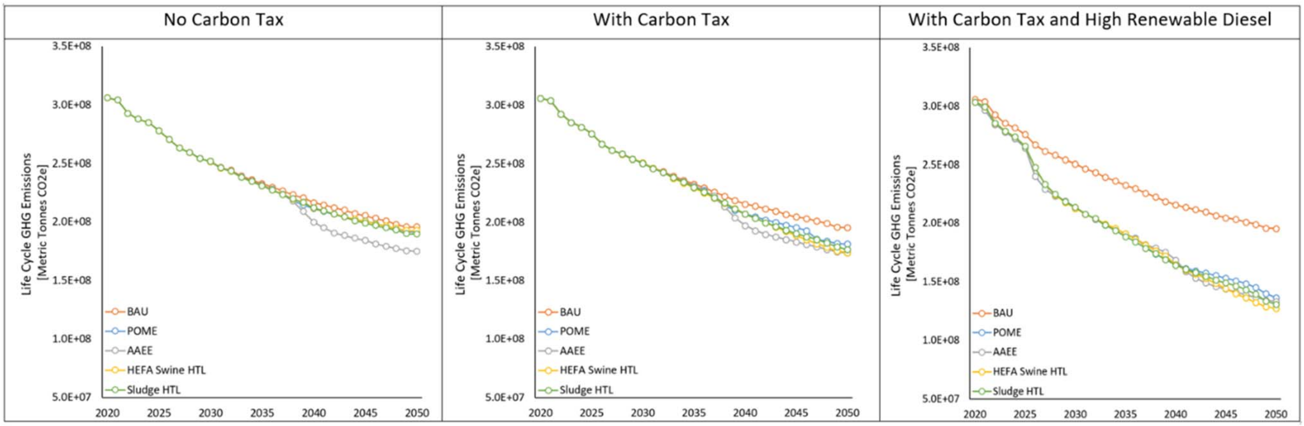

Fig. 8 Life-cycle GHG emissions of BAU and co-optimized scenarios. In this figure, the BAU in the case with carbon tax and high renewable diesel has no low-carbon RD fuels *via* offering national carbon credits.

in the final energy demand between the BAU with carbon tax and HEFA swine HTL case.

With carbon tax and high renewable diesel case. The high penetration of RD in the BAU reduced the GHG emissions by 49 million metric tons (25%) compared to the level with carbon tax only. In the co-optimized scenarios, POME and AAEE reduce GHG emissions by 10 million metric tons (7% decrease relative to BAU with carbon tax and high RD) and 13 million metric tons (or 9% decrease in emissions), respectively. The HEFA swine HTL and sludge HTL cases reduce GHG emissions by 13% (19

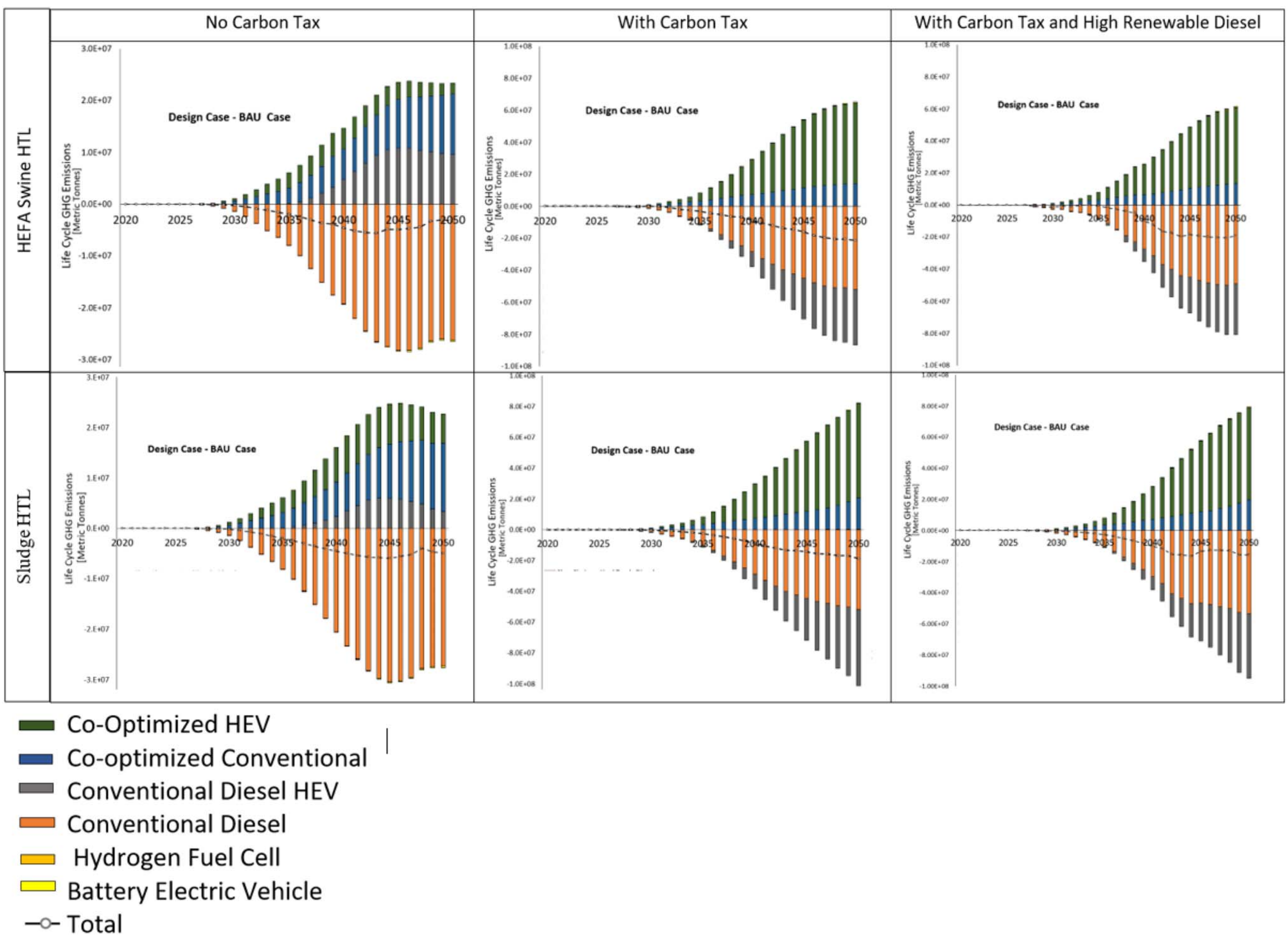

Fig. 9 Environmental impacts by vehicle–fuel pair in the HEFA swine HTL and sludge HTL scenarios.

million metric tons) and ~11% (16 million metric tons) in 2050, relative to the BAU with carbon tax and high RD. The higher GHG emissions benefit in the HEFA swine HTL scenario is primarily driven by the lower GHG intensity of RD from swine HTL relative to diesel (>100% lower GHG intensity due to avoided emissions from management of swine manure if not used for RD production[10]) given 7.5% HEFA swine HTL market penetration on an energy basis in 2050.

However, comparing the co-optimized scenarios with carbon tax and high RD against the BAU with carbon tax only (*i.e.*, BAU case with no low-carbon RD fuels *via* offering national carbon credits) will result in more significant emission reductions across all scenarios (Fig. 8). Emissions reduction could reach ~30%, 32%, ~35%, and 33% in the POME, AAEE, HEFA swine HTL, and sludge HTL MCCI fuel cases, respectively. This reflects the significant combined benefits of high RD penetration and co-optimized technologies adoption by displacing conventional powertrains that largely consume fossil fuels.

Fig. 9 illustrates the environmental impacts by vehicle–fuel pair in the HEFA swine HTL and sludge HTL cases. The no carbon tax case shows fleet turnover from conventional diesel ICEVs and BEVs to co-optimized conventional and HEVs as well as an increase in conventional HEVs. With the carbon tax, there is significant fleet turnover from conventional diesel HEVs and ICEVs to the co-optimized HEVs and co-optimized conventional and a slight increase in BEV and FCVs sales. In addition to major fleet turnover to co-optimized vehicles, decreasing diesel consumption results in substantial GHG emissions reduction with a carbon tax and high renewable diesel as policies such as a carbon tax and nationwide LCFS help ramp up MCCI renewable diesel fuels/vehicles. We highlighted these two scenarios because they showed higher adoption of co-optimized vehicles compared to POME and AAEE cases.

Job and economic impacts assessment

The net job effects, defined as the difference in jobs between a baseline without MCCI bio-blendstocks and a scenario with MCCI bio-blendstocks, are shown in Fig. 10 for three scenarios, *i.e.*, (1) no carbon tax, (2) with carbon tax, and (3) with carbon tax and high renewable diesel production. These results account for job gains or losses due to change in production in the entire diesel market which includes conventional diesel; MCCI bio-blendstock; biodiesel from soy oil, FOG, and DCO; and renewable diesel *via* HEFA from soy oil, FOG, and DCO. The results consider both temporary construction jobs from biorefineries and permanent operation and maintenance (O&M) jobs for a given year from 2020 to 2051 (for a breakdown, see the ESI†). The year 2051 was chosen instead of 2050 to portray the lasting economic impacts of the biorefineries, *i.e.*, the effect of biorefinery O&M alone, because it is the only year in which there are no temporary construction impacts.

The production dynamics in the diesel market simulated by BSM is shown in Fig. 11, which highlights the difference between scenarios and the penetration of MCCI bio-blendstocks in each simulation. While AAEE has the largest penetration in the market by 2051 (producing 3.1 billion gallons per year in the with carbon tax and high renewable diesel scenario), HTL bio-blendstocks have the smallest, with only 0.9 billion gallons per year from HEFA swine in the same year. The key similarities are (1) the penetration of co-optimized bio-blendstocks is relatively small under all scenarios, and (2) among the different co-optimized blendstocks, AAEE's penetration is most noticeable followed by POME. The main differences are (1) total fuel consumption appears higher under the carbon tax + renewable diesel scenario when compared to that under the other two scenarios. (2) While AAEE and POME have higher penetration, the increased use of these two bio-blendstocks leads to higher total energy consumption when compared to other blendstocks.

Fig. 12 shows the absolute or gross job impacts due to construction of a single MCCI bio-blendstock biorefinery (see facility sizes in Table A1 in ESI†) and its operation and maintenance (O&M). The higher O&M jobs for biorefineries in comparison to petroleum refineries reflect the fact that biorefinery production and collection of feedstocks tend to be more labor-intensive than crude oil extraction and petroleum refineries, which are mature industries and operate at higher economies of scale than biorefineries, resulting in fewer jobs per gallon produced.

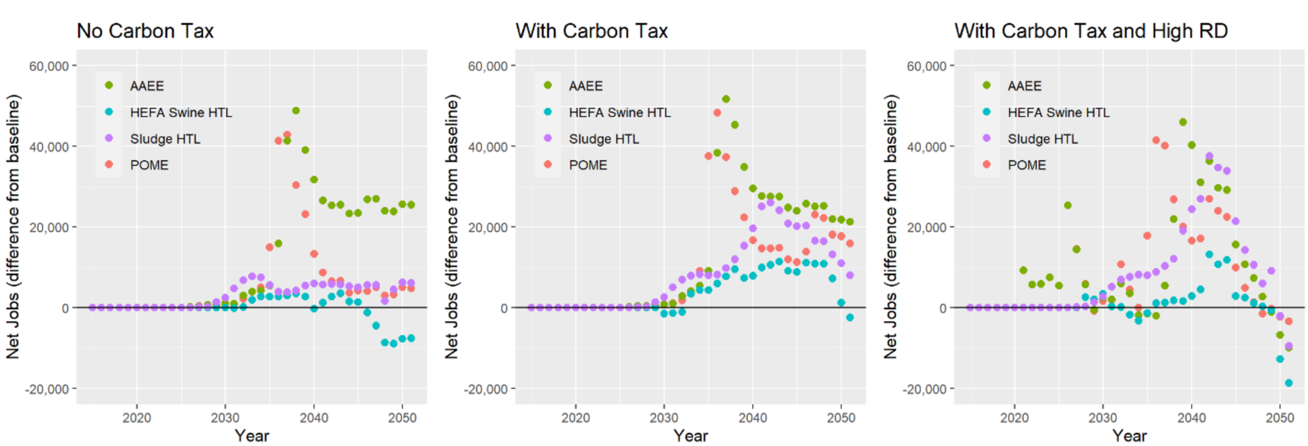

Fig. 10 Net jobs (FTE) by MCCI bio-blendstock, diesel market.

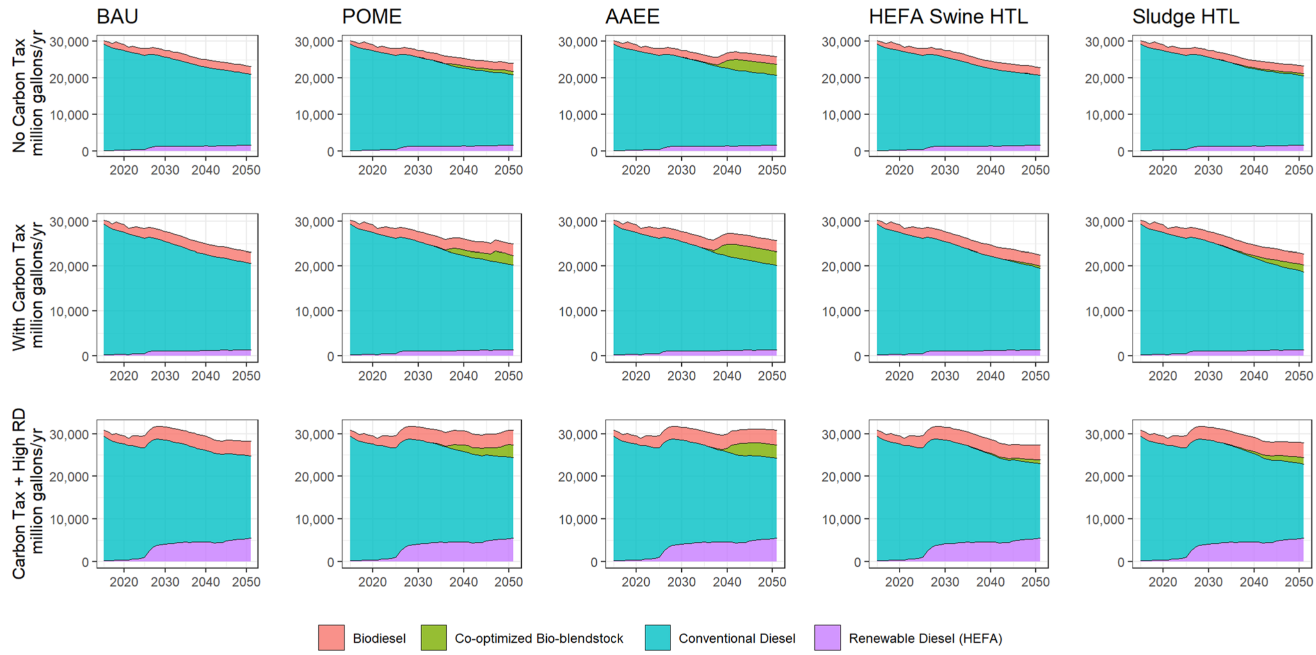

Fig. 11 Diesel market production volumes by MCCI bio-blendstock and scenario.

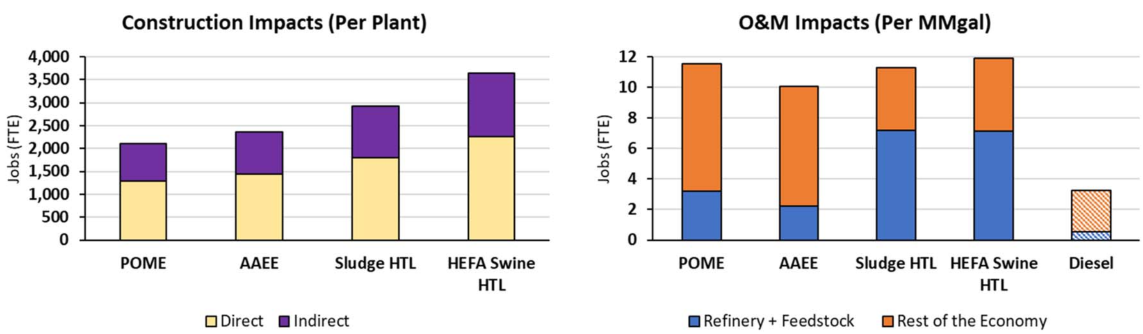

Fig. 12 Construction and O&M job impacts (FTE).

The net results for the POME bio-blendstock are mainly driven by the difference between job creation from the biofuel production, feedstock (woody biomass), and its supply chain (particularly supporting activities for agriculture), and job losses from conventional diesel production, renewable diesel from soybean oil and their related supply chains. In the no carbon tax scenario, by 2051 there is a net gain of around 4600 jobs with renewable diesel from soybean oil driving job losses as it accounts for most of the 15% decline in renewable diesel production observed in this scenario compared to the BAU (Fig. 13). In the carbon tax scenario, we estimate a net increase of around 16 000 jobs by 2051 despite a sharper decline in conventional diesel and renewable diesel production. The main driving factor behind this is the lower overall production volume of renewable diesel; although the production declines more than 15%, the reduction in production volume is not as large as in the carbon tax scenario. In the carbon tax and high renewable diesel scenarios, the higher production volumes for renewable diesel combined with a decline of more than 20% by 2051 relative to the baseline resulted in a net loss of 3500 jobs in that year.

The net job effects for the AAEE bio-blendstock are driven mainly by the same industries highlighted in the POME case, except for the biofuel feedstock (in this case, corn stover). Despite the lower O&M jobs per gallon in relation to POME (Fig. 12), the higher penetration of AAEE in the no carbon tax and with carbon tax scenarios (Fig. 11) leads to higher increase in net jobs. In the no carbon tax scenario, by 2051 there is a net gain of around 25 400 jobs with renewable diesel from soybean oil driving the losses as it accounts for most of the 10% decline in renewable diesel production observed in this scenario (Fig. 14). In the carbon tax scenario, by 2051 there is an increase in net gains of approximately 21 200 jobs despite a sharper decline in conventional diesel production and renewable diesel. In the carbon tax and high renewable diesel scenario, two contributing factors lead to a net loss of almost 10 000 jobs in 2051: (1) the higher overall production volumes for renewable diesel in this scenario in

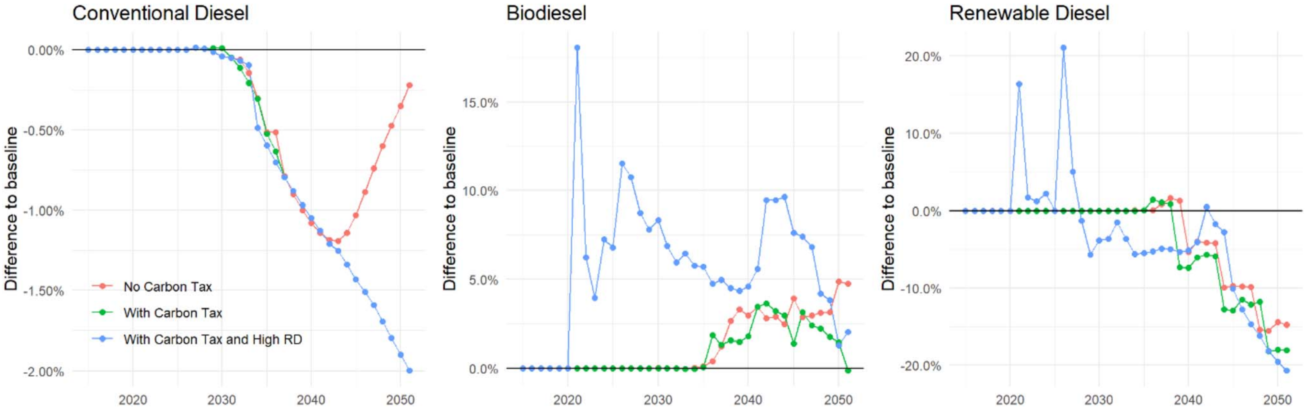

Fig. 13 Difference in production volumes by fuel, POME.

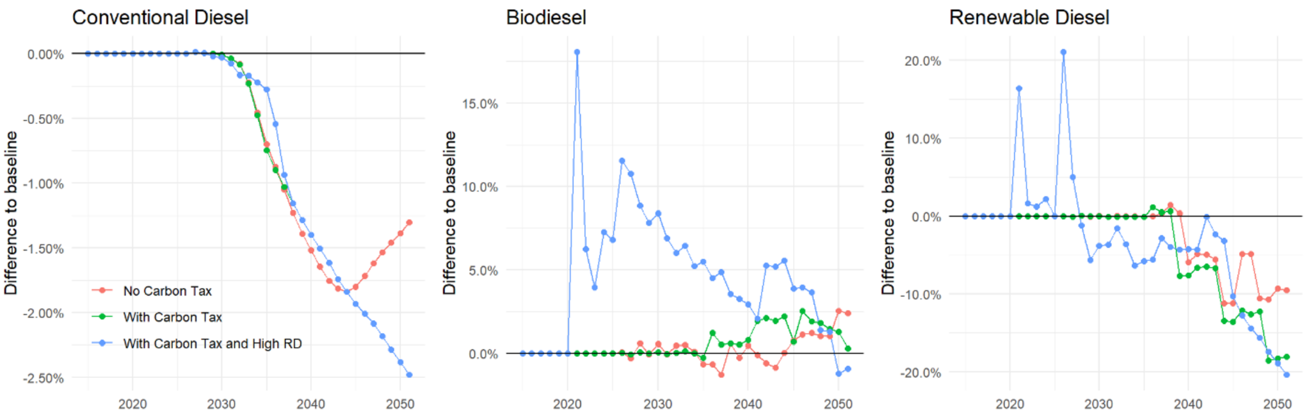

Fig. 14 Difference in production volumes by fuel, AAEE.

relation to the previous ones (Fig. 11) combined with a decline of about 20% (Fig. 14), and (2) a drop of 1% in biodiesel production.

Both HTL bio-blendstocks offer the smallest job increase in comparison to POME and AAEE bio-blendstocks because of higher reductions in conventional diesel production in these scenarios. Due to higher penetration of sludge HTL relative to HEFA swine HTL, the former shows net job gains in the no carbon tax and carbon tax scenarios by 2051, while the latter results in job losses throughout all scenarios. Jobs supported by lower production volumes of HTL bio-blendstocks barely offset the job losses from conventional diesel, biodiesel and renewable diesel in the scenarios (Fig. 15 and 16). Annual production in the carbon tax and high renewable diesel scenario only

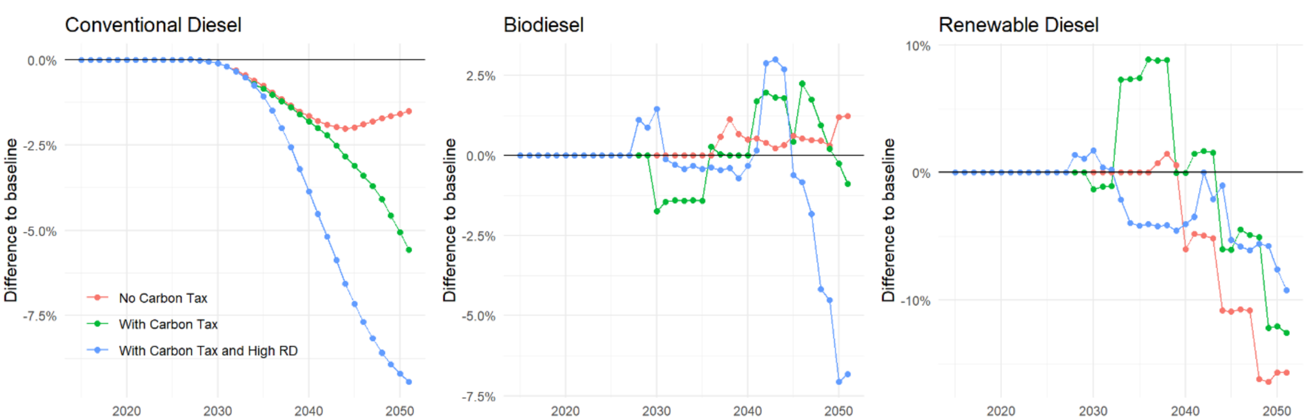

Fig. 15 Difference in production volumes by fuel, HEFA swine HTL.

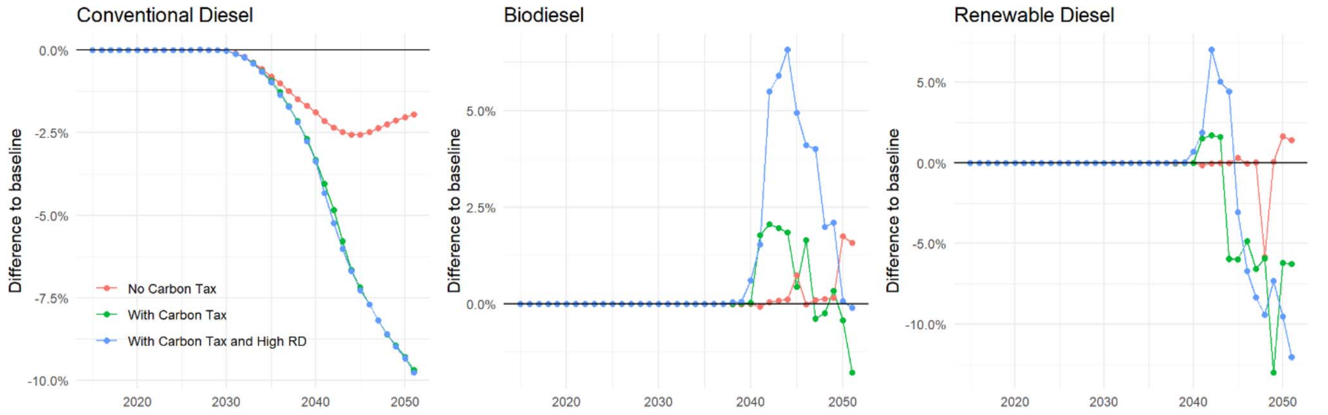

Fig. 16 Difference in production volumes by fuel, sludge HTL.

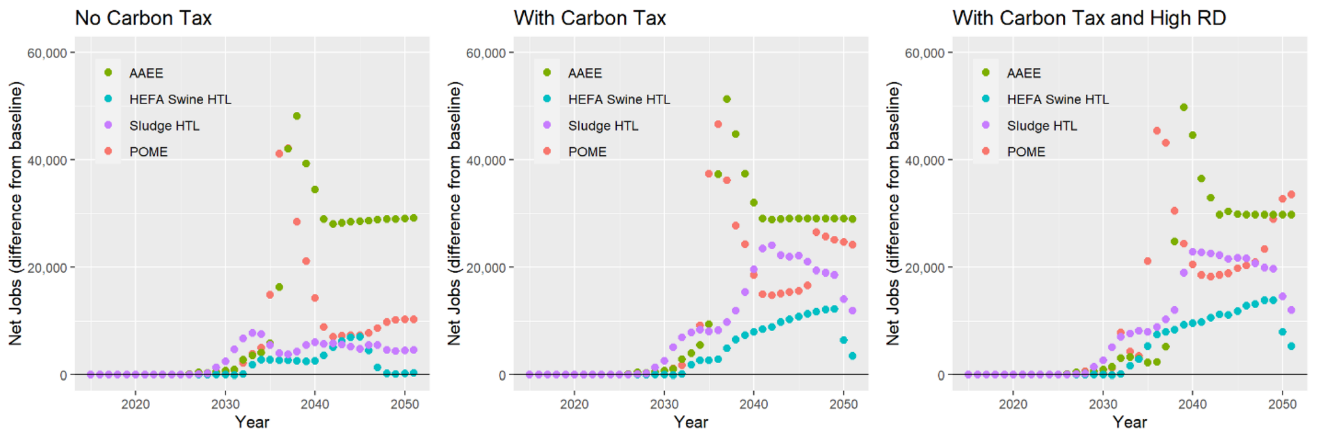

Fig. 17 Net jobs (FTE) by MCCI bio-blendstock, conventional diesel *vs.* bio-blendstock.

reaches 0.9 billion gallons for HEFA swine HTL and 1.5 billion gallons for sludge HTL.

Additional net results were calculated by only accounting for job gains from the MCCI bio-blendstocks and job losses from conventional diesel production (Fig. 17). Without considering the losses from renewable diesel production, gains in net jobs increase or net losses decrease across all scenarios and bio-blendstocks. Scenarios for HTL bio-blendstocks also show net job gains.

Although BEIOM accounts for changes in productivity for co-optimized biorefineries and fuel substitution over time, the production function (technology) of other sectors of the economy is assumed constant throughout the simulation. Additionally, the model also assumes fixed average import shares across sectors, to avoid the uncertainty of assuming any future global trade patterns or increased/reduced domestic supply chains in the U.S. Hence, the previous results show a conservative estimate of indirect net jobs. Also note that due to current data limitations in BEIOM, the job metric does not reflect which types of occupations were created/displaced; therefore, we cannot infer the distributional impacts of such changes. In future analyses, constant technology assumptions will be relaxed by using a non-linear input–output framework, and occupational characteristics such as job types and wages will be added to results.

Conclusions and discussion

This study has highlighted the potential of and barriers to co-optimized vehicles adoption and scaling up MCCI bio-blendstocks and could be adapted for other liquid fuel markets. The low energy density of some MCCI bio-blendstocks (especially POME/AAEE) is a key factor in their lack of competitiveness with petroleum diesel. Diesel replacement with POME/AAEE will result in higher cost per unit energy. With bio-blendstocks made from HEFA swine HTL and sludge HTL, this effect is minimal. Co-optimizing fuels and MCCI engines reduce life-cycle petroleum consumption and GHG emissions from the heavy-duty sector. However, the analysis shows that the contribution of various MCCI bio-blendstocks to reducing life cycle GHG emissions varies based on the energy densities and carbon intensities of fuels relative to petroleum diesel. MCCI bio-blendstocks *via* HEFA swine HTL and sludge HTL offer greater benefits because of equivalent energy densities and lower carbon intensities than petroleum diesel. Although POME and AAEE have lower carbon intensities than petroleum diesel, their energy densities are a barrier to co-optimized vehicle adoption. In all cases, rapid deployment of co-optimized fuels could be delayed due to feedstock availability, fuel price, investment costs, and construction constraints.

Of the different fuel options we considered, a carbon tax was most effective at accelerating the adoption of fuels with energy densities comparable to petroleum diesel. Without meeting this key fuel property threshold, increased cost per distance traveled outweighed the benefits of a carbon tax. In addition, when incentives are in place that dramatically expand RD production and use, life-cycle GHG emissions and petroleum consumption exhibit the greatest decline among the scenarios we considered. These policies should be viewed as examples for how incentives could make new technology more attractive than incumbent technology and not as a specific recommendation for policy intervention.

Jobs in the energy sector benefited slightly from increasing production of bio-based fuels co-optimized for use in MCCI engines. The long-term economy-wide net economic impacts of introducing MCCI bio-blendstocks are positive when compared to the displacement of conventional diesel, with POME and AAEE generating the largest economic gains (10–33 k FTE per year), and HTL bio-blendstocks marginally compensating for job losses in the conventional diesel industry due to their reduced market penetration (0.2–12 k FTE per year). However, when accounting for the dynamics of the entire diesel market (including renewable diesel production), both non-carbon tax and carbon tax scenarios lead to smaller positive net jobs for POME and AAEE (5–25 k FTE per year) as well as sludge HTL (6–8 k FTE per year), while HEFA swine HTL bio-blendstock is the worst performer, resulting in job losses in all scenarios (unable to compensate for reduction in jobs in the renewable diesel industry). In terms of short-term economic impacts from construction, additional annual jobs during peak building years varied between 8 and 49 k FTE depending on the MCCI bio-blendstock (with POME/AAEE showing the highest impacts).

In the current analysis, co-optimized fuels are restricted to a 20% blend level, which limits their capacity for GHG emissions reductions. Greater benefit could be achieved for co-optimized fuels if the blend fraction of the bio-blendstock could be increased. It is important to note that the findings from this study hold under the assumption that MCCI fuels could achieve cost parity (on a volume basis) with diesel. In addition, the deployment of co-optimized vehicles require multiple major technological breakthroughs including: (1) cost of biofuels can achieve cost parity with fossil fuels—something that has yet to materialize in the market and requires further research and development, (2) DFI cost is limited to \$100 which could be optimistic, (3) competition of limited biomass resources across sectors, *e.g.*, heavy-duty *vs.* aviation/marine sectors and potential breakthrough and adoption of electrification technologies in the heavy-duty sector.

One driver for Co-Optima's research on MCCI bio-blendstocks is to identify options to reduce the GHG footprint of MD/HD transportation. The weight and operational patterns of trucks pose additional challenges to the electrification of these vehicles, and they are expected to run on liquid fuel for a longer period. More sustainable, low-emission, vehicles such as those considered in this study will play an important role in reducing GHG emissions during that transition. Co-optimized MCCI fuels and engines can act as an effective bridge between conventional petroleum-fueled vehicles and a future fleet with increased electric trucks and can complement future heavy-duty electrification to reduce emissions beyond what electrification alone can achieve, supporting the national transition to a net-zero-carbon-emissions transportation system.

Author contributions

Doris Oke: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft, writing – review and editing, visualization; Lauren Sittler: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft, writing – review and editing, visualization; Hao Cai: conceptualization, methodology, software, validation, data curation, writing – original draft, writing – review and editing; visualization; Andre Avelino: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft, writing – review and editing, visualization; Emily Newes: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft, writing – review and editing, visualization; George G. Zaimes: conceptualization, methodology, software, writing – review and editing; Yimin Zhang: conceptualization, methodology, software, validation, formal analysis, data curation, writing – original draft, writing – review and editing, visualization; Longwen Ou: conceptualization, methodology, writing – review, and editing; Avantika Singh: conceptualization, project administration, funding acquisition; Jennifer Dunn: conceptualization, writing – review and editing, supervision, project administration, funding acquisition; Troy R. Hawkins: conceptualization, methodology, validation, writing – original draft, writing – review and editing, visualization, supervision, project administration, funding acquisition.

Conflicts of interest

The authors declare no conflict of interest.

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