Optimal Design and Allocation of Electrified Vehicles and Dedicated Charging Infrastructure for Minimum Greenhouse Gas Emissions

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ABSTRACT
Electrified vehicles, including plug-in hybrid electric vehicles (PHEVs) and battery electric vehicles (BEVs), have the potential to reduce greenhouse gas (GHG) emissions from personal transportation by shifting energy demand from gasoline to electricity. GHG reduction potential depends on vehicle design, adoption, driving and charging patterns, charging infrastructure, and electricity generation mix. We construct an optimization model to study these factors by determining optimal design of conventional vehicles (CVs), hybrid electric vehicles (HEVs), PHEVs, and BEVs and optimal allocation of vehicle designs and charging infrastructure in the fleet for minimum lifecycle GHG emissions over a range of scenarios. We focus on vehicles with similar size and acceleration to a Toyota Prius under urban EPA driving conditions. We find that under today's U.S. average grid mix, the vehicle fleet allocated for minimum GHG emissions includes HEVs and PHEVs with ~30 miles (48 km) of electric range. Allocating only CVs, HEVs, PHEVs, or BEVs will produce 86%, 1%, 0%, or 13+% more life cycle GHG emissions, respectively. Unlike BEVs, PHEVs do consume some gasoline; however, PHEVs can power a large portion of vehicle miles on electrical energy while accommodating infrequent long trips without need for a large battery pack, with its corresponding production and weight implications. Availability of workplace charging for 90% of vehicles optimistically reduces optimized GHG emissions by 0.5%. Under decarbonized grid scenarios, larger battery packs are more competitive and reduce life cycle GHG emissions significantly. Future work will relax modeling assumptions and address life cycle cost and cost-effectiveness of GHG reductions.

1. INTRODUCTION

Climate change and peak oil are among the most pressing issues faced by the world, and both are complicated by concerns about energy security. In the U.S., the transportation sector accounts for 33% of GHG emissions [1] and over 60% of petroleum consumption [2]. Reducing GHG emissions and fuel consumption in this sector is crucial. Electrified transportation can help to address both of those issues by shifting transportation energy use from gasoline to electricity, especially when that electricity comes from low-carbon generation sources [3]. A barrier to widespread adoption of personal electrified vehicles, especially BEVs, is the “chicken and egg” problem: manufacturers do not want to make vehicles that have no market, consumers do not want vehicles that have no refueling infrastructure, and no one wants to invest in refueling infrastructure for vehicles that do not exist [4]. Policymakers can help break this cycle by putting incentives in place. For instance, the Obama administration has set a target of one million plug-in vehicles on the road by 2015 and has provided incentives to manufacturers and consumers as well as support for research and development [5]. However, to promote cost effective GHG reductions, it is important to understand which outcomes should be incentivized, and this study is a step towards addressing this issue by analyzing best possible outcomes.

Several studies have examined potential transportation electrification scenarios from various perspectives. For example, the Electrification Coalition, in their 2009 Electrification Roadmap, suggests a goal, based on energy security goals and a GHG target of 450 ppm carbon dioxide equivalent (CO_2eq), of powering 75% of personal vehicle miles traveled (VMT) by electricity by 2040 [6]. To reach this goal, they suggest that 25% of new vehicle purchases should be “grid-enabled” by 2020, and 90% by 2030. The Electric Power Research Institute and the National Resources Defense Council found in a 2007 study that PHEVs have substantial potential for reducing GHG emissions and air pollution [7]. However, a 2009 Argonne National Laboratory report finds that electrified vehicles are likely to have “little or no” market penetration by 2050 without government subsidies, and government subsidies of $7,500/vehicle could increase penetration of PHEVs, leading to a 22% reduction in GHG emissions by 2050 compared to their base case [8]. Studies have concluded that GHG reductions from plug-in vehicles are not likely to be cost effective in the near term [8, 9, 10].

Several trade-offs must be considered to determine the best scenarios. One of the major design decisions for PHEVs and BEVs is selecting the battery size. A larger battery pack enables the vehicle to travel a longer distance on electricity alone (the all-electric range, or AER) without the use of gasoline, which reduces operation-associated GHG emissions over the vehicle life under today's average grid mix. However, a larger battery pack costs more upfront, has production implications, and may reduce vehicle efficiency due to its weight [11]. Availability of charging infrastructure at the workplace and/or in public locations can enable a longer effective AER with a smaller battery pack. Availability of such infrastructure also affects charge timing, which has implications for plant dispatch and resulting GHG emissions [3, 12, 13, 14]. In this study, we take a limited scope, ignoring charge timing and focusing on the effect of private home and workplace charging availability on vehicle allocation and battery sizing in vehicle design.

Prior studies compare and select among a small set of fixed vehicle configurations based on selected commercially available vehicles or a small set of simulated vehicle alternatives [3, 11, 12, 14, 15]. However, interactions among engine sizing, motor sizing, and battery sizing can be important in comparing vehicle characteristics, and optimal battery sizing represents a compromise among drivers with different travel patterns. We follow Shiau *et al.* 2010 and pose an optimization problem to determine the best configuration of vehicles in the design space in order to compare the best design of each CV, HEV, PHEV, and BEV model under performance constraints that ensure vehicles are comparable [9]. We further incorporate charging infrastructure decisions that determine which of the electrified vehicles should be only charged at home versus charged both at home and at the workplace. We then address three questions: (1) What mix of vehicles can minimize GHG emissions? (2) What is the GHG reduction potential of workplace charging infrastructure? and (3) What effect does workplace charging have on optimal vehicle allocation and battery sizing? We describe our approach in Section 2, present results in Section 3, address model limitations and future work in Section 4, and provide discussion and conclusions in Section 5.

2. APPROACH

We pose an optimization problem to minimize life cycle greenhouse gas emissions over a fleet of vehicles by jointly determining (1) the optimal design of each CV, HEV, PHEV, and BEV; (2) the optimal allocation of each vehicle design to vehicles in the fleet based on annual VMT; and (3) the optimal allocation of home and workplace charging infrastructure to electrified vehicles in the fleet. We also incorporate vehicle design constraints to ensure that vehicles have comparable performance characteristics and vehicle allocation constraints that allow BEVs to be assigned only if the BEVs have sufficient range to accommodate the vehicle's driving distance on most days. This formulation represents a best-case scenario for minimizing greenhouse gas emissions with vehicle technology; market outcomes would likely deviate.

The general form of the optimization problem that we would like to solve is

$$\begin{array}{lll} \underset{\mathbf{x}=[\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_n]}{\text{minimize}} & \int_{s=0}^{\infty} f_{\mathrm{O}}(\mathbf{x},s) f_{\mathrm{S}}(s)\,ds & \textit{minimize net GHG emissions,} \\ \text{subject to} & \mathbf{g}_j^{\mathrm{D}}(\mathbf{x}_j) \le \mathbf{0},\ \forall j \in J & \textit{s.t. design constraints,} \\ & \mathbf{x}_j \in \Re^{p_j},\ \forall j \in J & \\ \text{where} & f_{\mathrm{O}}(\mathbf{x},s) = \min_{\left\{j\in J \mid \mathbf{g}_j^{\mathrm{A}}(\mathbf{x}_j,s)\le \mathbf{0}\right\}} \left\{ f_{\mathrm{O}j}(\mathbf{x}_j,s) \right\} & \textit{where vehicles are optimally allocated based on VMT subject to allocation constraints} \end{array} \tag{1}$$

where s is the average daily VMT for a specific vehicle in the fleet; $f_{\mathrm{S}}(s)$ is the probability density function of average daily VMT over the fleet; $J=\{1,2,\ldots,n\}$ is the set of indices for all vehicle alternatives; $f_{\mathrm{O}j}(\mathbf{x}_j,s)$ is the annual life cycle GHG emissions of vehicle j defined by the vehicle design vector $\mathbf{x}_j$ when driven an average of s miles per day (daily variation is discussed later); $\mathbf{g}^{\mathrm{D}}_j(\mathbf{x}_j)$ is the vector of vehicle design constraints; $\mathbf{g}^{\mathrm{A}}_j(\mathbf{x}_j,s)$ is the vector of allocation constraints; and p_j is the size of vector $\mathbf{x}_j$. This optimization formulation models two questions: (1) the best vehicle from the set J for each average daily VMT s that minimizes life cycle GHG emissions while satisfying the corresponding allocation constraints and (2) the design variables $\mathbf{x}_j$ that define each vehicle $j\in J$.

This problem formulation presents two key difficulties for mathematical optimization: (1) the objective function contains an integral, and (2) the objective function contains a minimization function, which has derivative discontinuities. To avoid these difficulties, we reformulate the problem using numerical integration and binary selection variables. First, we select a finite upper limit for the integral s_{MAX} and partition $[0,s_{\mathrm{MAX}}]$ into equal adjacent segments $i\in\{1,2,\ldots,m\}$, each of size s_{MAX}/m. We introduce binary selection variables, $\alpha_{ij}\in\{0,1\}$, for each segment i and vehicle alternative j that define which vehicle is assigned to each segment ($\Sigma_j\alpha_{ij} = 1$: only one vehicle alternative can be selected for each segment), and we further partition each segment into $K = s_{\mathrm{MAX}}/m\Delta$ sub-segments of size Δ for numerical integration using the trapezoidal rule. The resulting formulation is

$$\begin{aligned}
&\underset{\substack{\mathbf{x}_j,\alpha_{ij},\forall j\in J\\ \forall i\in\{1,..,m\}}}{\text{minimize}} && \sum_{i=1}^{m}\sum_{k=K(i-1)}^{iK-1}\left(\frac{\sum_{j=1}^{n}\alpha_{ij}f_{\mathrm{O}j}\left(\mathbf{x}_j,s_{k\Delta}\right)f_{\mathrm{S}}\left(s_{k\Delta}\right)+\sum_{j=1}^{n}\alpha_{ij}f_{\mathrm{O}j}\left(\mathbf{x}_j,s_{(k+1)\Delta}\right)f_{\mathrm{S}}\left(s_{(k+1)\Delta}\right)}{2}\right)\Delta\\
&\text{subject to} && \sum_{j\in J}\alpha_{ij}=1,\quad \mathbf{g}_j^{\mathrm{D}}\left(\mathbf{x}_j\right)\le\mathbf{0},\quad \alpha_{ij}\mathbf{g}_j^{\mathrm{A}}\left(\mathbf{x}_j,s_{(k+1)\Delta}\right)\le\mathbf{0},\\
& && \mathbf{x}_j\in\Re^{p_j},\quad \alpha_{ij}\in\{0,1\},\quad \forall i\in\{1,..,m\},\quad \forall j\in J\\
&\text{where} && K=\frac{s_{\mathrm{MAX}}}{m\Delta}
\end{aligned}\tag{2}$$

We relax the binary α_{ij} variables into the continuous domain, $\alpha_{ij}\in\Re$, $0\le\alpha_{ij}\le 1$, to ease computation. For any fixed $\mathbf{x}^* = [\mathbf{x}_1, ..., \mathbf{x}_n]^*$, the optimization formulation in (2) is linear in α_{ij}, so we expect that the optimal solution set will always contain a corner solution, and that all corner solutions will be binary in this formulation.

In our application, the set of vehicle alternatives J is partitioned into CVs, HEVs, PHEVs and BEVs, so that $J = J_{\mathrm{CV}} \cup J_{\mathrm{HEV}} \cup J_{\mathrm{PHEV}} \cup J_{\mathrm{BEV}}$. The decision variable vector $\mathbf{x}_j = [x_{\mathrm{E}j}, x_{\mathrm{M}j}, x_{\mathrm{B}j}]^{\mathrm{T}}$ for each vehicle $j\in J$ includes x_{E} = gasoline internal combustion engine (ICE) peak power (kW), x_{M} = electric motor peak power (kW), and x_{B} = battery size (number of cells) for each vehicle j, where $x_{\mathrm{M}} = x_{\mathrm{B}} = 0\ \forall\ j\in J_{\mathrm{CV}}$ and $x_{\mathrm{E}} = 0\ \forall\ j\in J_{\mathrm{BEV}}$. The objective function $f_{\mathrm{O}j}(\mathbf{x}_j,s)$ for annualized life cycle GHG emissions (kg CO_2eq/vehicle-year) is

$$\begin{aligned}
f_{\mathrm{O}j}\left(\mathbf{x}_j,s\right)=&\underbrace{\frac{v_{\mathrm{V}}sd}{s_{\mathrm{LIFE}}}}_{\text{base vehicle production}}+\underbrace{\frac{v_{\mathrm{E}}\left(x_{\mathrm{E}j}\right)sd}{s_{\mathrm{LIFE}}}}_{\text{engine production}}+\underbrace{\frac{v_{\mathrm{M}}\left(x_{\mathrm{M}j}\right)sd}{s_{\mathrm{LIFE}}}}_{\text{motor production}}+\underbrace{\frac{v_{\mathrm{B}j}x_{\mathrm{B}j}\kappa_{\mathrm{B}j}sd}{s_{\mathrm{LIFE}}}}_{\text{battery production}}+\underbrace{\frac{v_{\mathrm{C}}q_{\mathrm{C}j}}{l_{\mathrm{C}}}}_{\text{charger production}}\\
&+\underbrace{\frac{v_{\mathrm{G}}s_{\mathrm{G}}\left(\mathbf{x}_j,s\right)d}{\eta_{\mathrm{G}}\left(\mathbf{x}_j\right)}}_{\text{gasoline usage}}+\underbrace{\frac{v_{\mathrm{ELEC}}s_{\mathrm{E}}\left(\mathbf{x}_j,s\right)d}{\eta_{\mathrm{E}}\left(\mathbf{x}_j\right)\eta_{\mathrm{C}}}}_{\text{electricity usage}}
\end{aligned}\tag{3}$$

where v_{V} is the GHG emissions from production of the base vehicle excluding engine, motor, and batteries; d is driving days per year; s_{LIFE} is the life of the vehicle, including the engine and motor (and, for simplicity, the battery), in miles; $v_{\mathrm{E}}(x_{\mathrm{E}j})$ is the GHG emissions from production of the engine; $v_{\mathrm{M}}(x_{\mathrm{M}j})$ is the GHG emissions from production of the motor; v_{B} is the GHG emissions per kWh of battery production; κ_{B} is the battery cell energy capacity in kWh; v_{C} is the GHG emissions from producing one charger; $q_{\mathrm{C}j}$ is the number of chargers allocated to vehicle j; l_{c} is the charger life in years, which we assume is equal to the life of the vehicle; v_{G} is the life cycle GHG emissions from gasoline consumption per gallon; $s_{\mathrm{G}}(\mathbf{x}_j,s)$ is the average distance for which the vehicle is powered by gasoline (charge sustaining mode) on a driving day; $\eta_{\mathrm{G}}(x_j)$ is the vehicle gasoline efficiency in miles per gallon (mpg); v_{ELEC} is the life cycle GHG emissions from electricity consumption per kW; $s_{\mathrm{E}}(\mathbf{x}_j,s)$ is the average distance for which the vehicle is powered by electricity (charge depleting mode) on a driving day; $\eta_{\mathrm{E}}(x_j)$ is the vehicle electrical efficiency in mi./kWh; and η_C is the charging efficiency. We focus on the all-electric control strategy and ignore PHEVs with blended control strategies. In Eq. (3), the motor, battery, charger, and electricity terms drop out for CVs; the charger and electricity terms drop out for HEVs; and the engine and gasoline terms drop out for BEVs. Table 1 summarizes the model parameters and defines base case and sensitivity values for each. We discuss the functions $\eta_G(x_j)$ and $\eta_E(x_j)$ in Section 2.1 and the functions $f_S(s)$, $s_E(\mathbf{x}_j,s)$, and $s_G(\mathbf{x}_j,s)$ in Section 2.3. The GHG emissions from production of the engine, $v_E(x_{Ej}) = 16.1x_E + 589$, is calculated from an engine cost scaling equation in Shiau *et al.* 2010 [9], adjusted to 2002 dollars using the Consumer Price Index (CPI) [16], and then converted to engine production GHG emissions (including supply chain) using the EIO-LCA 2002 U.S. producer price model, Sector #336300: Motor vehicle parts manufacturing, which includes NAICS sector 33631: Motor Vehicle Gasoline Engine and Engine Parts Manufacturing [17]. The GHG emissions from production of the motor, $v_M(x_{Mj}) = 21.0x_M + 411$, is calculated from a motor cost scaling equation in Shiau *et al.* 2010 [9], adjusted to 2002 dollars using the CPI [16], and then converted to motor production GHG emissions using the EIO-LCA 2002 U.S. producer price model, Sector #335312: Motor and generator manufacturing [17].

TABLE 1 Model notation and parameter values for the base case and the sensitivity analysis

	Description	Unit	Base Value	Range	Ref
	Variables				
x_B	Number of battery cells	-	$0\ \forall\ j\in J_{CV}$; $168\ \forall\ j\in J_{HEV}$;	$200\text{-}1000\ \forall\ j\in J_{PHEV}$; $200\text{-}9000\ \forall\ j\in J_{BEV}$	
x_E	Peak engine power	kW	$126\ \forall\ j\in J_{CV}$; $57\ \forall\ j\in J_{HEV}$	$30\text{-}60\ \forall\ j\in J_{PHEV}$	
x_M	Peak motor power	kW	$0\ \forall\ j\in J_{CV}$; $52\ \forall\ j\in J_{HEV}$;	$50\text{-}110\ \forall\ j\in J_{PHEV}$; $70\text{-}250\ \forall\ j\in J_{BEV}$	
α_{ij}	Binary selection variable for each segment *i* and vehicle alternative *j*	-		{0,1}	
	Functions				
$f_S(s)$	PDF of annual VMT over the fleet		§2.3		
$s_{AER}(\mathbf{x}_j)$	All-electric range of vehicle alternative *j*	mi.	§2.1	$12\text{-}60\ \forall\ j\in J_{PHEV}$; $15\text{-}301\ \forall\ j\in J_{BEV}$	
$s_E(\mathbf{x}_j,s)$	Average distance powered by electricity per driving day for a vehicle driven an average of *s* miles per day	mi.	§2.3		
$s_G(\mathbf{x}_j,s)$	Average distance powered by gasoline per driving day for a vehicle alternative *j* driven an average of *s* miles per day	mi.	§2.3		
$s_\phi(s)$	Driving distance of ϕ^{th} percentile day for a vehicle given average daily distance *s*	mi.	§2.3		
$t_E(\mathbf{x}_j)$	0-60 mph acceleration time on electric power for vehicle *j*	sec.	§2.1	$7.3\text{-}19\ \forall\ j\in J_{PHEV}$; $6\text{-}36.5\ \forall\ j\in J_{BEV}$	
$t_G(\mathbf{x}_j)$	0-60 mph acceleration time on gasoline power for vehicle *j*	sec.	§2.1	$6.7\text{-}14.6\ \forall\ j\in J_{PHEV}$	

	Description	Unit	Base Value	Range	Ref
$v_E(x_{Ej})$	Engine production GHGs for vehicle alternative j	kg CO_2eq	§2 2620 $\forall\ j \in J_{CV}$; 1510 $\forall\ j \in J_{HEV}$	1070-1560 $\forall\ j \in J_{PHEV}$	
$v_M(x_{Mj})$	Motor production GHGs for vehicle j	kg CO_2eq	§2 1500 $\forall\ j \in J_{HEV}$	1460-2720 $\forall\ j \in J_{PHEV}$; 1880-5660 $\forall\ j \in J_{BEV}$	
$\eta_E(\mathbf{x}_j)$	Electrical efficiency of vehicle j	mi. / kWh	§2.1	4.98-5.39 $\forall\ j \in J_{PHEV}$; 2.34-5.75 $\forall\ j \in J_{BEV}$	
$\eta_G(\mathbf{x}_j)$	Gasoline efficiency of vehicle j	mi. / gal	§2.1 29.5 $\forall\ j \in J_{CV}$; 60.1 $\forall\ j \in J_{HEV}$;	55.9-61.8 $\forall\ j \in J_{PHEV}$	
			Parameters		
b_B	Scaling factor for number of battery cells	-	1/1000		
b_E	Scaling factor for peak engine power	-	1/57		
b_M	Scaling factor for peak motor power	-	1/52		
d	Driving days per year	days / year	243.82		
K	Number of integration steps per segment	-	$s_{MAX} / m\Delta$ (1000)		
l_c	Charger life	years	s_{LIFE}/sd		
m	Number of segments for vehicle allocation	-	20		
n	Size of set J (number of vehicles in choice set)	-	10	1-10	
q_C	Number of chargers allocated to vehicle j	chargers	{1,2}		
s_{LIFE}	Vehicle life	mi.	150,000		
s_{MAX}	Maximum daily VMT considered in the model	mi.	200		
t_{MAX}	Maximum allowed 0-60mph acceleration time	sec.	10.5		
v_{Bj}	GHG emissions from li-ion battery production $\forall\ j \in J_{PHEV} \cup J_{BEV}$	kg CO_2eq / kWh	120		[3]
	GHG emissions from NiMH battery production $\forall\ j \in J_{HEV}$	kg CO_2eq / kWh	230		[3]
v_C	GHG emissions from producing a charger	kg CO_2eq	536 (§2.2)		
v_{ELEC}	GHG emissions from electricity generation	kg CO_2eq / kWh	0.752	0.066-0.9	[3, 9]
v_G	GHG emissions from gasoline	kg CO_2eq / gal	11.34		[9]

	Description	Unit	Base Value	Range	Ref
ν_V	GHG emissions from vehicle production excluding batteries	kg CO_2eq	5965		[3]
β_{abc}	PSAT metamodel coefficients	-	§2.1		
β_f	Shape parameter of Weibull distribution of VMT over the fleet	-	1.372		
Δ	Integration step size	mi.	10^{-2}		
η_C	Vehicle charging efficiency	%	88%		[9]
κ_{Bj}	Energy capacity of one li-ion battery cell $\forall\, j \in J_{PHEV} \cup J_{BEV}$	kWh / cell	0.0216		[9]
	Energy capacity of one NiMH battery cell $\forall\, j \in J_{HEV}$	kWh / cell	0.00774		[9]
λ_f	Scale parameter of Weibull distribution of VMT over the fleet		38.22		
σ_j	Battery swing for vehicle $j \in J \backslash \{J_{CV}\}$	%	80%		[9]

The design constraint vector $\mathbf{g}^D{}_j(\mathbf{x}_j)$ ensures that each vehicle satisfies comparable performance criteria. These include a maximum 0-60 miles per hour (mph) acceleration time t_{MAX} = 10.5 seconds for all vehicles, in both gasoline and electric mode: $g_1{}^D{}_j(\mathbf{x}_j) = t_G(\mathbf{x}_j) - t_{MAX} \leq 0\ \forall\, j \in J_{CV} \cup J_{HEV} \cup J_{PHEV}$, $g_1{}^D{}_j(\mathbf{x}_j) = 0\ \forall\, j \in J_{BEV}$, $g_2{}^D{}_j(\mathbf{x}_j) = t_E(\mathbf{x}_j) - t_{MAX} \leq 0\ \forall\, j \in J_{PHEV} \cup J_{BEV}$, and $g_2{}^D{}_j(\mathbf{x}_j) = 0\ \forall\, j \in J_{CV} \cup J_{HEV}$, where $t_G(\mathbf{x}_j)$ and $t_E(\mathbf{x}_j)$ are the 0-60 mph acceleration time of vehicle $\mathbf{x}_j$ in gasoline and electric mode, respectively, as discussed in Section 2.1. We also incorporate simple bounds 30kW $\leq x_{Ej} \leq$ 60kW, 50kW $\leq x_{Mj} \leq$ 110kW, and 200 cells $\leq x_{Bj} \leq$ 1000 cells $\forall\, j \in J_{PHEV}$ and x_{Ej} = 0 kW, 70 kW $\leq x_{Mj} \leq$ 250 kW, and 200 cells $\leq x_{Bj} \leq$ 9000 cells $\forall\, j \in J_{BEV}$ to avoid extrapolation beyond our simulation data. Finally, the allocation constraints $g^A{}_j(\mathbf{x}_j,s) = s_\phi(s) - s_{AER}(\mathbf{x}_j) \leq 0\ \forall\, j \in J_{BEV}$, and $g^A{}_j(\mathbf{x}_j,s) = 0\ \forall\, j \in J \backslash J_{BEV}$ ensure that BEVs are only allocated to vehicles if ϕ percent of days have VMT lower than the vehicle's range. We discuss the $s_{AER}(\mathbf{x}_j)$ function in Section 2.1 and the s_ϕ function in Section 2.3.

2.1 Vehicle Performance Model

To estimate the electrical $\eta_E(\mathbf{x}_j)$ and gasoline $\eta_G(\mathbf{x}_j)$ efficiencies and the acceleration performances $t_G(\mathbf{x}_j)$ and $t_E(\mathbf{x}_j)$ of vehicle j defined by design variables $\mathbf{x}_j$, we utilize Argonne National Laboratory's Powertrain System Analysis Toolkit (PSAT) vehicle simulation software [18] and construct a cubic metamodel fit to a discrete set of simulation points in the design space $\mathbf{x}_j$ using the Urban Dynamometer Driving Schedule (UDDS) driving cycle [19]. We use the 2004 Toyota Prius model as the baseline vehicle and our HEV model, and we construct our PHEV model by substituting Li-ion batteries for the Prius Nickel metal hydride (NiMH) batteries and increasing the pack size. One kilogram of structural weight is added to the vehicle per kilogram of battery, engine, and motor to support the weight of those components [11]. We base our CV model on a scaled Honda Accord powertrain, adjusted to have a Toyota Prius vehicle body for fair comparison to the HEV, PHEV, and BEV [9]. Our BEV model has a generic BEV drive train modified to use the same body, motor, and batteries as the PHEV. We ignore the possibility of using different battery designs on BEVs vs. PHEVs.

Because the performance of CVs and HEVs are independent of s, we identify the optimal designs for these vehicles *a priori*. For the CV, $\mathbf{x}_j$ = [126 kW, 0 kW, 0 cells], $\eta_G(\mathbf{x}_j) = 29.5$ mpg and $t_G(\mathbf{x}_j) = 11.0$ seconds. For the HEV, $\mathbf{x}_j$ = [57 kW, 52 kW, 168 cells] with $\eta_G(\mathbf{x}_j) = 60.1$ mpg, and $t_G(\mathbf{x}_j) = 11.0$ seconds. For the PHEV and BEV cases, we construct cubic metamodels fit to an array of points tested within the bounds of the design space. The resulting models, of the form $\Sigma_{a,b,c\in\{0,1,2,3\}|a+b+c\leq 3}\, \beta_{abc}\, (b_E x_E)^a\, (b_M x_M)^b\, (b_B x_B)^c$, where $b_E = 1/57$, $b_M = 1/52$, and $b_B = 1/1000$ are scaling factors, have coefficients fit using least squares regression listed in Table 2 (for BEVs, the terms involving x_E drop out). The error for all metamodels is within 0.7 seconds, 0.05 mpg, and 0.1 mi./kWh over the set of data points used for fitting.

Based on the metamodel for electrical efficiency $\eta_E(\mathbf{x}_j)$ for PHEVs and BEVs, we calculate the AER $s_{AER}(\mathbf{x}_j) = \eta_E(\mathbf{x}_j)\kappa_{Bj}x_{Bj}\sigma_j$, where σ_j is the battery swing (state of charge window) for vehicle *j*. The effective AER is the AER multiplied by the number of chargers, q_{Cj} (i.e. number of charges per day).

TABLE 2 Metamodel coefficients

	$\eta_E(\mathbf{x}_j)$ $\forall\, j\in J_{PHEV}$	$\eta_G(\mathbf{x}_j)$ $\forall\, j\in J_{PHEV}$	$t_E(\mathbf{x}_j)$ $\forall\, j\in J_{PHEV}$	$t_G(\mathbf{x}_j)$ $\forall\, j\in J_{PHEV}$	$\eta_E(\mathbf{x}_j)$ $\forall\, j\in J_{BEV}$	$t_E(\mathbf{x}_j)$ $\forall\, j\in J_{BEV}$
β_{300}	0.008	2.214	1.457	3.334		
β_{030}	0.154	1.087	-5.496	-2.266	0.004	-0.328
β_{003}	0.353	5.578	-28.456	-20.257	0.000	-0.015
β_{210}	-0.005	-0.815	0.913	0.414		
β_{120}	-0.005	0.510	-0.881	-3.524		
β_{201}	-0.025	1.562	-1.050	-0.286		
β_{102}	0.000	2.212	-0.308	-10.111		
β_{021}	-0.057	-0.613	2.044	1.951	-0.006	0.096
β_{012}	-0.043	0.254	15.610	10.309	-0.004	0.050
β_{111}	-0.016	-0.159	0.336	5.808		
β_{200}	-0.001	-8.906	-4.634	-6.932		
β_{020}	-0.805	-6.095	31.478	15.800	-0.022	4.015
β_{002}	-0.656	-15.208	34.017	39.198	0.041	0.052
β_{110}	0.057	0.089	1.153	7.901		
β_{101}	0.080	-3.274	1.169	6.582		
β_{011}	0.342	2.498	-32.057	-30.119	0.101	-1.600
β_{100}	-0.191	2.622	3.405	-6.734		
β_{010}	1.189	9.285	-54.473	-26.385	-0.266	-15.659
β_{001}	-0.347	5.837	9.570	-4.098	-0.835	4.637
β_{000}	4.960	57.680	44.231	32.102	6.337	25.435

2.2 Charging Infrastructure Scenarios

We consider the following two charging scenarios: (1) only home slow charging (120 or 240 volts AC, up to 3.3 kW [20]), and (2) home slow charging with additional dedicated workplace slow charging (at the same power level): we do not consider additional charging methods such as fast charging, battery swapping, smart charging, or vehicle to grid power. We implement these two charging scenarios in the model by partitioning J_{PHEV} and J_{BEV} each into two subsets $J_{PHEV} = J_{PHEV(1)} \cup J_{PHEV(2)}$ and $J_{BEV} = J_{BEV(1)} \cup J_{BEV(2)}$, where the numbers indicate 1 charger (home) or 2 chargers (home + work). Each 2-charger partition is identical to the corresponding 1-charger partition (equal design variables) except that $q_C = 2$ instead of 1. This allows each vehicle design to be assigned to some drivers with one charger and also to other drivers with two chargers. To find v_C, the GHG emissions from producing one charger, we use the EIO-LCA 2002 U.S. producer price model [17] and assume that a charger is reasonably represented by $1000 (2008 dollars, adjust to 2002 dollars using the CPI [16]) of purchases from Sector #33441A: Electronic capacitor, resistor, coil, transformer, and other inductor manufacturing.

2.3 Driving Patterns

To estimate the probability density function $f_S(s)$ of annual VMT, we fit a Weibull distribution, shown in Figure 1, to the weighted average daily distance traveled (based on odometer readings) from the U.S. from the 2001 National Household Travel Survey (NHTS) [21]. The distribution takes the form $f_S(s) = \frac{\beta_f}{\lambda_f}\left(\frac{s}{\lambda_f}\right)^{\beta_f - 1} \exp\left(-\left(\frac{s}{\lambda_f}\right)^{\beta_f}\right)$ where $\lambda_f = 38.22$ and $\beta_f = 1.372$. This distribution accounts for the variability in average daily VMT across the U.S. vehicle fleet (across vehicle), but does not account for variability in VMT of the same vehicle across days (within vehicle). NHTS data do not contain information on within-vehicle variability, since each household was only surveyed on one day, so we use detailed trip data collected for 133 vehicles in Minnesota in 2004-2005 to estimate this variability across days [22]. Since the average annual VMT is similar across the two data sets (11,800 miles in NHTS odometer readings [21] and 11,900 miles in the Minnesota data set [22]), we believe the Minnesota data set is reasonably representative for providing an estimate of U.S. within-vehicle variability.

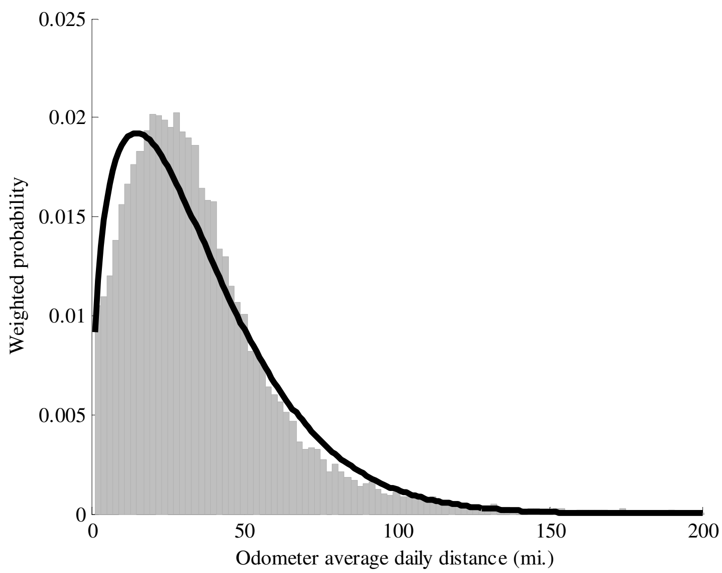

FIGURE 1 Weibull fit to odometer average daily distance from NHTS 2001 data [16]

We represent the variability in daily driving distances across days by first removing days in which the vehicle was not driven, leaving an average of $d = 243.8$ driving days per year (we observed no clear trend in d vs. s, so d is assumed constant across s) [22]. Next, we fit a curve through the mean distance on driving days: $\mu(s)=1.110s+13.33$. Finally, a family of exponential distributions is defined with random variable σ indicating distance driven on a particular day.

The cumulative distribution function (CDF) of σ is set to $F_{\sigma}^{V}(\sigma) = 1 - \exp\left(\frac{-\sigma}{1.110s + 13.33}\right)$ so that the mean of σ for a given s is equal to $\mu(s)$. In practice, the shape of the distribution of daily distance driven in the Minnesota data set varies across vehicles, including unimodal and multimodal distributions. However, the exponential assumption provides a reasonable rough approximation of the general trend in daily variability while offering a closed form CDF to facilitate estimation of the portion of miles driven beyond a PHEV's all-electric range (and the distance on the vehicle's 95th percentile day, for comparison to a simple linear fit to the 95$^{\text{th}}$ percentile day distance data). Using a linear fit to the data, the 95$^{\text{th}}$ and 99$^{\text{th}}$ percentile daily driving distances can be calculated as $s_{95\%}(s) = 2.62s + 40.3$ miles and $s_{99\%}(s) = 3.61s + 108$ miles, respectively. By using the $s_{95\%}$ function as a minimum AER constraint for allocating BEVs, we ensure that the BEV has sufficient range to accommodate 95% of driving days for a vehicle with the given annual VMT. We can also perform sensitivity analysis on this constraint using the $s_{99\%}(s)$ function and the $\mu(s)$ function. Figure 2 shows both of these functions, along with the 95$^{\text{th}}$ and 99$^{\text{th}}$ percentiles of the family of exponential distributions, for comparison. While the exponential assumption deviates somewhat from the 95th percentile trend, the approximation is optimistic toward electrification.

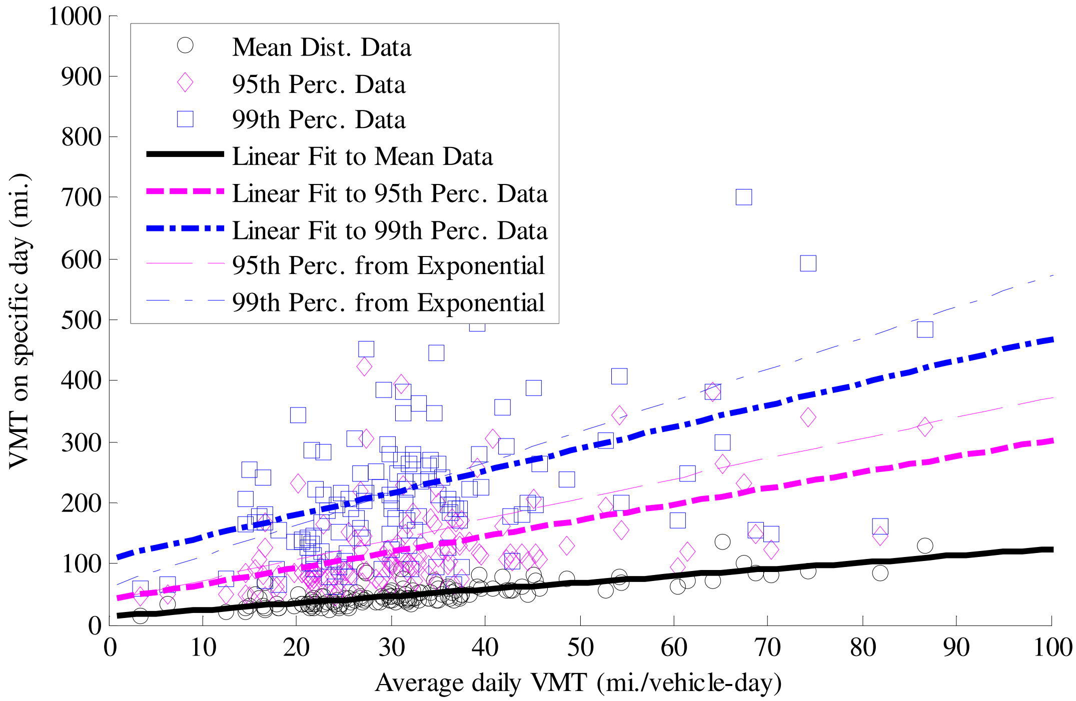

FIGURE 2 Mean, 95$^{\text{th}}$ percentile, and 99$^{\text{th}}$ percentile driving distance on driving days for 133 vehicles versus average daily VMT (including non-driving days), with linear fits, and with 95$^{\text{th}}$ and 99$^{\text{th}}$ percentiles as calculated from a family of exponential distributions calibrated to match a linear fit to the mean.

Using the exponential fit, we calculate $s_G(\mathbf{x}_j, s)$, the average portion of driving day distance powered by gasoline, and $s_E(\mathbf{x}_j, s)$, the average portion of driving day distance powered by electricity:

$$s_{\mathrm{G}}\left(\mathbf{x}_j, s\right) = s\exp\left(\frac{-q_{\mathrm{C}j}s_{\mathrm{AER}}\left(\mathbf{x}_j\right)}{1.110s+13.33}\right)$$
$$s_{\mathrm{E}}\left(\mathbf{x}_j, s\right) = s - s_{\mathrm{G}}\left(\mathbf{x}_j, s\right) \tag{4}$$

We assume that the presence of workplace charging will provide a charging opportunity sufficient to recharge the battery at distance $s/2$, effectively doubling the AER on an average day (we ignore workplace charging for the 95th percentile day). This assumption is optimistic about the benefits of PHEVs and of workplace charging, since daily distance variability typically reflects trips taken to locations other than the workplace, rather than variable distance to the workplace. Because we use the UDDS driving cycle for all drivers, we also do not account for the correlation between driving distance and driving style (and therefore efficiency). We leave incorporating such considerations for future work.

3. RESULTS

In this section, we describe the results obtained from the optimization formulation defined in Eq. (2). First, we show lifecycle GHG emission results for several representative vehicle designs. Later, we present total GHG emission results for several scenarios in which vehicles are optimally designed and allocated.

The first graph in Figure 3 shows an example plot of GHG emissions per mile, $f_{\mathrm{O}j}(\mathbf{x}_j,s)/sd$, versus average daily driving distance s for two hypothetical vehicles. The lowest vehicle curve at any point s represents the best vehicle for that driving distance. While GHG emissions per VMT are independent of daily VMT for CVs, HEVs, and BEVs, daily VMT and charger availability affect the portion of PHEV distance traveled on electricity vs. gasoline and thus the resulting GHG emissions. The second graph in Figure 3 shows $f_{\mathrm{O}j}(\mathbf{x}_j,s)f_{\mathrm{S}}(s)$, the population-weighted life cycle GHG emissions per vehicle-year and the integrand of the objective in Eq. (1), for the same representative vehicles. The area under each curve represents

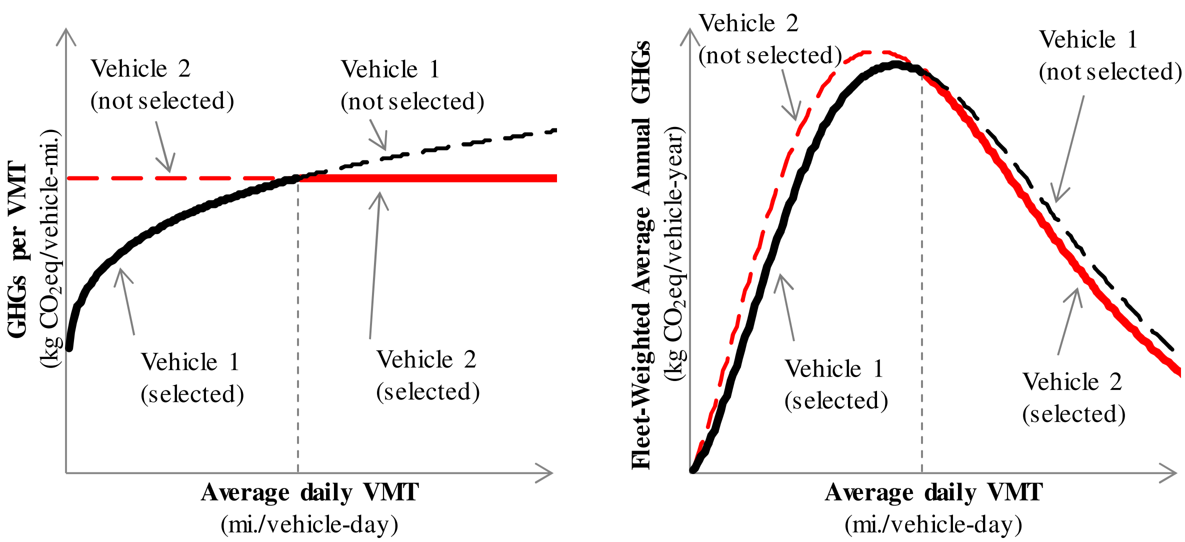

FIGURE 3 Left: Example GHG emissions per VMT vs. average daily VMT. Right: Example fleet-weighted average annual GHG emissions vs. average daily VMT (integral is average annual GHG emissions per vehicle per day).

the total annual emissions if all vehicles were of the corresponding design and charging scenario, and the area under the piecewise smooth curve defined by the solid lines represents total annual emissions if the two vehicles are allocated optimally for minimum GHGs.

Table 3 summarizes the optimal results for several scenarios, where we define each scenario relative to the base case. For each scenario, we report the total annual GHG emissions both in metric tons of CO_2 equivalent (mt CO_2eq) per vehicle per year and as a percent change from the base case result. We also show the vehicle designs allocated in each scenario, as well as the range of average daily driving distances for which each vehicle is allocated, the percent of the vehicle fleet represented by that vehicle, the percent of VMT represented by that vehicle, and the percent of total annual lifecycle GHG emissions from that vehicle. In the base case, the optimal solution involves a PHEV29 allocated with both home and work charging to replace vehicles that are driven on average 0-30 miles per day, a PHEV32 with both home and work

TABLE 3 Optimal solutions for selected scenarios. Percentages may not sum to 100% due to rounding

Scenario		Min GHGs (mt CO_2eq per vehicle year)	% Change in GHGs from Base Case	Allocated Vehicles	# of Chargers	Allocated Range (mi)	% of Fleet	% of VMT	% of GHGs
Base case Vehicle alternatives {*CV, HEV, PHEV$_A$, PHEV$_B$, BEV$_A$, BEV$_B$*}; {*1,2*} *chargers for PHEV/BEV alternatives; U.S. avg. grid mix* (*0.752 kgCO_2/kWh*); *ϕ=95% BEV allocation constraint*		1.94		PHEV29	2	0-30	51	23	23
				PHEV32	2	30-70	39	51	51
				HEV	0	70-200	10	26	26
Vehicle availability	CV only	3.61	+86%	CV	0	0-200	100	100	100
	HEV only	1.96	+1%	HEV	0	0-200	100	100	100
	PHEVs only	1.94	+0%	PHEV29	1	0-20	1	5	5
				PHEV29	2	110-200	34	11	10
				PHEV31	2	20-110	65	84	85
	BEVs only (with ϕ=mean allocation constraint for feasibility)	2.20	+13%	BEV102	1	0-80	93	82	76
				BEV235	1	80-200	7	18	24
Infrastructure availability	Home charging only	1.95	+0.5%	PHEV30	1	10-40	26	16	16
				PHEV 32	1	0-10, 40-50	51	35	35
				HEV	0	50-200	24	49	49
Electricity generation mix (for vehicle charging only)	Coal electricity (*0.9 kg CO2eq/kWh*)	1.96	+1%	HEV	0	0-200	100	100	100
	Natural gas electricity (*0.47 kg CO_2eq/kWh*)	1.55	-20%	BEV67	1	0-10	15	2	2
				PHEV54	2	10-40	51	35	33
				PHEV76	2	40-200	34	63	65
	IGCC-CCS electricity (*0.252 kg CO_2eq/kWh*)	1.19	-39%	BEV67	1	0-10	15	2	2
				PHEV60	2	10-30	37	21	19
				PHEV88	2	30-200	49	77	79
	Nuclear electricity (*0.066 kg CO_2eq/kWh*)	0.87	-55%	BEV67	1	0-10	15	2	2
				PHEV69	2	10-30	37	21	17
				PHEV88	2	30-200	49	77	81

charging for vehicles that average between 30 and 70 miles per day, and an HEV above 70 miles per day. Figure 4 visually summarizes the fleet allocation. In the base case solution, workplace charging is allocated to the 90% of vehicles. The optimal design and allocation result in 1.94 mt CO_2eq per vehicle per year.

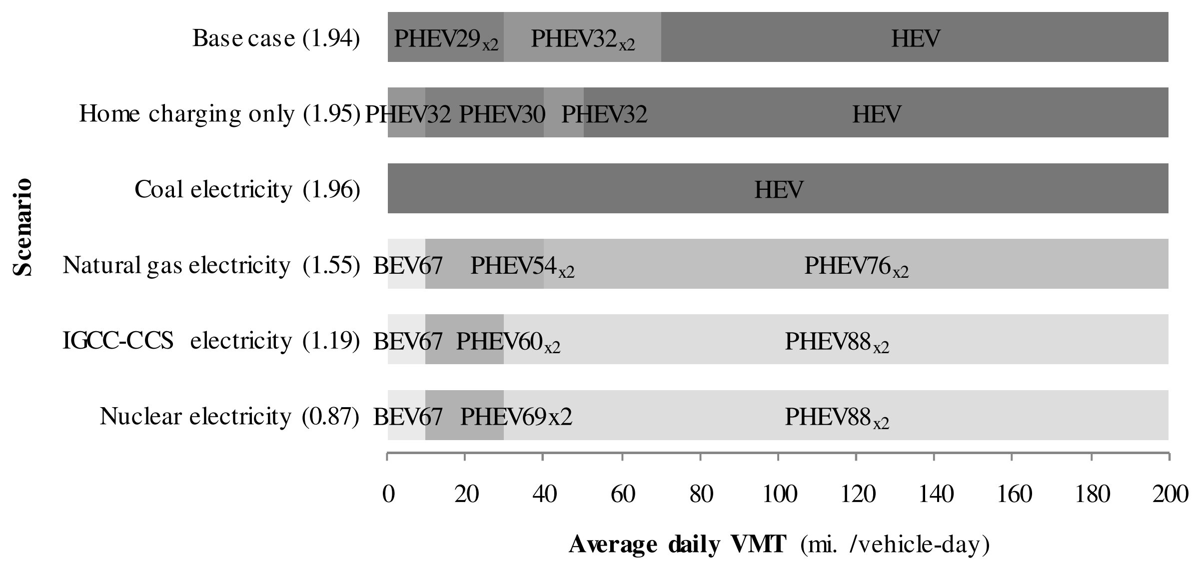

FIGURE 4 GHG-emission-minimizing vehicle allocations for various scenarios, with total scenario GHG emissions shown in mt CO2eq in parentheses. Lighter colors represent larger battery packs.

Relative to the base case solution, GHG emissions would increase by 86% if all vehicles were CVs of comparable size and performance, by 1% if all vehicles were HEVs, and by 0% if all vehicles were PHEVs. The case with all BEVs is not feasible in this model because battery packs large enough to accommodate the 95th percentile trip for vehicles that average over 100 miles/day are outside of scope. To establish an optimistic reference point, we allow the BEV-only case to allocate BEVs whose battery pack is large enough to accommodate the average trip. This results in a net increase of GHG emissions by 13%. In practice, range anxiety may cause consumers to demand even greater range from BEVs than the 95th percentile distance in the absence of widespread, convenient public charging infrastructure, since accommodation of the 95th percentile longest trip still leaves 18-19 days each year where trip distance is longer than vehicle range.

If dedicated workplace charging is not available, the optimal solution results in about a 0.5% increase in GHG emissions with a smaller portion of PHEVs (of approximately the same sizes) allocated. This is because without the benefit of additional miles of electric travel provided by the second charge, PHEVs compete with HEVs over a smaller range of *s* values. This case is calculated under the optimistic assumption that workplace charging occurs at the halfway point for daily distance for each driver. Under more realistic assumptions, the benefit of workplace charging would be lower, suggesting that availability of dedicated workplace charging is not a significant factor in driving overall life cycle GHG emissions under today's electricity grid.

Under high-carbon coal generation, HEVs have lower lifecycle GHG emissions for all drivers. Under lower-carbon electricity scenarios, the optimal fleet involves larger battery packs and allocation of some BEVs for short-distance vehicles that do not require large battery packs to meet the $s_{95\%}$ range allocation constraint. Lifecycle GHG emissions are reduced significantly with increased grid decarbonization. Future marginal dispatch electricity associated with PHEV and BEV charging will vary by location and charge timing, but the grid scenarios examined here provide a bounding analysis over a wide range of grid GHG intensity.

4. LIMITATIONS AND FUTURE WORK

Several important limitations in the current model call for care in interpreting results. Key limitations include assumptions about vehicle driving and charging patterns, vehicle design options, and electricity generation mix.

One important set of assumptions relates to driving and charging patterns. Assuming that workplace charging allows a charge exactly halfway through daily travel is optimistic for PHEVs, although GHG reduction potential is marginal even under this optimistic assumption. Additionally, we use the UDDS driving cycle to calculate efficiency for all vehicles and do not account for the correlation between driving distance and driving cycle characteristics. Research has shown that real-world driving cycles typically require more energy than standard EPA cycles [23], and longer distances are likely to involve a greater portion of highway travel, where conventional vehicles are more competitive. We lack information on driving cycle characteristics in the NHTS and Minnesota data sets and are unable to account for correlation with daily VMT. We also do not account for other factors such as air conditioning use that affect vehicle energy use. We would expect these factors to make PHEVs and BEVs somewhat less attractive for long distances.

A second important set of assumptions is design options, such as the use of a single scaled engine design, similar to Toyota Prius to model each electrified powertrain alternative. In particular, we do not examine advancements to ICEs that improve fuel economy, such as direct injection, low friction lubricants, variable valve timing, etc. [24], and we do not include PHEVs with blended control strategies due to complexity in modeling the control variable space [25]. Additionally, we do not account for degradation requiring replacement of batteries and chargers prior to the end of vehicle life. Battery degradation will tend to affect smaller battery packs more severely than large packs because processed energy is spread over a larger number of cells in a larger pack.

Third, while we do consider a wide range of possible electricity generation scenarios, we vary these independently in sensitivity analysis and do not consider the effect that vehicle allocation might have on marginal grid mix. If assigning vehicles with larger battery packs leads to greater charging demand, it may have systematic effects on electricity grid mix that vary by region and time and would be expected to change in future scenarios with high penetration of electrified vehicles [7, 12, 14]. In general, marginal electricity associated with charging PHEVs in future grid scenarios may be of somewhat lower carbon intensity than today's U.S. average grid mix in some regions, although it may be higher intensity in other regions. Across regions and assumptions, grid implications should be bounded by our sensitivity scenarios.

5. CONCLUSIONS

We pose an optimization model to minimize annual GHG emissions from the personal vehicle fleet by selecting (1) engine, motor, and battery size for conventional, hybrid, plug-in hybrid, and battery electric vehicles and (2) allocation of those vehicles and of home and workplace charging stations to the vehicle fleet based on annual VMT. Results indicate a best-possible scenario for GHG reductions given existing driving patterns, rather than likely market outcomes.

We find that hybrid electric vehicles and plug-in hybrid vehicles provide the greatest reduction in GHG emissions under most scenarios. Under the current average U.S. grid mix, allocation of conventional vehicles produces 86% more life cycle GHG emissions, HEVs produce 1% more GHG emissions, and BEVs produce over 13% more GHG emissions due to battery production and vehicle weight. Availability of workplace charging has marginal potential for reducing GHG emissions, providing only 0.5% reductions under optimistic assumptions.

Carbon intensity of the electricity grid has a significant effect on GHG emissions of electrified vehicles. Low-carbon scenarios make larger battery packs more competitive; however, the optimal PHEV pack under the current average U.S. grid mix holds about 30 miles (48 km) of charge. Larger battery packs would allow longer travel on electricity, rather than gasoline, but the GHG benefit is offset by greater emissions in battery production and lower efficiency of heavier vehicles. Under our modeling assumptions, BEVs are allocated only to a small subset of the population under decarbonized grid scenarios, and they may not offer substantial GHG reductions over PHEVs.

In future work, we aim to address remaining model limitations while also examining life cycle cost and petroleum consumption.

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