Supporting Information for Potential Adoption and Benefits of Co-optimized Multimode Engines and Fuels for U.S. Light-duty Vehicles

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Definitions of Acronyms Used in Figure 1

ADOPT: Automotive Deployment Options Projection Tool

GREET: Greenhouse gases, Regulated Emissions, and Energy use in Transportation

Bioeconomy AGE: Bioeconomy Air Emissions, Greenhouse Gas Emissions, and Energy Consumption

BSM: Bioenergy Scenario Model

EIA: Energy Information Administration

FASTSim: The Future Automotive Systems Technology Simulator

BTS: Bureau of Transportation Statistics

BLM: Biomass Logistics Model

USDA: United States Department of Agriculture

BT16: Billion-Ton 2016

NREL: National Renewable Energy Laboratory

POLYSYS: Policy Analysis System Model

Additional Information on Multimode Engine Efficiency Improvement

Table S1. Blending properties* of co-optimized fuels

Bioblendstock	Blending Vol. (%)	Blending Motor Octane Rating [bMON]	Blending Research Octane Rating [bRON]	Blending Octane Sensitivity [bS]
Ethanol	10%	106.1	132.8	26.8
	20%	112.7	145.9	33.2
	30%	102.4	128.4	26.0
	Neat	90.0	109.0	19.0
Isopropanol	10%	102.8	117.2	14.4
	20%	109.4	127.7	18.3
	30%	102.5	120.6	18.2
	Neat	96.7	112.5	15.8
Isobutanol	10%	95.1	110.3	15.1
	20%	99.0	118.4	19.5
	30%	93.6	113.0	19.4
	Neat	93.0	107.0	14.0

*Obtained from the Co-Optima Fuel Property Database[1]

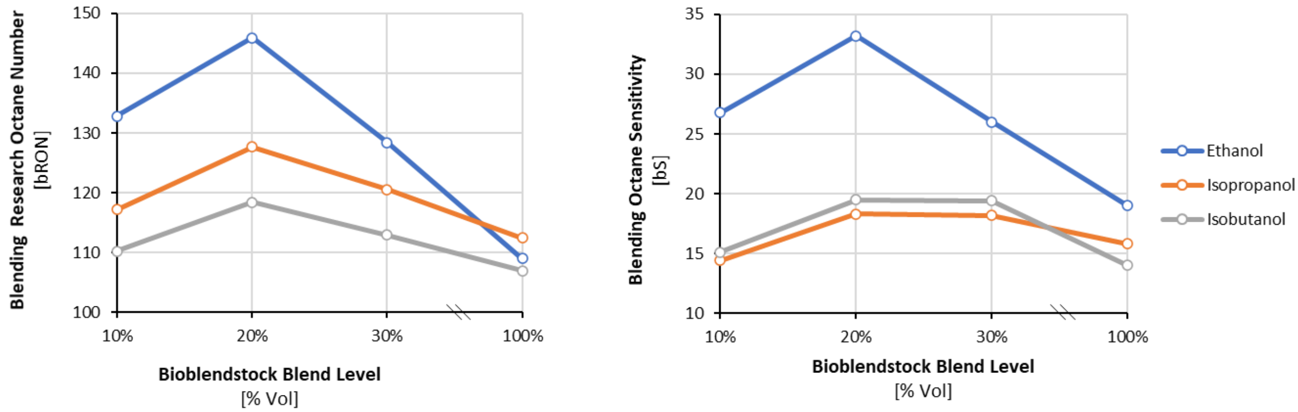

Fig. S1: Blending Research Octane Number and Octane Sensitivity for select co-optimized fuels, as a function of bioblendstock blending level.

National Average Electricity Grid Mix Used in the Analysis

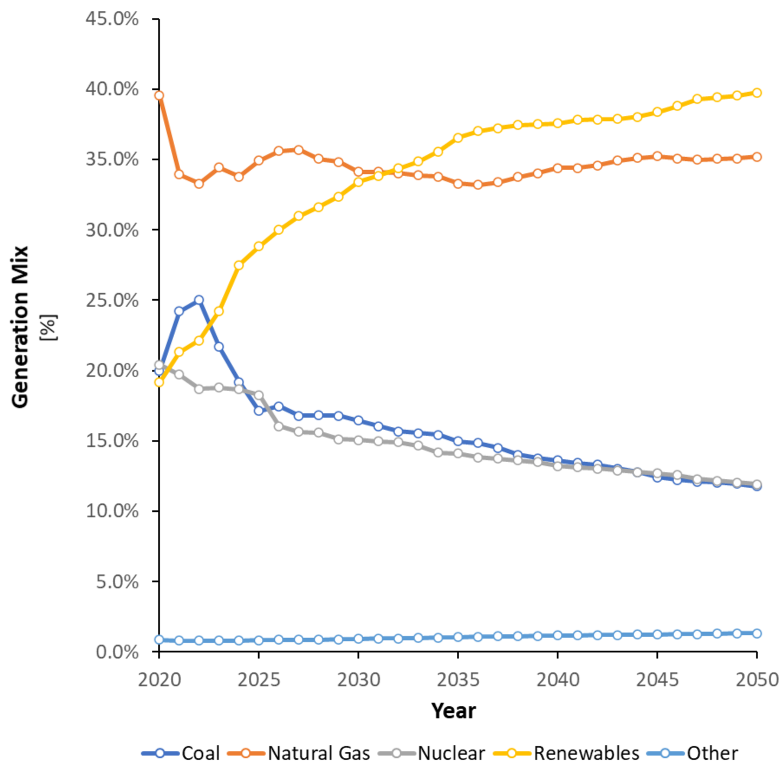

Fig. S2: Forecasted U.S. electricity generation mix[2].

Additional Information on Autonomie

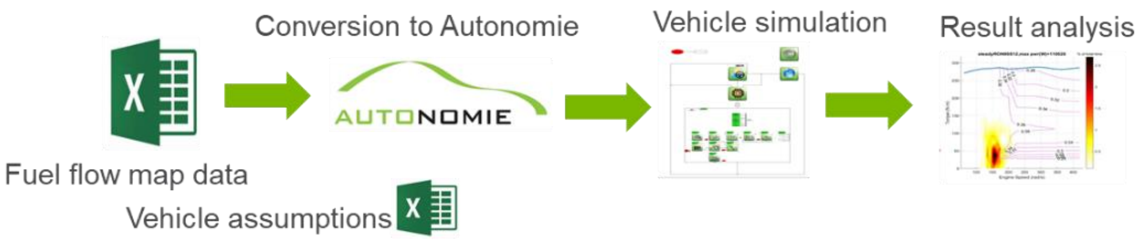

Fig. S3: Autonomie workflow for evaluating engines using vehicle simulation.

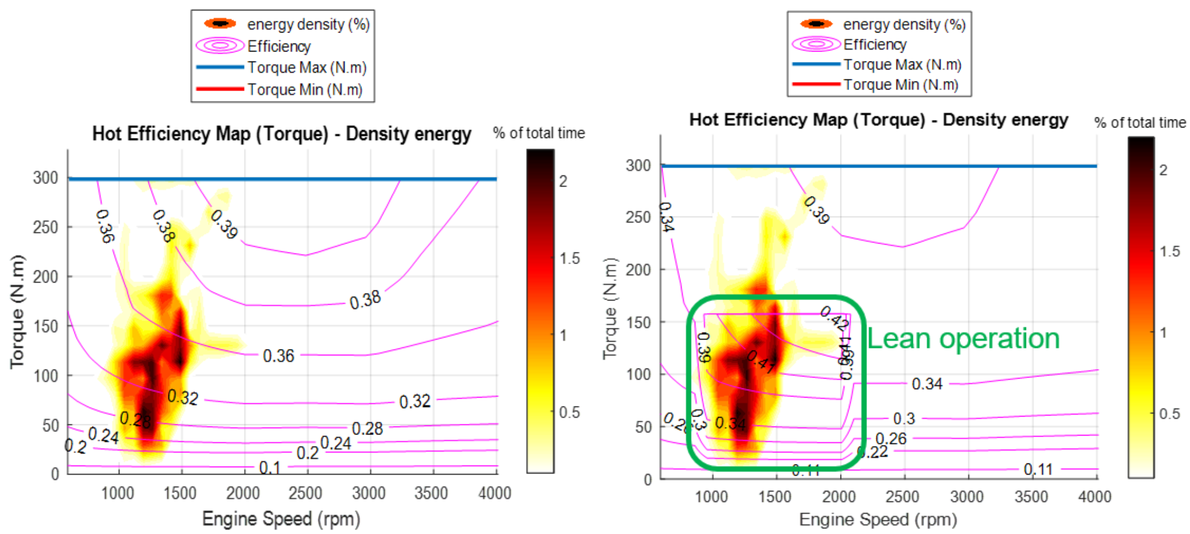

Fig. S4: Density plot showing the engine operating region where most of the fuel consumption occurs in city driving conditions.

Additional Information on ADOPT Simulation Inputs for the Screening and High Electrification Scenarios

Table S2. Light duty multimode isobutanol bounding scenarios with favorable electrification condition

Bio-blendstock	Engine Eff. Gain: Merit Function	Engine Eff. Gain: MM Combustion	Total Engine Efficiency Gain			Incremental Cost (USD, 2021)	Blending Level (% Vol)	Incentives for PEV Sales	CAFE Regulations	Battery and Fuel Cell Technology Prices
			Co-Optima: MM Conventional (%)[1]	Co-Optima: MM HEV (%)[2]	Co-Optima: MM PHEV (%)[2]					
Isobutanol (98 RON)	6.7%	8%	18.7% [6.7% + 12%]	10%	10%	-$1000, $0, $1,000 $2,000 $3,000	26.9%	$2500-$75000 based on kWh up to 600,000 per manufacturer	Extended Regulations	Aggressive
Isobutanol (98 RON)	6.7%	16%	18.7% [6.7% + 12%]	10%	10%	-$1000, $0, $1,000 $2,000 $3,000	26.9%	$2500-$75000 based on kWh up to 600,000 per manufacturer	Extended Regulations	Aggressive

CAFE Coefficient Scenario Inputs

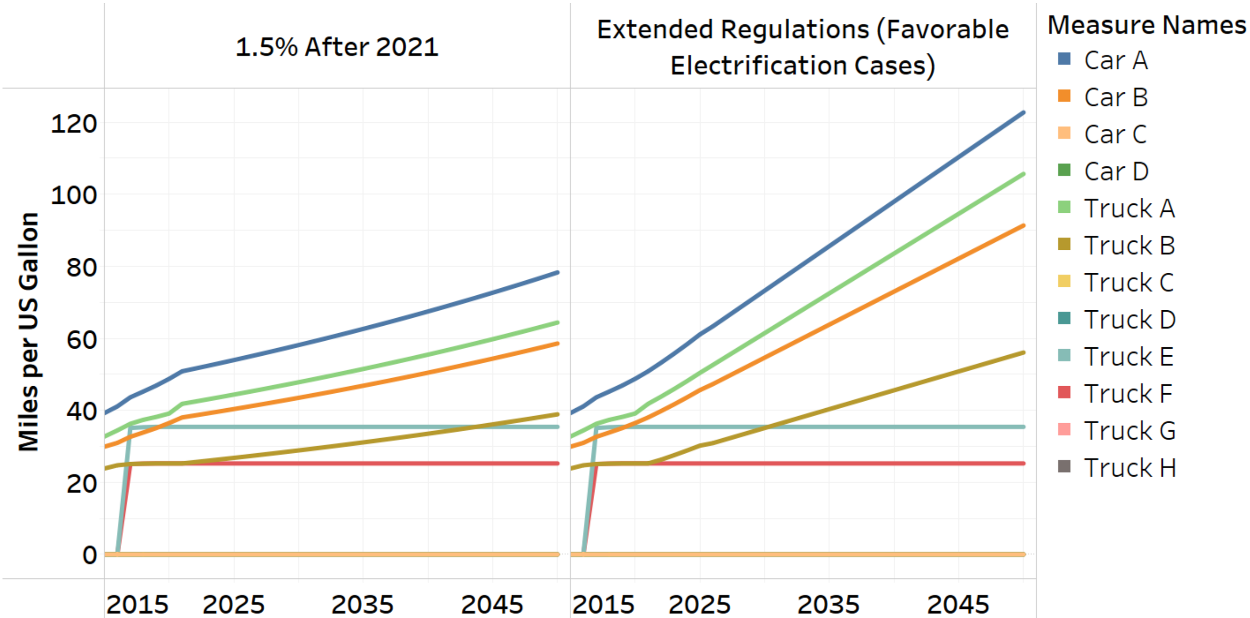

Fig. S5: CAFE coefficients with input from the CAFE standards[3]

Plug-in Electric Vehicle (PEV) Incentive Scenario Inputs

Table S3. PEV incentives by scenario with input from the Internal Revenue Service (IRS) credits[4]

Incentive Parameter Description	Screening Run Scenarios	High Electrification Scenarios
Minimum PEV Incentive	2500	2500
PEV Sales per Manufacturer Limit	200000	600000
Base kWh for Additional PEV Incentive	4	4
Dollar Incentive per Additional kWh	417	417
PEV Incentive Start Year	2010	2010
Maximum PEV Incentive	7500	7500
	0.55	0.55

Technology Cost and Performance Scenario Inputs

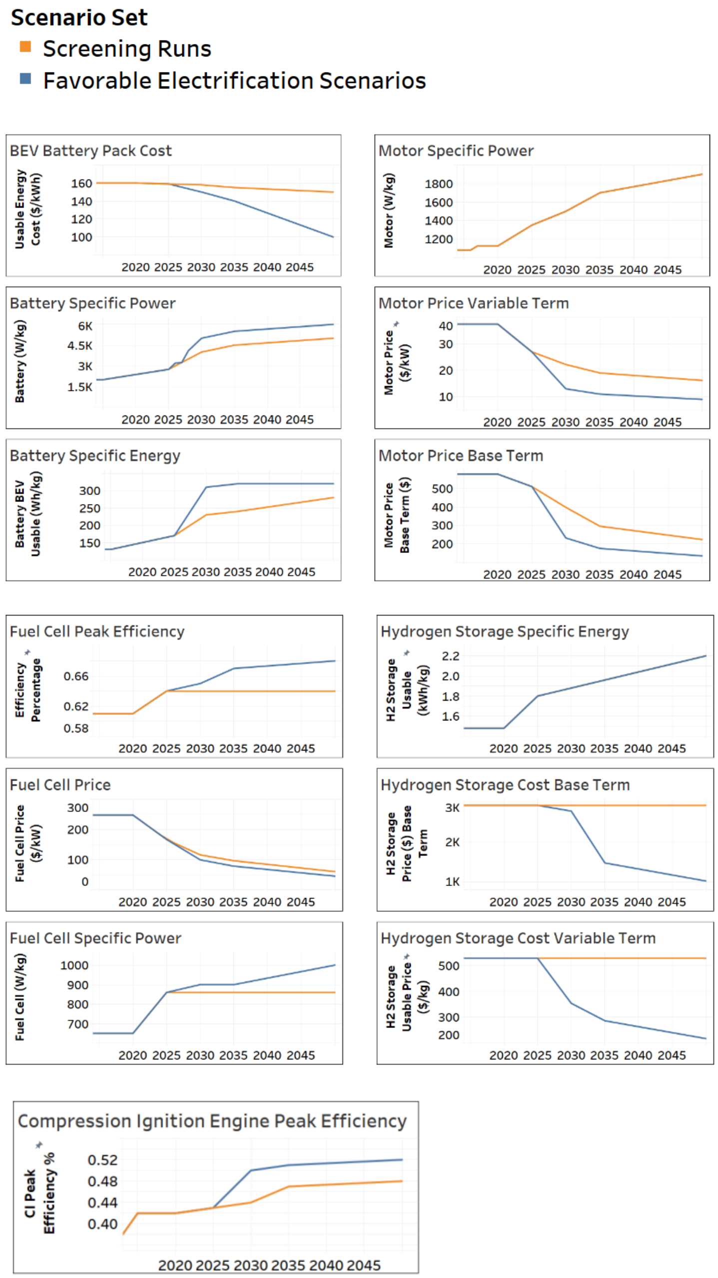

Fig. S6: Technology cost and performance scenario inputs.

Additional Information on Favorable Electrification Scenario Results

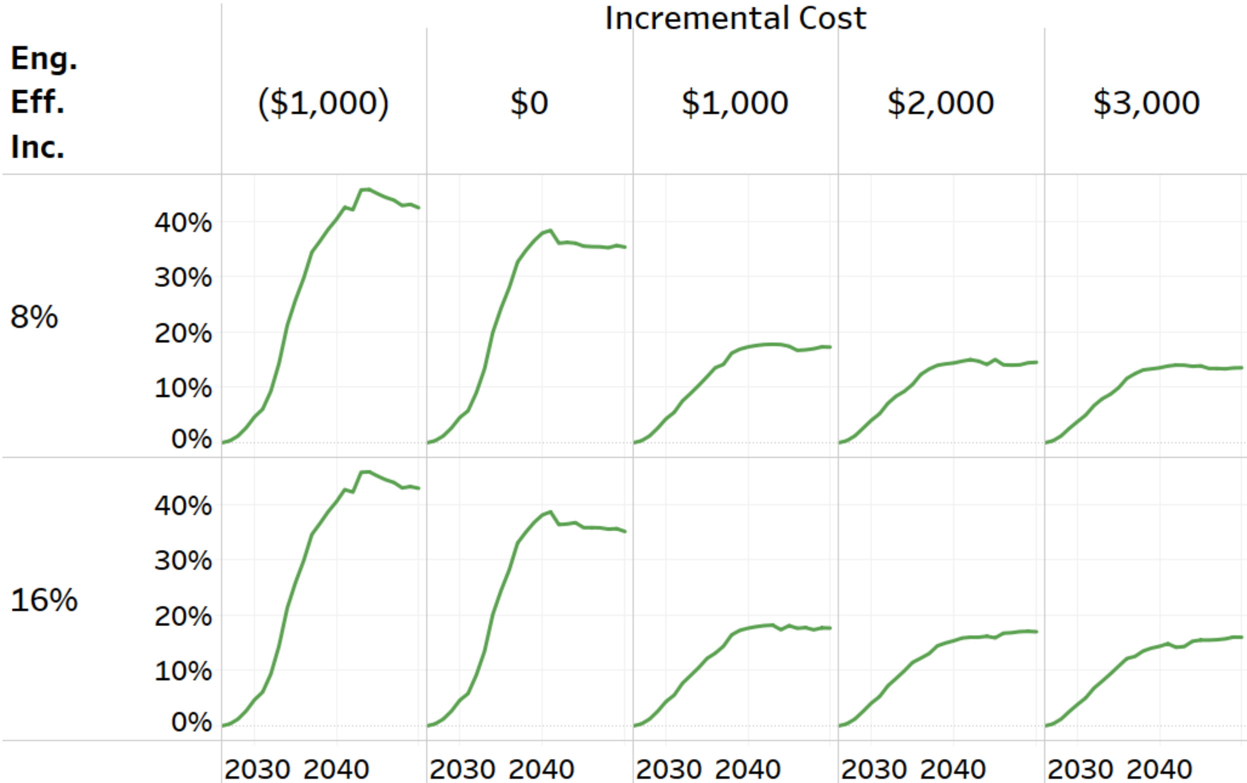

Fig. S7: Percentage of LDV sales that are co-optimized vehicles from 2026 through 2050 for the light duty multimode isobutanol bounding scenarios presented in Table 3.

Additional Information on Environmental Impacts of Scenarios

In the scenario with no co-optimized vehicles, water consumption declines from 2020 to 2042 due to decreased motor gasoline consumption, leading to reduced ethanol consumption that is water-intensive to produce (Fig. 5 in the manuscript). Water consumption then increased from 2043 to 2050 owing to increased penetration of battery electric vehicles (BEVs) and plug-in hybrid electric vehicles (PHEVs) and to a lesser extent, fuel cell electric vehicles (FCEVs) and natural gas vehicles. PHEVs and BEVs consume water-intensive electricity, especially hydroelectricity, which somewhat outweighs the water reduction effect of reduced conventional ethanol consumption in the later years.

In the MM scenarios, water consumption increased in 2050 across all cases compared to the scenario with no co-optimized vehicles. Water consumption remains the same as in scenario with no co-optimized vehicles case until 2033, after which increased adoption of co-optimized vehicles in the following years lead to higher water use due to the high water intensity of isobutanol fuel. At the lower incremental costs ($-1,000 to $1,000), water consumption increased between 10 – 24 billion gallons for both efficiencies gains scenarios. At the higher incremental costs ($2,000 and $3,000), water consumption increased by 1 billion gallons at lower efficiency gain for $2000, but slightly decreased by 0.7 billion gallons at $3000. At higher efficiency gain, water consumption increased by ~6 and 7 billion gallons in 2050 at $2,000 and $3,000 incremental costs respectively. The difference in the level of water increase between the two efficiency gains at higher incremental cost despite nearly the same level of co-optimized vehicles adoption reflects the difference in BEVs adoption. While BEVs adoption is comparable with the reference scenario at 16% efficiency gain and high incremental costs, the adoption is lesser at 8% engine efficiency gain and high incremental costs compared to the scenario with no co-optimized vehicles.

Co-optimized vehicles with advantageous blendstocks largely displace gasoline fueled vehicles.

Fig. S8 and Fig. S9 are a detailed analysis of GHG emissions contribution by vehicle types and fuel types for 16% engine efficiency gain and $0 incremental cost scenario. These figures intend to show the contribution of different vehicle and fuel categories to the overall LCA results, using a series of pair-wise comparisons with the scenario with no co-optimized vehicles. The bars show the “net” emissions between the MM scenario and the scenario with no co-optimized vehicles for each powertrain or fuel type. For blended fuels (Fig. S9), we use a ‘mixer’ wherein we consider the supply chains of the different blendstocks and then use a generic profile for fuel combustion. For example, for motor gasoline, the contribution of gasoline blendstock (e.g., crude extraction, T&D, crude-processing) is denoted as ‘Gasoline Blendstock,’while the upstream contribution of ethanol is denoted by the ‘Conventional Ethanol’ categories. The combustion/use phase emissions from motor gasoline are denoted as ‘Gasoline.’ This allows us to consider the impacts of the individual supply chain contributions. Emissions from a powertrain or fuel type will end up as a positive bar if there are more such powertrains or fuel type in the MM scenario than in the scenario with no co-optimized vehicles and vice versa.

At $-1,000 and $0 incremental costs, the emissions benefits can be attributed to the significant fleet turnover from conventional gasoline ICEVs, PHEVs, HEVs, and BEVs to co-optimized vehicles that consume fuel with lower GHG intensity than motor gasoline (E10/E15). However, at higher incremental costs ($2,000 and $3,000), the benefit is majorly associated with fleet turnover from conventional gasoline ICEVs and BEVs to co-optimized vehicles for the 8% engine efficiency gain scenario.

Reduction in electricity consumption driven by the adoption of co-optimized vehicles becomes the primary driver of emissions benefits in 2050 at higher incremental costs, while the contribution is also significant at the lower costs. For the 16% efficiency gain at higher incremental costs, the transition from conventional gasoline ICEVs, PHEVs, and HEVs to their more efficient co-optimized counterparts (hence reduced motor gasoline consumption) is the driver behind the emissions benefits achieved.

In some cases, the vehicle cycle impact bar ends up in the negative domain because of the low penetration of electric vehicles in the MM scenario compared to the scenario with no co-optimized vehicles (Fig. S9). In such cases, the changes in the vehicle composition of the fleet in the MM scenario result in lower vehicle cycle impacts as BEVs demonstrate higher per unit vehicle cycle impacts relative to other powertrain types.

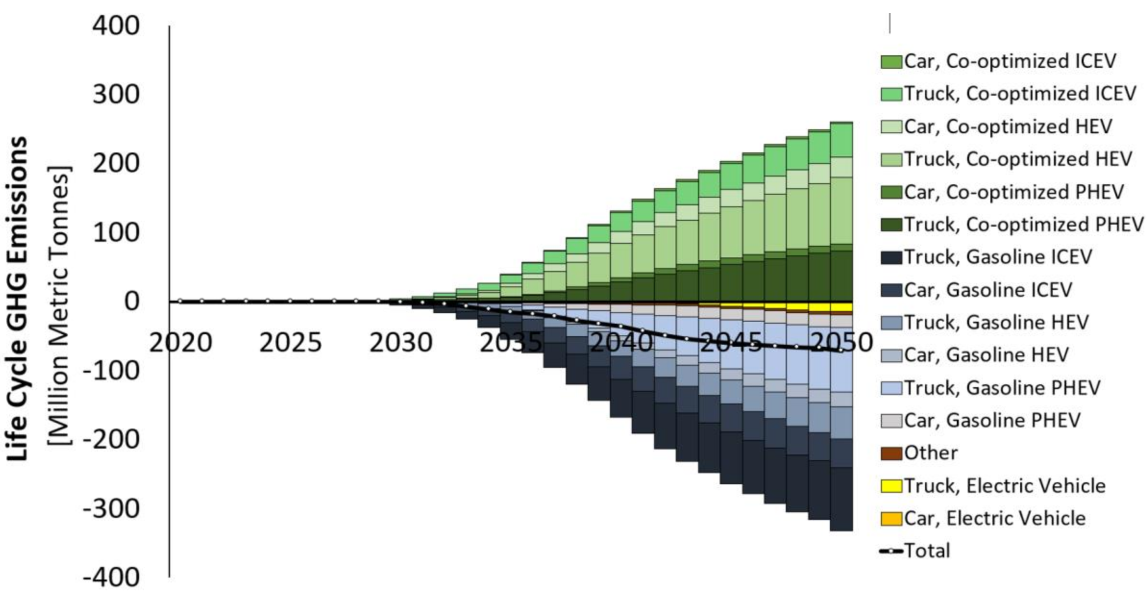

Fig. S8: Fleet-wide GHG contribution by vehicle type at 16% engine efficiency gain and $0 incremental cost. The bars show the “net” emissions between the MM scenario and the scenario with no co-optimized vehicles for each powertrain.

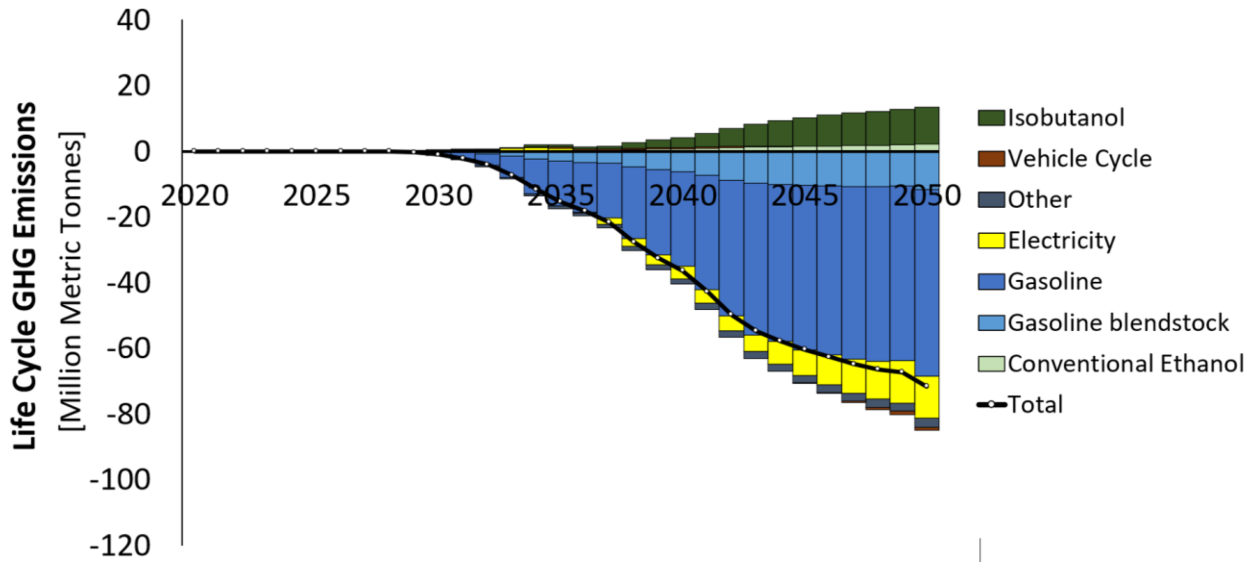

Fig. S9: Fleet-wide GHG contribution by fuel type at 16% engine efficiency gain and $0 incremental cost. The bars show the "net" emissions between the MM scenario and the reference case for each fuel type.

References

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