UNIVERSITY OF CALIFORNIA,
IRVINE

Alternative Light- and Heavy-Duty Vehicle Fuel Pathway and Powertrain Optimization

DISSERTATION

submitted in partial satisfaction of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

in Mechanical and Aerospace Engineering

by

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DEDICATION

To Tracy

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NOMENCLATURE

AD	anaerobic digestion
AER	all electric range
APEP	Advanced Power and Energy Program
BER	battery electric range
BEV	battery electric vehicle
bhp	brake horsepower
BoP	balance of plant
BTU	British thermal unit
CA	California
CAP	criteria air pollutant
CARB	California Air Resources Board
CD	charge depleting
CH_4	methane
CO_2	carbon dioxide
CO_{2e}	carbon dioxide equivalent
CRF	capital recover factor
CS	charge sustaining
d	day
FASTSim	Future Automotive Systems Technology Simulator
FCEV	fuel cell electric vehicle
FOM	fixed operations and maintenance
FT	Fischer-Tropsch
FUF	fleet utility factor
g	gram
GGE	gallon of gasoline equivalent
GHG	greenhouse gas
GJ	gigajoule
GVWR	gross vehicle weight rating
GW	gigawatt
h	hour

H_2	hydrogen
HEV	hybrid electric vehicle
HRS	hydrogen refueling station
IC	internal combustion
ICE	internal combustion engine
ICV	internal combustion vehicle
kg	kilogram
kW	kilowatt
kW_{th}	kilowatt, thermal
kWh	kilowatt-hour
LDV	light-duty vehicle
LEV	low emission vehicle
LP	linear programming
MILP	mixed integer linear programming
MPa	megapascal
MPGDE	miles per gallon of diesel equivalent
MPGGE	miles per gallon of gasoline equivalent
MSRP	manufacturer's suggested retail price
MSW	municipal solid waste
MW	megawatt
NHTS	National Household Travel Survey
N_2O	nitrous oxide
NO_x	nitrogen oxides
OM	operations and maintenance
PEV	plug-in electric vehicle
PFCEV	plug-in fuel cell electric vehicle
PHEV	plug-in hybrid electric vehicle
PM	particulate matter
SMR	steam methane reformation
SNG	substitute natural gas
SUV	sport utility vehicle

ULEV	ultra-low emission vehicle
US	United States
V	volt
VMT	vehicle miles traveled
VOC	volatile organic compound
VOM	variable operations and maintenance
WTW	well-to-wheels
yr	year
ZEV	zero-emission vehicle
^{o}C	degrees Celsius

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CONFERENCE PRESENTATIONS

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ABSTRACT OF THE DISSERTATION

Alternative Light- and Heavy-Duty Vehicle Fuel Pathway and Powertrain Optimization

By

Blake Alexander Lane

Doctor of Philosophy in Mechanical and Aerospace Engineering

University of California, Irvine, 2019

Professor G. Scott Samuelsen, Chair

An increasing number of alternative vehicle fuel and powertrain options are evolving for both light-duty vehicles (LDVs) and heavy-duty vehicles (HDVs) to combat climate change and degraded air quality. Electricity, hydrogen, substitute natural gas, renewable gasoline, and renewable diesel are examples of alternative fuels, while internal combustion engines, fuel cell engines, plug-in battery engines, hybrids, plug-in hybrids, and electrical drivetrains are examples of components comprising powertrains. With such a diverse set of options for LDVs and HDVs, a systematic evaluation of the options that meet environmental goals at a minimum cost is required.

Using linear programming with fuel pathway and vehicle costs, emission constraints, realistic growth scenarios for travel and technology, and fuel feedstock availability, a methodology is developed ("Transportation Rollout Affecting Cost and Emissions, TRACE") to assess combinations of fuel and vehicle pathways. Each pathway has an associated efficiency, cost, and emission of greenhouse gases (GHGs) and criteria air pollutants (CAPs). Techno-economic data from the literature and Wright's Law project the cost of infrastructure to produce, distribute, and dispense fuel, and to produce vehicles through 2050.

The results from a Reference Case, comprised of business-as-usual fossil fuel and internal combustion vehicles (ICVs), projects costs of $1.43 trillion. For current LDV regulations in California, the optimization suggests adoption of ICVs fueled by renewable gasoline in the early years with many plug-in hybrid electric vehicles, a large population of zero-emission battery electric vehicles starting in 2030, and significant plug-in fuel cell electric vehicle (PFCEV) adoption in 2050. For all modeled HDV vocations (linehaul, drayage, refuse, and construction), TRACE projects ICVs fueled by renewable diesel until 2045, after which hybrids and PFCEVs are adopted for all vocations except refuse. This LDV and HDV rollout is projected to cost $1.28 trillion by 2050, 10% less than the Reference Case. Significant factors affecting results include battery costs, change in vehicle miles traveled, and zero-emissions vehicles (ZEV) constraints. For cases with proactive ZEV inducements, plug-in FCEVs displace ICVs while satisfying the long range and short fueling attributes provided today by ICVs, reducing GHGs an additional 18% and CAPs up to an additional 40%.

1. INTRODUCTION

1.1 Motivation

The transportation sector is amidst a time of major changes in various regards. Numerous factors such as energy independence, air quality, climate change, more renewable electricity production, and pieces of legislation aimed at transportation and emissions are forcing the fuels and powertrains of vehicles to evolve. This has caused automakers to offer a wide variety of vehicles that are powered by different, sometimes multiple, fuels and unconventional powertrains, such as batteries and fuel cells. This wide variety of options is only increasing as research into other carbon-free or carbon-neutral fuels, new fuel production pathways, and advanced powertrains all improve their viability and marketability. The wide array of options is vast compared to the traditional use of gasoline-fueled light-duty vehicles (LDVs) and diesel-fueled heavy-duty vehicles (HDVs).

Consider a trip to a local car dealership. If one were to go intending to buy a car today, a salesperson would offer the option of purchasing a conventional car that runs on gasoline, but they could mention the option of a car that also uses electricity as a fuel, or another one that only uses electricity, or a fourth option that uses hydrogen as a fuel. With all of these options and more, it is impossible for the average consumer to judge what might be best for themselves in terms of fuel cost and driving characteristics. It is even more challenging for the average consumer to judge what is best for society as a whole, considering the intricacies of cost, efficiency, and emissions of various kinds at the many stages of fuel production and vehicle use.

At the same time as options for vehicle fuels and powertrains are increasing dramatically, the world is facing growing issues of climate change and air quality. Transportation accounts for over a quarter of greenhouse gas (GHG) emissions in the U.S., and 14% of GHG emissions

worldwide, as shown in Figure 1 [1], [2]. These GHGs exacerbate climate change. Transportation is also responsible for 38% of criteria air pollutants (CAPs) in the U.S. [3]. These CAPs are what lead to poor air quality, respiratory issues, and a number of other health hazards for those that breathe them [4]–[6]. It is clear from these data that the transportation sector is an important area of research to meet air quality and climate change goals.

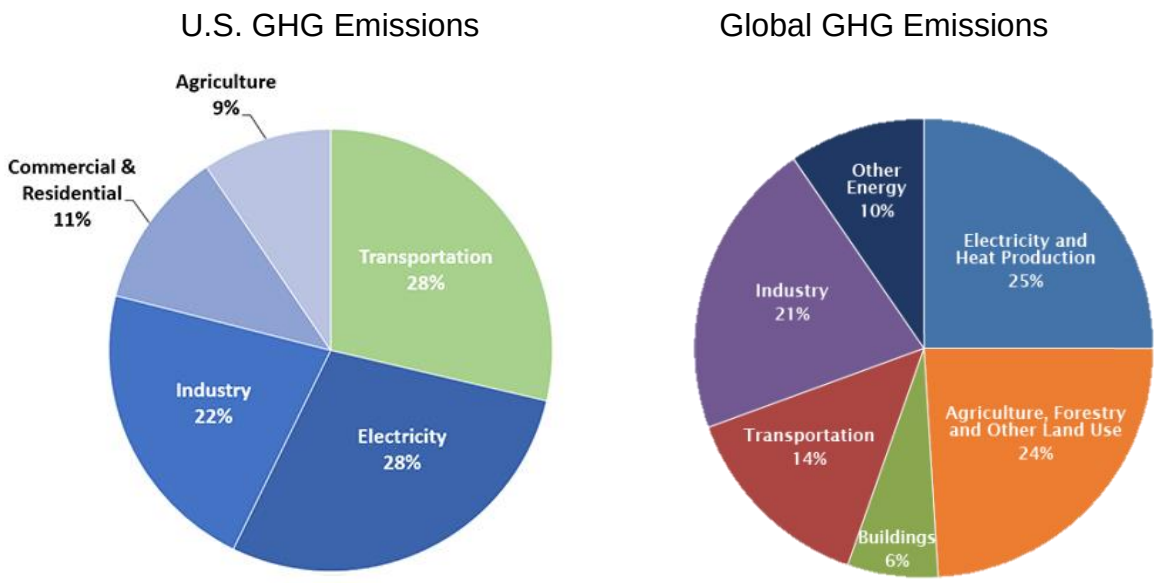

Figure 1. Left chart: U.S. GHG emissions per economic sector in 2016, from U.S. EPA [1]; Right chart: Global GHG emissions per economic sector in 2014, from U.S. EPA [2]

Focusing on California, transportation is the largest emitter of GHG emissions, responsible for 41% of GHG emissions. Furthermore, about 90% of these GHG emissions are from LDV and HDVs [7].

As a politically progressive state with some areas burdened by poor air quality, California has a number of pieces of legislation as well as goals relating to the environment. Table 1 lists a variety of legislation and goals either directly or indirectly relating to transportation.

Table 1. California transportation legislation and goals

Climate Change	
AB 32: Global Warming Solutions Act [8]	Reduce GHG emissions to 1990 amounts by 2020
SB 32: California Global Warming Solutions act of 2006 [9]	Reduce GHG emissions to 40% below 1990 amounts by 2030
California Governor's Executive Order # S-03-05 [10]	Reduce GHG emissions to 80% below 1990 amounts by 2050
SB 2: Renewable Energy Resources [11]	33% of electricity is renewable by 2020
SB 350: Clean Energy and Pollution Reduction Act of 2015 [12]	50% of electricity is renewable by 2030
SB 100: California Renewables Portfolio Standard Program [13]	100% of electricity is zero-carbon by 2045
SB 375: Sustainable Communities [14]	Reduce GHG emissions by community planning for transportation and land use
Transportation Fuel	
Low Carbon Fuel Standards [15]	Reduce carbon in transportation fuel by 10% in 2020
AB 1007: State Alternative Fuels Plan [16]	Plan to use more alternative fuels in CA, including details on how to increase hydrogen use
AB 118: California Alternative and Renewable Fuel, Vehicle Technology, Clean Air, and Carbon Reduction Act [17]	Provides funding for technologies that improve local air quality
Zero Emissions Vehicle Action Plan[18]	Plan to achieve 1.5 million ZEVs in CA by 2025
AB 8: Alternative Fuel and Vehicle Technologies [19]	Allocates $20 million each year for hydrogen fueling stations until 100 are built
SB 1505: Environmental Standards for Hydrogen Production [20]	Requires that hydrogen be 33.3% renewable, and have 30% lower GHG and 50% lower CAP emissions than gasoline
Heavy-Duty Vehicles	
AB 739: State vehicle fleet: purchases [21]	A minimum of 15% of certain state-purchased heavy-duty vehicles must be ZEVs by 2025 and 30% by 2030
AB 1073: California Clean Truck, Bus, and Off-Road Vehicle and Equipment Technology Program [22]	Extended funding for heavy-duty trucks, according to California's Clean Truck, Bus and Off-Road Vehicle program
Goods Movement Emission Reduction Plan [23]	$1 billion allocated to a collaboration between California Air Resources Board and local agencies to reduce pollutant emissions in freight corridors
California Sustainable Freight Action Plan [24]	Creates 2050 goals for cleaner freight system, targets for 2030, and assistance in starting pilot projects
San Pedro Bay Ports Clean Air Action Plan, 2018 Update [25]	Newly-registered trucks at the Ports of Long Beach and Los Angeles must be model year 2014 or newer

Three key ideas are found in these goals and pieces of legislation: (1) California is actively pursuing methods to reduce GHG and CAP emissions from both the electric grid and the transportation sector, which are increasingly overlapping; (2) various fuels ranging from electricity to hydrogen to others that are actively being researched are potential methods of these emissions reductions; and (3) all classes of vehicles, including LDVs and HDVs, have room to reduce emissions and support California's efforts.

A study that analyzes the wide range of potential fuel pathways and powertrain configurations for vehicles and optimizes an evolution of the transportation sector has yet to be completed. Furthermore, there has not been a study that includes the breadth of vehicle fuels and included a vehicle powertrain component of the optimization as well. This encompassing work, however, is necessary due to the wide array of options. Simply analyzing a few of the fuels in isolation from the powertrains, or a general analysis of the powertrains without including a detailed study of the associated fuel pathways does not allow for a meaningful result that can direct the evolution of the transportation sector at this critical time.

Both cost and emissions are two key components of these technologies. Cost is a necessary consideration. If a technology has promising emissions reductions but is prohibitively expensive, the technology will not be widely adopted due to economic constraints. Regarding emissions, the aim is to combat climate change and improve air quality. Therefore, technologies that reduce emissions and thereby allow for compliance with previously-introduced legislation and goals should be prioritized. Therefore, a combined analysis of cost and emissions is needed to better understand what technologies should be pursued.

This dissertation explores the future of the automobile, with emphasis on the fuels and powertrains envisioned for alternative vehicles. With such a wide range of fuel pathways and

powertrain configurations, it is wise to establish an objective methodology to determine which combination provides the most economical method of meeting our environmental goals. Constructing a methodology that works for the bulk of the transportation sector, including LDVs and HDVs, will yield the most insight and have the broadest impact on air quality and climate change. While medium-duty vehicles (MDVs) are important to commerce, the GHG and CAP emissions are relatively negligible when compared to the LDVs and HDVs modeled in the present work.

1.2 Goal

The goal of this dissertation is to establish viable fuel pathways and powertrain configurations for LDVs and HDVs that meet environmental constraints at the lowest cost. This work develops a methodology to characterize and project various fuel pathways and powertrain configurations techno-economic data and then determine a fleet to meet transportation needs into 2050. The results of this work will inform the transportation industry and policy makers how society might effectively transform the transportation sector in a future of stricter environmental regulations.

1.3 Objectives

To meet this dissertation goal, the following objectives will be completed:

1. Establish the fuel pathways for LDVs and HDVs.
2. Establish the powertrain configurations for LDVs and HDVs.

3. Develop efficiency, cost, and emissions data out to 2050 for the fuel pathways established in Objective 1 and the vehicle powertrain configurations established in Objective 2.
4. Establish the constraints of the optimization problem using California legislation and executive order for emissions, realistic growth scenarios for travel and technology, and feedstock availability.
5. Determine optimization tool to use given the results of Objectives 3 and 4, and establish the formal optimization problem.
6. Solve the optimization problem established in Objective 5 to determine the emissions and cost impacts of the optimum cases. Compare these results to the Reference Case.
7. Systematically assess the results to establish viable fuel pathways and powertrain configurations for LDVs and HDVs that meet the constraints of this problem.

2. BACKGROUND

Areas of study that are relevant to this work include vehicle fuel production methods, vehicle powertrain configurations, and optimization techniques. Each of these three areas will be discussed in the following sections in as much detail as is needed to follow the work of this dissertation.

The scope of analysis for this work is known as well-to-wheels (WTW). This includes the production of fuel from its feedstock, the distribution of the fuel, the dispensing of the fuel, and the use of the fuel in vehicles.

2.1 Vehicle Fuels

Five alternative fuels are likely to be used in the next few decades in LDVs and HDVs. These fuels are electricity, hydrogen, substitute natural gas (SNG), renewable gasoline, and renewable diesel [26]–[30].

Each of the above fuels can be produced in a variety of manners. Some constraint on the scope of this work is used to focus on pathways that are, according to the state of the art of this writing, more likely to be viable from cost and efficiency perspectives. This does not preclude the fact that future technology advancements may introduce new fuels or pathways. It is important to note that while these potential future advancements could mean reality may be different from the projections of the present work, the advancements can be integrated into the methodology introduced herein at the time that they are discovered. It is recommended that the current state of the art be updated from time to time to ensure the most accurate data are used.

2.1.1 Fuel Feedstocks

A fuel feedstock is an input that is converted to a fuel through one of a multitude of fuel production technologies that are available. For the five alternative fuels introduced, there are two broad feedstock categories: electricity and biomass.

2.1.1.1 Electricity

Electricity is widely familiar throughout society as a means of turning on lights, running fans, charging phones, and many other daily necessities of the modern world. Less familiar to most is using electricity as a main input for making vehicle fuels. Most would understand how electricity might be used in various processes of refining gasoline for cars. However, for some alternative fuels for vehicles, electricity is a main feedstock. Furthermore, certain kinds of vehicles, known as plug-in electric vehicles (PEVs), use electricity directly as a fuel.

As a fuel feedstock, electricity is primarily used to convert water into hydrogen in a process known as electrolysis. Water could be considered a co-feedstock along with electricity. However, given the techno-economic nature of this work, and the fact that water costs will likely stay a small fraction of overall fuel costs, which will be discussed in more detail later in this dissertation, the water feedstock is not further considered in this work. It should be noted, however, that future electrolytic fuel production should be located in an area with water availability to increase efficiency and cost-effectiveness.

2.1.1.2 Biomass

Biomass comes from both plant and animal sources. In the scope of the present work, biomass can be used for producing either electricity or gaseous, liquid, or solid fuel. Biomass is therefore quite flexible as a feedstock category.

Biomass availability, for both the U.S. and California in particular, is sourced from the U.S. Department of Energy's Billion Ton Report [31]. Biomass is separated into seven crop type categories in the Billion Ton Report, as follows: (1) agriculture residues, (2) energy crops, (3) food waste, (4) forest residue, (5) manure, (6) municipal solid waste (MSW), and (7) tree. The individual feedstocks that compose each of these crop types are listed in Table 2.

Table 2. Biomass feedstocks by crop type according to Billion Ton Report [31]

Agriculture residues	**Energy crops**	**Food waste**	**Forest residue**	**Manure**	**MSW**	**Tree**
Barley straw	Miscanthus	Food waste	Hardwood, lowland, residue	Hogs, 1,000+ head	Construction and demolition waste	Hardwood, lowland, tree
Citrus residues	Poplar		Primary mill residue	Milk cows, 500+ head	MSW wood	Hardwood, upland, tree
Corn stover			Secondary mill residue		Other	Softwood, natural, tree
Cotton gin trash			Softwood, natural, residue		Paper and paperboard	Softwood, planted, tree
Cotton residue			Softwood, planted, residue		Plastics	
Non-citrus residues					Rubber and leather	
Rice hulls					Textiles	
Rice straw					Yard trimmings	
Tree nut residues						
Wheat straw						

Note that one defining factor of these biomass feedstocks that will play a role in determining which fuel production technologies that can be used is moisture content. Both food

waste and manure categories are high-moisture biomass categories, whereas the rest are typically dry.

Additionally, the non-organic portions of the MSW, which include plastics, rubber, and leather, are not included in this analysis as potential fuel production feedstocks. The feedstock quantities that will later be shown reflect this removal of the non-organic MSW from the original Billion Ton Report data.

2.1.2 Fuel Production

What follows are descriptions of the various methods of fuel productions for the five fuels considered in this work, categorized first by the fuel being produced and then by the specific fuel production technology adopted.

2.1.2.1 Electricity Production

From the perspective of PEVs, electricity is the fuel itself, and not simply a feedstock as introduced previously. This work assumes the electricity production feedstocks and methods as projected by entities such as Energy and Environmental Economics (E3) [32] and Argonne National Laboratory's GREET Model [33]. The reasoning for this is that the electricity sector is larger than simply the demand for transportation. There are legislation and goals for the electric grid in particular, and therefore it is reasonable to assume that a transportation analysis will not dramatically impact the evolution of the feedstock portfolio for electricity generation. However, it is important to note that transportation and electricity generation are increasingly intertwined as vehicle electrification increases.

Electricity is generated from a wide variety of sources, ranging from fossil fuels such as natural gas used in gas turbines to renewable sources such as solar panels. Due to the wide variation in the production of electricity that is beyond the scope of this work, the PATHWAYS model by E3 is used to determine how the electricity grid composition will change with time [32]. This model shows the projected evolution of the electric grid from 2015 to 2050 along various evolution scenarios. The one used for this dissertation is the “Straight Line” scenario which assumes a linear reduction in emissions to reach emissions reductions goals in 2050, and also complies with the recent SB 100 legislation that was introduced in Table 1.

Detailed electricity production discussion is outside the scope of this work for the reasons stated above. However, some general facts are important to note. Figure 2 displays the electricity generation sources in California for February 2019 with data from the U.S. Energy Information Administration [34]. Natural gas is used in combustion electricity generators known as gas turbines. There are various evolutions of the gas turbine plant, including combined cycle plants which use waste heat of the gas turbine as heat input for a steam turbine to produce additional electricity from the same natural gas fuel input. Nuclear power, while somewhat significant in terms of power generated, is set to be phased out of California when the last nuclear plant at Diablo Canyon is shut down in 2025 [35]. Coal has been almost completely phased out, with only one plant still producing electricity from coal [36], and it is unlikely to return due to the strict environmental regulations of the State.

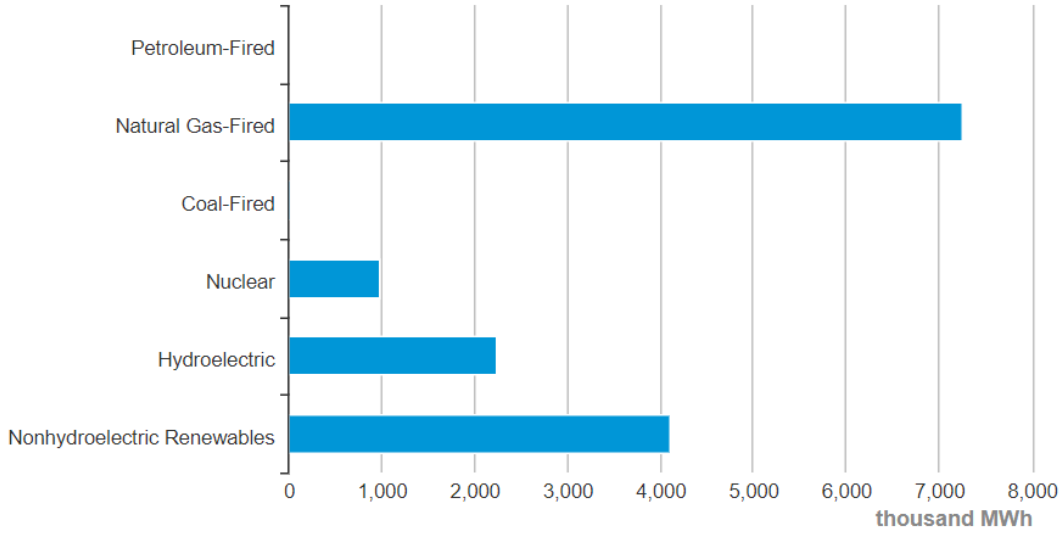

Figure 2. Electricity Sources in California in February 2019, from U.S. Energy Information Administration [34]

It is clear that natural gas is a major feedstock for the California electric grid. The rest of the electricity comes from renewables such as solar and wind, hydroelectric, and nuclear power. As the last remaining California nuclear generators will be decommissioned in 2025 [35], natural gas, renewables, and hydroelectric plants will make up the demand that is now served by nuclear. Therefore, electricity either as a fuel or a fuel feedstock will either be associated with an emission-free technology such as renewables or hydroelectric plants, or it will come from a natural gas-powered plant, which does have emissions from combustion. However, it is possible that these natural gas-fueled electricity generators can start to use SNG which have varying emissions impacts, just as vehicles are set to use SNG instead of fossil-source natural gas. While these competing uses of biomass feedstocks are not considered in this work, it is important to keep in mind that the biomass feedstocks considered herein could potentially be used for broader electricity demand such as those of the commercial or industrial sectors.

2.1.2.2 Hydrogen Production

Hydrogen is a gaseous fuel at ambient temperature and pressure, though it is often stored at higher pressures to increase volumetric energy density. Hydrogen can be combusted like current fossil fuels in vehicles, but in this work it is assumed that hydrogen is a fuel only for fuel cells. Fuel cells are electrochemical conversion devices, and more detailed information about them will come later in the section discussing the various vehicle powertrain configurations. Suffice it to say for now that fuel cells are an alternative to combustion engines which do not have any harmful emissions when fueled by hydrogen.

Hydrogen can be made from one of three major production methods. First, hydrogen can be produced from electrolysis of water, meaning production efficiency and associated emissions are heavily dependent on those of the electricity used. Second, hydrogen can also be produced from biomass gasification. Gasification involves heating dried biomass without an oxidant (air) to produce bio-oils, a process known as pyrolysis. Next, the bio-oils are further heated with an oxidant (such as air) and water. Fuels produced from biomass feedstocks, such as hydrogen from biomass gasification, are known as biofuels. Thirdly, hydrogen can be produced from steam methane reformation (SMR). SMR is a process in which methane and water react at high temperatures to produce hydrogen. The methane being reformed can come from one of the SNG processes described in the relevant section of this dissertation.

a) Electrolytic Hydrogen Production

Electrolysis splits water with electricity to produce hydrogen and oxygen using electrolyzers of three main varieties: alkaline electrolytic cells (AECs), proton exchange membrane electrolytic cells (PEMECs), and solid oxide electrolytic cells (SOECs). AECs are the

most mature form of electrolyzers of these three in that they have been available commercially for the longest time. PEMECs are the next most mature. SOECs are the least mature electrolyzer, with no commercially available examples available and a technology readiness level (TRL) of 2-4 in 2014 [37].

Power-to-gas (P2G) is an emerging technology that transforms energy in the form of electricity to energy in the form of a gaseous fuel such as hydrogen (or methane, which will be detailed shortly). This is useful due to the increasing amount of renewable energy such as wind and solar which are intermittent and not easily predictable. P2G can be used as a form of energy storage in that the gas that is produced from electricity can be stored in containers or even the natural gas grid for later use either as a vehicle fuel or fuel for other purposes.

P2G is flexible due to the numerous possible pathways for energy to flow. These pathways are depicted in Figure 3. P2G can connect the electric grid and the natural gas grid, two large energy distributors of the modern day. This allows the benefits of both grids to be utilized while downplaying their characteristic issues. For example, P2G can use the highly efficient electric grid when possible (meaning there is demand for more electricity), but also use the natural gas grid when there is not an immediate demand for power (making use of the natural gas grid's inherent storage ability). P2G also enables other transfers of energy, such as fueling vehicles that run on hydrogen, natural gas, or electricity.

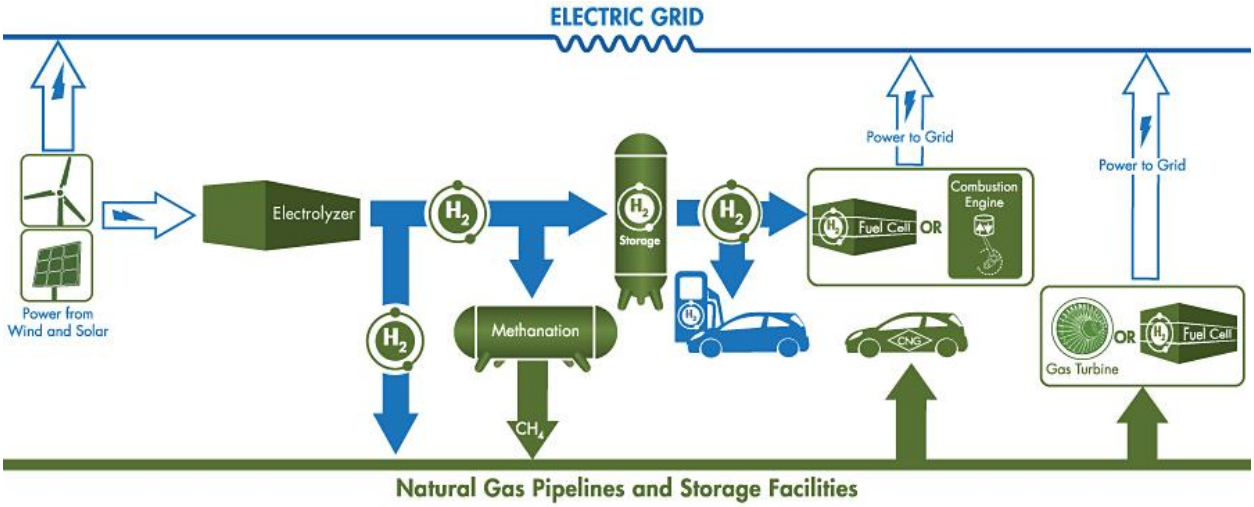

Figure 3. Schematic of P2G Pathways, from the Advanced Power and Energy Program [38]

As seen from Figure 3, the first step in P2G, no matter which pathway is being followed, is using electricity in an electrolyzer to produce hydrogen. Therefore, the emissions associated with P2G are directly tied to the emissions associated with the production of the electricity used by the electrolyzer. While Figure 3 only shows renewable sources of electricity, P2G can also use fossil sources of electricity which do have emissions.

A particularly attractive use of P2G comes from using what would be curtailed, or wasted, electricity from renewable energy sources such as solar panels and wind turbines [39]. As mentioned above, both wind and solar power are intermittent and hard to predict precisely. P2G is able to use electricity from these renewable sources at times when the electric grid might not be able to accept them, which is brought about by the fact that electricity must continually be used at the same time as it is generated. This means more of the renewable electricity generated would be used in other areas such as making renewable hydrogen for vehicle fuel. Increasing renewable energy usage will decrease the emissions associated with both the electric grid and the natural gas grid, which are both intertwined with the advent of P2G.

To focus on the work conducted within this dissertation, it is beneficial to summarize the pathways and technologies used herein. Figure 4 is a flowchart that includes all such pathways for electrolytic hydrogen production. The overall idea of these pathways is to use electricity (produced from either fossil fuels or non-fossil fuels such as solar and wind power) to produce hydrogen from water. This gaseous fuel can be made by any of the three electrolyzer technologies displayed below.

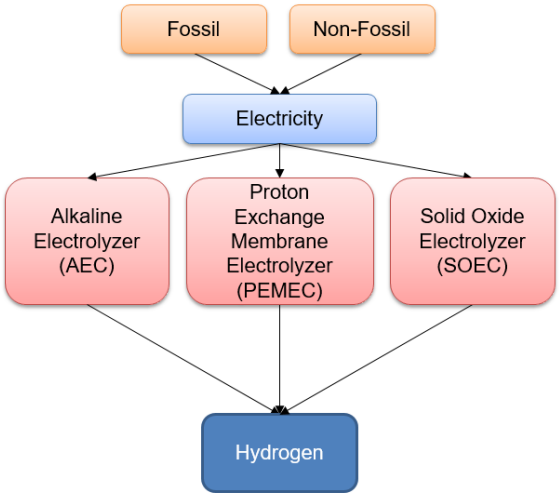

Figure 4. Flowchart of analyzed electrolytic hydrogen production pathways

b) Gasification Hydrogen Production

Gasification is a thermochemical process in which solid biomass is heated in the absence of oxygen to produce a gaseous mixture known as syngas [40]. This syngas is composed primarily of hydrogen and carbon monoxide. Hydrogen can then be separated from this mixture [41][42][43], [44][45]–[52].

Note that gasification is most efficient with dry biomass [40]. Drying would be required for higher moisture content biomass, and the efficiency loss there would make gasification less attractive than an alternative process such as anaerobic digestion, which will be introduced later.

Therefore, this work assumes only dry biomass as potential feedstocks for gasification, including agricultural residues, MSW, forestry residues, trees, and energy crops. Food waste and manure are not considered feedstocks for gasification in this work as they would require significant drying which would decrease overall efficiency.

c) Steam Methane Reformation Hydrogen Production

SMR is a chemical reaction in which methane (CH_4) is converted to hydrogen (H_2) according to the following reaction in Equation 1.

Equation 1. Steam methane reformation reaction

$$\mathrm{CH_4 + H_2O \rightarrow CO_2 + 4H_2}$$

This process is currently used on natural gas, a fossil fuel, to make 95% of hydrogen in the U.S. [53]. Additionally, some biogas is put through SMR to meet SB 1505, the requirement that one-third of hydrogen sold at fueling stations is renewable.

Due to this work's focus on increasing adoption of renewable fuels and the roundabout method of production using SMR which lowers efficiency by about 70% [54] (first biogas would need to be produced from the primary biomass by one of the methods to be introduced shortly, and then that biogas would be converted to hydrogen), this production method is not considered in this work.

2.1.2.3 SNG Production

Substitute natural gas (SNG) is a drop-in fuel, meaning it can be integrated into current natural gas infrastructure, including pipelines and dispensing stations, and be used in current vehicles that are fueled by natural gas. Being a drop-in fuel allows for easy integration of a fuel that can be made in a more environmentally-friendly manner, and using resources that may be

more prevalent in any given area. One potential benefit of drop-in fuels such as SNG is time of transition: it may take less time to reduce emissions by changing the fuel than by changing the vehicle, either with efficiency improvements or alternative powertrain technologies.

Three methods of producing SNG are considered in this dissertation. Those three methods are electrolytic methanation and biomass conversion by either anaerobic digestion or gasification. Electrolytic production of SNG uses electricity as its feedstock. This process begins the same as electrolytic hydrogen production, and is followed by a methanation step to convert that hydrogen into methane using carbon dioxide. Anaerobic digestion (AD) is a biochemical process that uses microbes to break down organic matter to methane and carbon dioxide. Gasification for SNG production, as for hydrogen mentioned previously, requires lower moisture biomass. Again, these dry biomass feedstocks are agricultural residues, MSW, forestry residues, trees, and energy crops.

a) Electrolytic SNG Production

Electrolytic methanation starts in the same way as electrolytic hydrogen, but there is a following methanation step. This production method also belongs to the umbrella term P2G introduced previously.

Methanation is the chemical reaction that turns hydrogen and carbon dioxide into methane and water. This chemical reaction is also known as the Sabatier reaction, and it is exothermic, meaning heat is a product. The chemical equation is listed below with the correct stoichiometric coefficients in Equation 2. Each mole of reaction gives off 165 kilojoules of heat [55].

Equation 2. Sabatier reaction

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$

Literature was consulted for technologies that provide carbon dioxide for making SNG from hydrogen as well as technologies to make use of the heat produced during the methanation process. Both of these technologies are needed because the Sabatier reaction (1) is an exothermic reaction that requires a heat sink for sustained reaction without overheating equipment, and (2) requires carbon dioxide as input to convert hydrogen into methane [56].

The primary benefit of methanation is the ability to take advantage of the natural gas infrastructure. Without methanation, hydrogen is the main product of P2G. However, there is not much infrastructure in the U.S., or even the world, for hydrogen. Therefore, the extra step of methanation makes P2G much simpler to integrate into the power grid of today and transport to areas of demand. Use of natural gas pipelines and storage throughout the country and much of the rest of the world make P2G more practical today. The tradeoff for this practicality is the loss of efficiency by adding the extra step of methanation as well as the additional emission of carbon wherever the SNG is eventually used.

Because methanation can take place at a range of temperatures and its efficiency is benefitted by some pressurization, it is wise to include a range of temperatures and an above-ambient pressure in calculations [55]. An equilibrium analysis using NASA's Chemical Equilibrium with Applications code at 5 atmospheres of pressure at 400, 500, and 600°C leads to an average methanation efficiency of 0.7904 [57]–[59]. This is calculated by analyzing the products of the Sabatier reaction at the given pressure and temperatures, and determining what fraction of the products is methane, the desired product.

Methanation is pressure dependent in such a way that it is more efficient at producing methane at higher pressures [60]. Methanation efficiency is highly dependent on reaction temperature. At 400°C with a 4 to 1 molar ratio of hydrogen to methane input (the stoichiometric ratio of the Sabatier reaction), the methanator output is 92% methane; at 500°C, the output is 81% methane; and at 600°C, the output is 64% methane. Therefore, operating at a lower temperature would increase the amount of methane coming out of the methanator, which could also remove the need for any gas cleanup before injection into the natural gas pipeline. However, it is important to keep in mind other effects of lowering the temperature of the methanator. One major impact is there will be lower quality waste heat which would be used in other P2G processes to be expanded upon later. This could lower the overall process efficiency, even if the amount of methane is decreased. A more careful analysis would be needed based upon an individual plant design.

See Figure 5 for equilibrium species concentration of a methanator at 5 atmospheres of pressure. Note that some methanators may not allow for the full expected conversion of carbon dioxide and hydrogen to methane due to time reacting. Because the calculations discussed are for equilibrium concentrations, and equilibrium takes time to achieve, actual methanation efficiency may be lower than calculated if time spent reacting in the methanator does not allow for equilibrium to be reached. Therefore, it is important to ensure reactor design does so, or account for the drop in conversion efficiency of the methanator used.

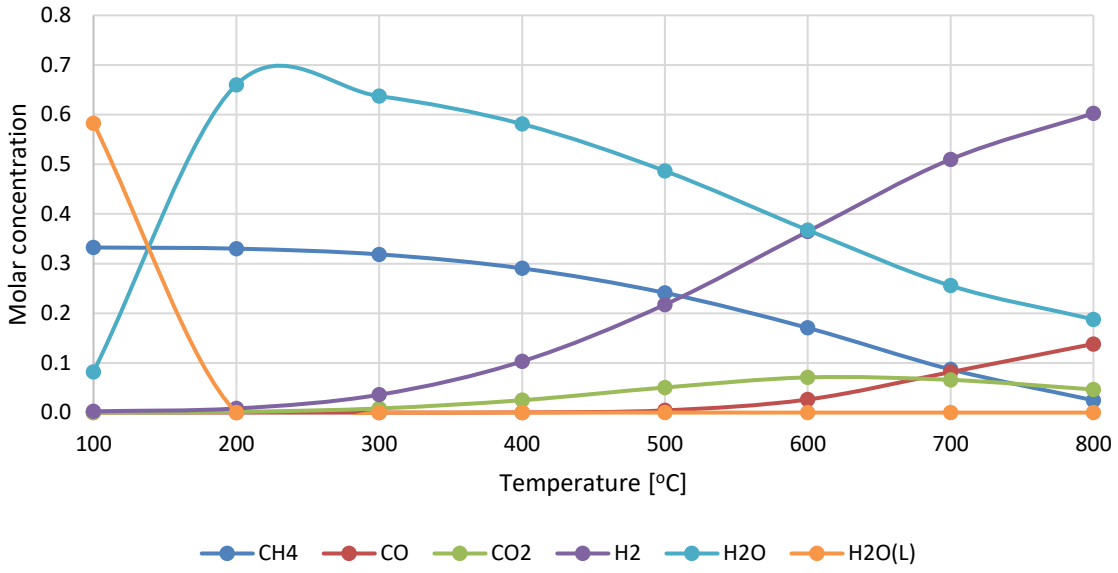

Figure 5. Methanator equilibrium species concentrations at 5atm

Lastly, the energy required for the methanation process itself as well as any necessary gas cleanup before injecting must be considered. Two steps are required: (1) carbon dioxide removal and (2) water removal. Carbon dioxide removal is accomplished using amines, organic compounds are used as solvents to capture carbon dioxide. This carbon dioxide can be recirculated back into the methanator to improve process efficiency. Water removal is accomplished through cooling of the gas mixture and collecting the water as it condenses back out. This water can be recirculated back to the electrolysis step, also improving process efficiency. These two cleanup steps produce gas that is able to be injected into the natural gas grid [61]. In some scenarios, simply a removal of the water is all that is needed to produce natural gas pipeline-quality gas [62]. According to Collet et al., when a nearly stoichiometric ratio of hydrogen and carbon dioxide are input to the methanator, the above two processes account for a mere 1.3% of the amount of energy input to the electrolyzer [63]. Therefore, these two processes can be assumed to be of negligible energy requirement for the overall P2G process. However, it is important to remember that gas cleanup will be needed, and that need

increases as the methanator temperature increases because less methane will be output from the methanator as the temperature increases.

A diagram showing the various electrolyzers, heat sinks, and carbon dioxide sources analyzed in this work for electrolytic SNG production is shown below in Figure 6.

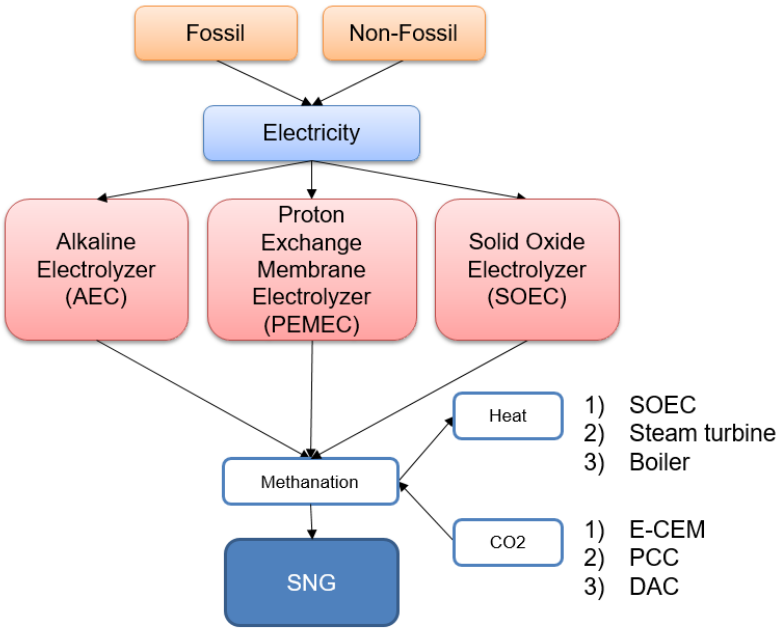

Figure 6. Flowchart of analyzed electrolytic SNG production pathways

The three electrolyzer types have already been introduced in the discussion of electrolytic hydrogen production. What follows are the various heat sink and carbon dioxide source technologies.

Heat Sink

The heat sink technologies for the methanation process that have been considered are SOECs, steam turbines, and boilers to produce steam. The TRLs for each of these are shown in Table 3.

Table 3. Heat sink TRLs

Heat sink technology	TRL
SOEC	5
Steam turbine	9
Boiler	9

Solid Oxide Electrolyzers

SOECs are high temperature electrolyzers which take in electricity and water and output hydrogen and oxygen. Because they operate at high temperatures of up to 800°C or sometimes higher, they often require heat input to achieve those high temperatures. Coincidentally, the range of operation temperatures of methanation reactors is similar to that of SOECs, so SOECs can serve as heat sinks for the methanation process to achieve a slight increase in efficiency [64], [65].

SOECs stand out in this application because they can be used to produce more hydrogen, which can in turn make more SNG. With the heat coming from the Sabatier reaction at a high temperature, the only other needed input is water to produce hydrogen with the SOECs. However, SOECs have a lower TRL than other heat sink technologies, so they need some more time to develop before they can be widely adopted. As they are, they also react slower than other electrolyzer technologies and therefore need to improve their dynamics for P2G applications, but this improvement is expected to be realistic [66], [67].

Steam Turbines

Steam turbines are another attractive option as they produce electricity with the waste heat of the Sabatier reaction, and this electricity could be used to power components of the SNG production plant or be put into the electric grid. Steam turbines are used in a Rankine cycle to produce electricity. They are a well-established technology that come in various power

capacities, making them flexible for different-sized SNG production plants in the future. Steam turbines would be sized to take advantage of the waste heat from the methanation process and produce as much electricity as possible.

Steam Production

The last option considered, producing steam, would be able to provide heat to any components of the SNG production plant or be piped to any nearby industrial or other facility in the vicinity that might need steam. Like steam turbines, the heat exchangers that could produce the steam are a well-established technology. Furthermore, they can also be easily sized to meet the heat sink requirement of the methanation process at SNG production plants.

Carbon Dioxide Source

The carbon dioxide source technologies that have been considered are post-combustion capture (PCC), direct air capture (DAC), electrolytic cation exchange modules (E-CEM), and co-location with a biofuel plant. The TRLs of each are shown in Table 4, with the biofuel plant technology omitted as it the technology used is the same as PCC.

Table 4. Carbon dioxide source TRLs

Carbon dioxide source technology	**TRL**
PCC	9
DAC	5
E-CEM	3

Post-Combustion Capture

PCC pulls carbon dioxide from the exhaust stream of a power plant, a stream that is relatively dense in carbon dioxide compared to ambient air. Various solvents, sorbents, and

membranes are used to capture the carbon dioxide from the exhaust stream as the carbon dioxide-containing exhaust flows through the PCC system. Solvents and sorbents capture carbon dioxide and release it under certain conditions such as heating or compressing. Membranes allow only specific molecules, such as carbon dioxide in the case of PCC, to pass through, and other molecules are blocked from passing [68], [69].

The relatively high concentration of carbon dioxide in the exhaust stream of a power plant makes capturing carbon more efficient compared to a less-concentrated source such as ambient air. Priority should be given to the largest sources of carbon dioxide, such as very large power plants, so these PCC installations can capture the most emissions with the least effort of installing systems.

One consideration for PCC placement is the effect on nearby ecosystems due to the decreased carbon dioxide in the air. Particularly for vegetation downstream of the exhaust, the drastic decrease in carbon dioxide can affect growth, which may have undesired effects on the ecosystem as a whole [70]. Of course, the amount of carbon dioxide emitted worldwide must be reduced; the preceding comment is included just to make the reader aware of potential side-effects of the technologies studied herein.

Direct Air Capture

DAC also involves a sorbent to capture carbon dioxide from the ambient air [70]. Because of the lower density of carbon dioxide in ambient air compared to the exhaust stream of a power plant, DAC is not as efficient as PCC.

Due to the nature of carbon dioxide's effect on climate change, DAC units can be placed anywhere and have the same impact. A given amount of carbon dioxide captured has the same

effect on climate change no matter where that carbon dioxide is captured. However, it would be wise to place the DAC units in places with cheap and clean power to make operation more economical and more beneficial to the environment. Additionally, ambient air characteristics affect performance of the DAC systems, so placement should be done based on careful analysis. Humidity has a significant effect on performance due to the water molecules' interference with carbon dioxide capture. Similarly, other molecules in the air such as pollution can effect carbon dioxide capture by either their physical presence or chemical reactions with parts of the DAC system [70].

Similar to that which was discussed for PCC, a further consideration for DAC is the effect it has on ecosystems. Because DACs take in ambient air, the concentration of carbon dioxide is lower than in the exhaust for power plants. Therefore, DAC has the potential to deplete carbon dioxide to a level that could affect downstream ecosystems [70]. And again, carbon dioxide levels should be reduced; this is simply a side-effect that should be considered.

Electrolytic Cation Exchange Module

E-CEM technology is being pursued by the U.S. Navy and is promising due to its ability to capture both carbon dioxide and hydrogen from seawater [71]. Here, the carbon dioxide would be used as an input to the Sabatier reaction, and the hydrogen again is useful as a fuel or as more reactant for the Sabatier reaction. E-CEM was originally developed for jet fuel production in the sea to overcome the need for resupply of fuel on military missions involving aircraft carriers. However, the basic technology can be adapted to P2G by removing the final fuel synthesis step and instead stopping with carbon dioxide and hydrogen as the desired products, which are exactly what are needed for the methanation reaction.

The process is powered by ocean thermal energy conversion (OTEC), which uses the temperature difference in water at different depths. While circulating through the OTEC process, small amounts of the carbon in water, in the form of dissolved carbon dioxide, can be captured. Further carbon dioxide can be captured from the carbonates in seawater with additional capture materials and power from OTEC. Hydrogen is produced by PEMEC or AEC technology, using the electricity produced by OTEC [72]. While not mentioned in the report, SOEC technology could be used for hydrogen production as well.

The technology readiness level for E-CEM is low and therefore the option may not be ready in time for use in 2030 or 2050.

Co-location of Electrolytic SNG Production with Biofuel Plants

A fourth source of carbon dioxide is from biofuel plants. These biofuel plants produce carbon dioxide which can be captured with some additional plant equipment [73]. Biorefineries such as those producing biofuels from AD, pyrolysis, hydrolysis, and gasification have streams with relatively high concentrations of carbon dioxide [74]–[80]. The carbon dioxide can be separated from the streams rather efficiently, typically using differences in condensing temperatures of the stream constituents or any of the various methods used by PCC and DAC technologies. Note that this separation technology is effectively the same as that of PCC mentioned previously. Each of the above mentioned production methods will have different concentrations of carbon dioxide in various streams, so the efficiency and quantity of carbon dioxide will be different for each. However, there is an expected synergy of co-locating a P2G plant with a biorefinery due to the much higher concentration of carbon dioxide in the stream so of the biorefinery compared to the ambient air (in the case of a DAC) and the seawater (in the

case of E-CEM). This is similar to the high carbon dioxide concentration utilized in PCC, but biorefineries have the added benefit of using biomass as input, drastically improving the carbon impact of these facilities.

This concept is particularly attractive in situations in which the biofuel processing plants are co-located with electrolysis plants with solar or wind power on-site. The coalescing of these pieces of equipment create a synergy of fuel production, of both the original fuel of the biofuel plant and the electrolytic SNG. The main benefit of this layout is to take advantage of low electricity costs due to on-site renewable generation and the otherwise-wasted carbon dioxide from the biomass at a low marginal cost.

b) Anaerobic Digestion SNG Production

SNG can also be produced using a biochemical process known as anaerobic digestion. Anaerobic digestion involves microbes (hence biochemical), in the absence of oxygen, breaking down organic matter to methane and carbon dioxide. This process works with high moisture biomass, so only the moist biomass sources including manure and food waste can be used in AD [81]–[84]. One could co-digest a lower-moisture content biomass feedstock such as a somewhat moist agriculture waste (for example, fresh yard trimmings). This would require the feedstocks be added in such a ratio as the overall slurry has a high enough moisture content to work in the AD [83]. The work of this dissertation is not spatially resolved, so this constraint is not able to be considered. Given the fact that this co-digestion is rare in the literature, this simplification should not have much impact on practical results. Therefore, only manure and food waste will be considered feedstocks for anaerobic digestion.

The gas mixture of mostly methane and carbon dioxide can be cleaned to improve the purity of methane using methods previous introduced, creating SNG. The wet material remaining after AD, known as digestate, can be used as a fertilizer for farming applications [85].

c) Gasification SNG Production

Gasification was previously introduced as a method of producing hydrogen from dry biomass. Again, the actual product of gasification is termed syngas, which is composed primarily of hydrogen and carbon monoxide. This syngas can be turned into SNG by the same methanation process described previously to convert electrolytic hydrogen and carbon dioxide into methane [86], [87], [96]–[104], [88]–[95][105], [106], [115], [116], [107]–[114].

Just as before with hydrogen gasification, producing SNG by gasification is also most appropriate with a relatively dry biomass, which saves energy on the drying process. Therefore, this work assumes only dry biomass as potential feedstocks for gasification, including agricultural residues, MSW, forestry residues, trees, and energy crops. Food waste and manure are not considered feedstocks for gasification in this work as they would require significant drying which would decrease overall efficiency.

2.1.2.4 Renewable Gasoline and Renewable Diesel Production

Renewable gasoline and renewable diesel are both drop-in fuels, just as SNG is. Therefore, these liquid fuels can be used in the current gasoline and diesel infrastructure, including the many dispensing stations open today, as well as the vehicles that are fueled by gasoline and diesel. Taking advantage of the vast incumbent gasoline and diesel infrastructure

and vehicles provides a significant timing and cost benefit to the renewable gasoline and renewable diesel.

Renewable gasoline and diesel can both be produced from biomass using one of four processes: liquefaction, gasification followed by Fischer-Tropsch, pyrolysis, and hydrolysis. The three former production methods are thermochemical, whereas hydrolysis is biochemical. These production methods will be discussed in further detail shortly. The differentiation between renewable gasoline and diesel comes about through the refining process, similar to how fossil gasoline and fossil diesel are differentiated from crude fossil oil. There are no distinctions made for the different biomass feedstocks when producing either renewable gasoline or diesel. Also important to note is that each of these four fuel production methods use the nearly the same biomass feedstocks, which are relatively dry: agriculture, waste, forestry, tree, and energy crops. However, liquefaction can also use moist biomass, so food waste and manure are included as feedstocks for liquefaction [81], [117]–[119].

a) Liquefaction Renewable Gasoline and Renewable Diesel Production

Liquefaction is a direct conversion from biomass to liquid oils, and it is not as technologically developed as some of the other liquid fuels production methods that will be discussed. It involves heating and pressurizing biomass without oxidant at roughly 250-325ºC and 50-200 atmospheres of pressure. The result is a bio-oil which is then treated and refined to produce the desired hydrocarbon, either renewable gasoline or renewable diesel. The treatment process involves removing oxygen through hydrotreating, creating hydrocarbon chains of desirable length through hydrocracking, and then distilling to get the desired spectrum of hydrocarbons [81], [117]–[119][120][121]. In this work, the desired product is gasoline or diesel,

so the correct spectrum of hydrocarbons for either of these fuels is the design goal. A schematic of a liquefaction plant is shown in Figure 7.

Note that each of the treatment processes described above is also present in fossil gasoline and fossil diesel, so lessons learned in these areas from the fossil fuel counterparts can be applied here for the renewable fuels.

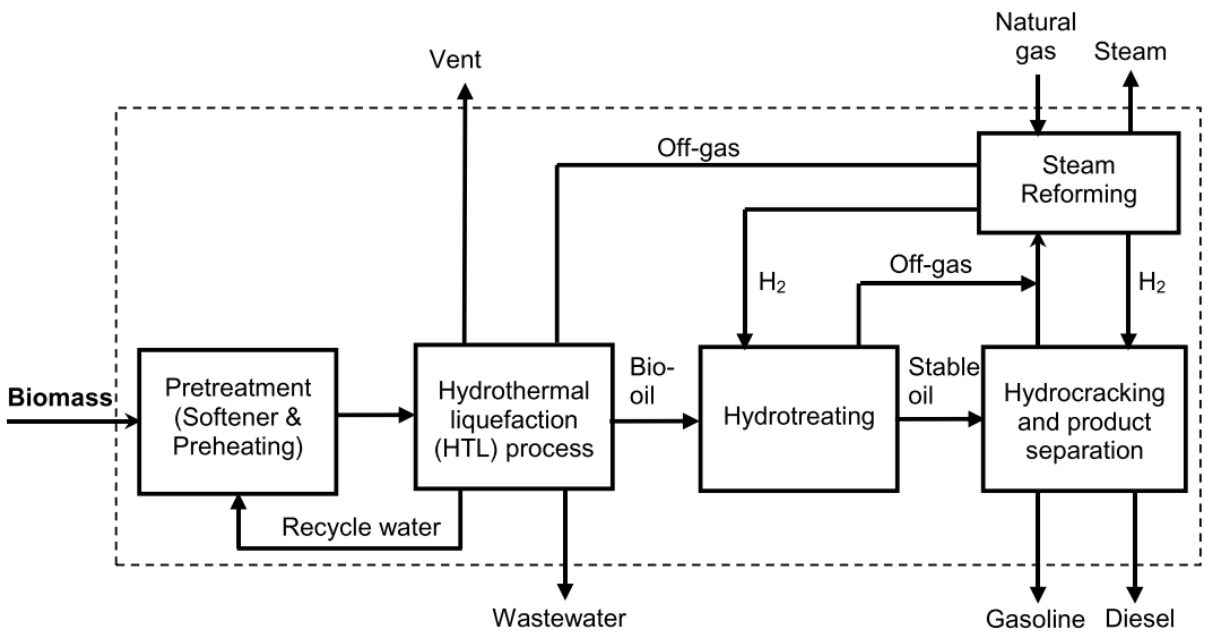

Figure 7. Liquefaction fuel production diagram for renewable gasoline and renewable diesel, from U.S. Department of Energy [120]

b) Gasification and Fischer-Tropsch Renewable Gasoline and Renewable Diesel Production

In addition to being used to make both hydrogen and SNG, gasification shows up again as the first step in a process to create liquid fuels. Gasification produces syngas (mainly hydrogen and carbon monoxide), and that syngas then goes through the Fischer-Tropsch (FT) process. FT converts the syngas into hydrocarbon chains of various lengths according to Equation 3, where *n* is an integer. The overall process of gasification followed by FT will be referred to by the shorthand of gasification-FT hereafter.

Equation 3. Fischer-Tropsch process, from [122]

$$(2n + 1)H_2 + n\ CO \rightarrow C_nH_{2n+2} + n\ H_2O$$

This process uses a catalyst to produce the hydrocarbon products. As before in liquefaction, the resulting products are hydrotreated, hydrocracked, and distilled for the final desired products of either renewable gasoline or diesel. See Figure 8 for a flow diagram of the gasification and Fischer-Tropsch process.

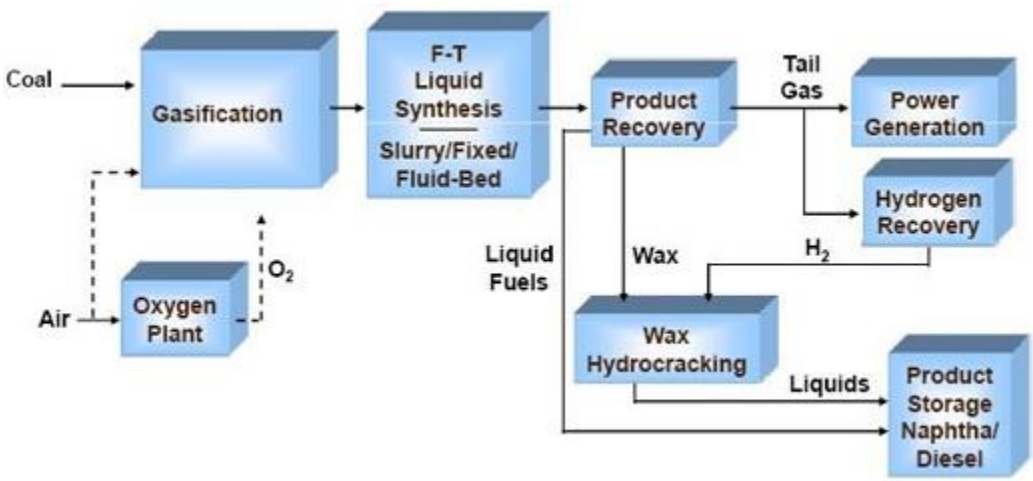

Figure 8. Gasification and Fischer-Tropsch production diagram for renewable gasoline and diesel, from U.S. Department of Energy [122]

c) Pyrolysis Renewable Gasoline and Renewable Diesel Production

In pyrolysis, the dried biomass is pressurized to 1 to 5 atmospheres and heated up to 300-500ºC without an oxidant to produce bio-oils which are then refined to produce either gasoline or diesel. Once again, the resultant bio-oil is hydrotreated, hydrocracked, and distilled to produce either renewable gasoline or diesel [81], [117]–[119].

d) Hydrolysis Renewable Gasoline and Renewable Diesel Production

In hydrolysis, the cellulose of biomass (a structural component of plant cell walls) is broken down by enzymes and water to produce hydrocarbons. These hydrocarbons can then be processed through the same hydrotreating, hydrocracking, and distilling to obtain renewable gasoline or diesel. Like gasification, hydrolysis is relatively early in its development state. Unlike the other production methods, hydrolysis is a biochemical process due to the enzymes that convert the biomass [81], [117]–[119].

2.1.2.5 Summary of Fuel Production Pathways

Having finished the introduction of each of the fuel pathways to be considered in this work, Figure 9 summarizes them. Note the many pathways options, particularly with respect to some of the biomass feedstocks that have several process options available. This diagram highlights the need for an objective methodology of determining which pathways should be pursued to fuel transportation needs into the future.

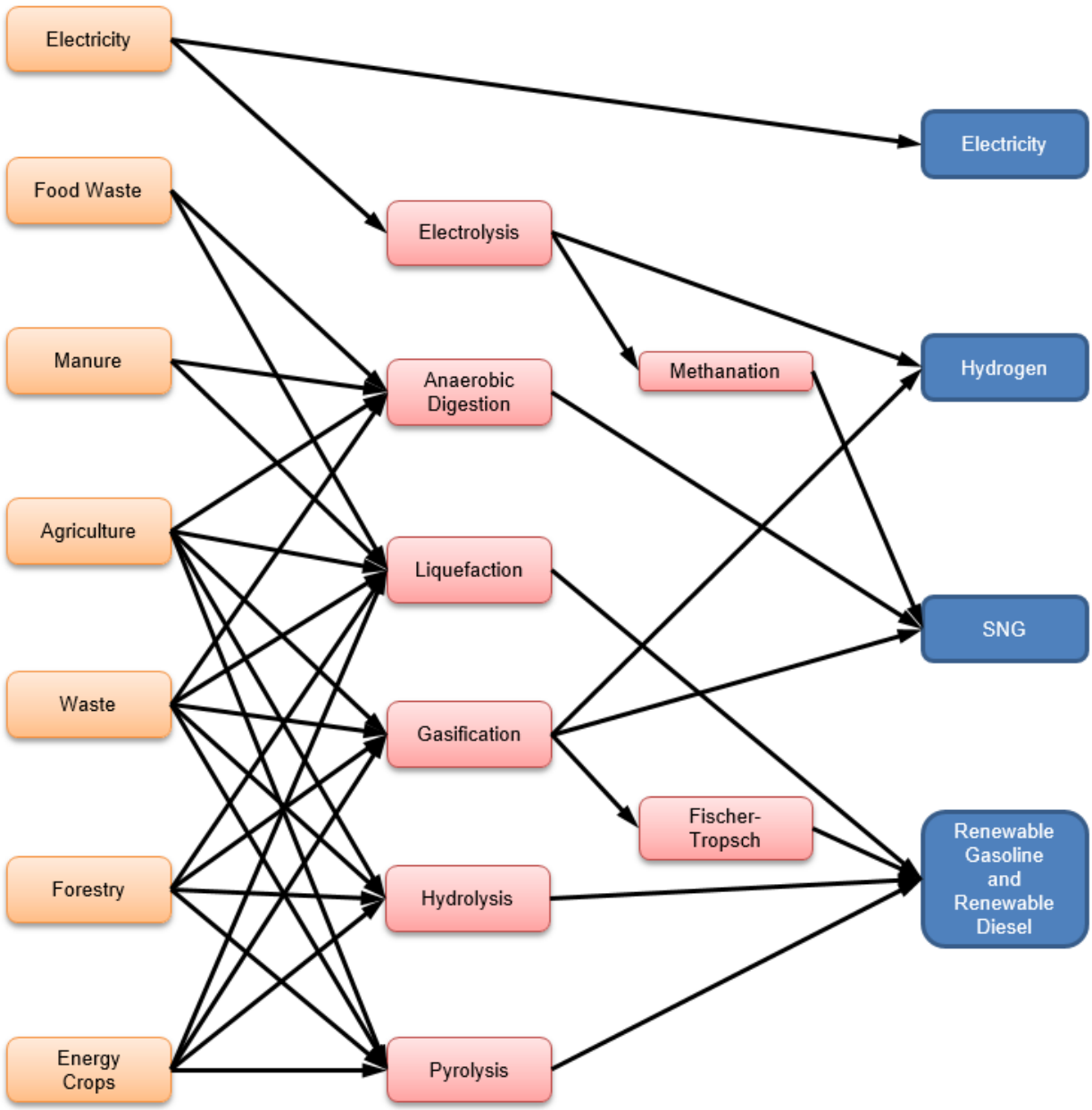

Figure 9. Flow diagram of fuel production pathways

2.1.3 Fuel Distribution

Once the fuels have been produced, it is then necessary to distribute them to locations at which drivers can refuel their vehicles. Due to the physical differences between these fuels, there are also major differences in how these fuels may be distributed.

2.1.3.1 Electricity Distribution

Electricity is distributed on the electric transmission and distribution grid, as shown in Figure 10. Transmissions lines move electricity long distances at high voltages to reduce electric losses, making the transmission more efficient. Distribution lines move electricity at lower voltages for shorter distances, typically around neighborhoods and office areas. While moving the electricity at lower voltages in distribution lines is less efficient, the distances covered by distribution lines is much lower than transmission lines and therefore the lower efficiency is acceptable. The lower voltage is then easier to handle for end-uses such as homes, business, and industrial facilities.

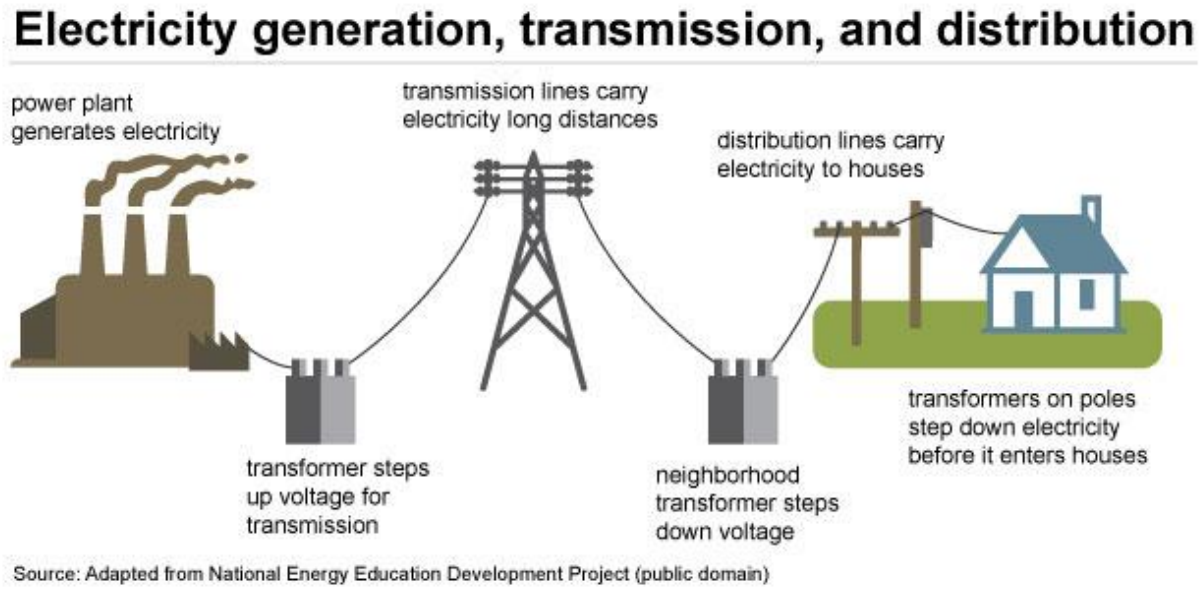

Figure 10. Diagram of electricity transmission and distribution network, from U.S. Energy Information Administration [123]

Equipment for electricity distribution, which again is both the transmission and distribution network of the electric grid, includes substations which house transformers that change voltage significantly, individual transformers that voltage at lower levels than entire

substations, and electric lines that carry the electricity from one place to another. Depending on the power of charging for PEVs as well as the PEV population, some or all of this distribution equipment may need upgrading to handle the increased electric load on the grid [124][125].

2.1.3.2 Hydrogen Distribution

Hydrogen is a gaseous fuel, and being a gaseous fuel means it is less energy dense by volume than a liquid fuel. Therefore, distribution of hydrogen has a challenge of keeping cost-effectiveness high.

A dedicated hydrogen pipeline to distribute hydrogen is a consideration, as is blending hydrogen into the natural gas grid. A dedicated hydrogen pipeline is a serious technical feat that would take decades to roll out with significant logistical challenges such as securing rights to dig and implement the pipeline. Blending hydrogen into the natural gas pipeline is an option, with a practical limit of about 15% of the pipeline by volume, or 5% by energy, before there are any serious concerns of safety or integrity [126], [127]. Blending hydrogen into the natural gas grid would also require interconnections to be built to connect to the grid itself, increasing cost significantly [128]. Lastly, blending hydrogen into the natural gas grid for distribution would then require extracting that hydrogen out of the grid downstream. This would most likely be done by SMR, which as previously mentioned lowers efficiency to the point that it would not be competitive with the other pathways considered herein [54]. Therefore, pipeline delivery of hydrogen, either through a dedicated pipeline or through the natural gas pipeline, is not considered in this work.

The remaining option for hydrogen delivery is trucking. One could consider trucking either as a compressed gas, or first liquefying the hydrogen and then trucking that. The benefit of

liquefying is increasing the density, but that comes with the tradeoff of energy input to liquefy the hydrogen.

There are two key components of hydrogen distribution: the terminal, and the delivery. The terminal is the point from which hydrogen is to be collected and then delivered to the dispensing stations. Terminals are needed to ensure smooth logistics in moving hydrogen from production location to dispensing stations [127].

2.1.3.3 SNG Distribution

SNG, like hydrogen, is a gas at ambient temperature and pressure. Because it is chemically comparable to natural gas (a reminder here that SNG is simply the methane molecule that has been produced either electrolytically or from biomass), SNG can be injected into the natural gas pipeline without any limitation or blending requirement. Due to the robust natural gas infrastructure in place, with nearly all homes, offices, and buildings already connected to the natural gas grid in the U.S., the distribution method for SNG in this work is assumed to be the natural gas pipeline.

Another option for SNG is to truck it, either as a compressed gas or as a liquid, similar to hydrogen. However, the efficiency and cost-effectiveness of the ability to take advantage of the robust natural gas infrastructure makes trucking SNG unwise. Therefore, SNG can be assumed to be distributed using the natural gas pipeline infrastructure.

2.1.3.4 Renewable Gasoline and Diesel Distribution

Renewable gasoline and diesel are effectively the same product as fossil gasoline and diesel. Therefore, it is safe to assume that distribution of renewable gasoline and diesel will take

the same form as fossil gasoline and diesel. This method is trucking. Because both gasoline and diesel are liquid fuels, they are relatively energy dense and therefore trucking is an effective method of distribution.

2.1.4 Fuel Dispensing

Once each of the fuels has been distributed from the point of production, there needs to be some station to allow for fueling of the corresponding vehicle types. This is the role of the dispensing station. While each of the following dispensing station types is currently open for public use, there is a wide gap between them in terms of availability and maturity.

2.1.4.1 Electricity Dispensing

Electricity dispensing takes the form of electric chargers for PEVs. These electric chargers come in a range of powers, with higher power electric chargers refueling PEVs faster. The PEV charging equipment is often referred to as electric vehicle supply equipment (EVSE), but this dissertation notes the ambiguity of that name due to the fact that there are types of electric vehicles that do not refuel by electric charging.

The lowest power charger is known as level 1, and it gives about 2 to 5 miles of charge per hour with power output of 1.44-1.9 kilowatts (kW). Level 1 charging is done at 120 volts (V), which is the same as is commonly available at homes and commercial locations. Therefore, conventional wall power outlets are able to support PEVs with level 1 charging, and no special equipment must be installed. Typically, level 1 charging is done at drivers' homes, but some workplaces offer level 1 charging as well.

Next is level 2 charging, which gives about 10 to 20 miles of charge per hour. Level 2 charging is done at 240 V at homes and 208 V at residential areas with power output of 3-19.2 kW. Level 2 charging does require additional equipment, which increases the cost of this charging compared to level 1. Level 2 charging is appropriate for homes, workplaces, and in public charging locations such as shopping centers or dedicated charging locations.

Last is level 3 charging, often known as DC fast charging, which can give 180-240 miles of driving per hour with power output of 25 kW and above. Level 3 charging operates at 480 V, which make these chargers most appropriate for public charging locations where PEV throughput is high and drivers may be going long distance [129].

Both level 1 and level 2 charging share the same connector, while level 3 uses a more robust connector to handle the higher charging powers. Therefore, any PEV that has a range extender (a PHEV or a PFCEV) could likely suffice without a level 3 charging port as the range extender negates the need for fast charging. However, a BEV may do well with a level 3 charging port to allow for convenient fast charging. See in Figure 11 an example of what the PEV charging connectors look like. While the level 1 and level 2 connector is mostly standard, there are some variations for level 3 connectors.

Figure 11. PEV charging connectors for level 3 on the left and levels 1 and 2 on the right, from U.S. Department of Energy [129]

For LDVs, over 80% of drivers charge their PEVs at home, and level 1 charging is most common there [129]. For HDVs, the relatively large battery capacity that is needed to move such a large vehicle for any sustained travel would make level 1 charging impractical. Higher power charging may be needed for these vehicles.

One last practical note for electricity dispensing is the amount of time that is required. While there are many factors such as vehicle battery capacity and the power of electric chargers, typical charging times are on the order of a few hours for a BEV. Therefore, it should be noted that the rapid refueling of conventional gasoline and diesel vehicles would be drastically changed for BEVs. Even with very high-powered chargers of the future and not charging to 100% battery capacity, charging an LDV can take close to 20 minutes [130]. That is not to mention the battery degradation associated with such fast charging [131][132]. Therefore, this work assumes that

more modest charging powers of level 1 and level 2 charging will be used to prevent damage to the battery, in addition to economic considerations that will be discussed later.

2.1.4.2 Hydrogen Dispensing

Hydrogen dispensing stations, often called hydrogen refueling stations (HRSs), are new, rare, and expensive. There are 40 stations open in California as of May 2019 [133]. There are some stations on the east coast [134], but otherwise hydrogen dispensing stations are non-existent in the rest of the U.S. Therefore, any significant future adoption of hydrogen vehicles will require hydrogen dispensing station construction. Current small-scale hydrogen stations costing on the order of $1 million each [135].

Note that the hydrogen station schematic is quite similar to that of the SNG station, as seen in Figure 12. One major difference is that because pipeline distribution of hydrogen is not modeled in this work, the "gas line" of the SNG station would be a tube trailer of liquid hydrogen that is delivered by truck.

2.1.4.3 SNG Dispensing

SNG is distributed just like compressed natural gas (CNG). CNG stations, while mature like gasoline and diesel stations, are not nearly as common. CNG is an option for HDVs and was until recently an option for LDVs. There are 116 public CNG stations that can support fueling for HDVs as of June 2019 [136]. However, neither the LDV nor HDV options have become as prevalent as the gasoline and diesel options, and similarly neither have CNG dispensing stations become as prevalent as gasoline and diesel dispensing stations. Therefore, any significant future adoption of SNG vehicles will require SNG fueling station construction [137].

A schematic representation of a SNG station is shown in Figure 12, with the “gas line” input being the natural gas pipeline that is used for distribution of SNG.

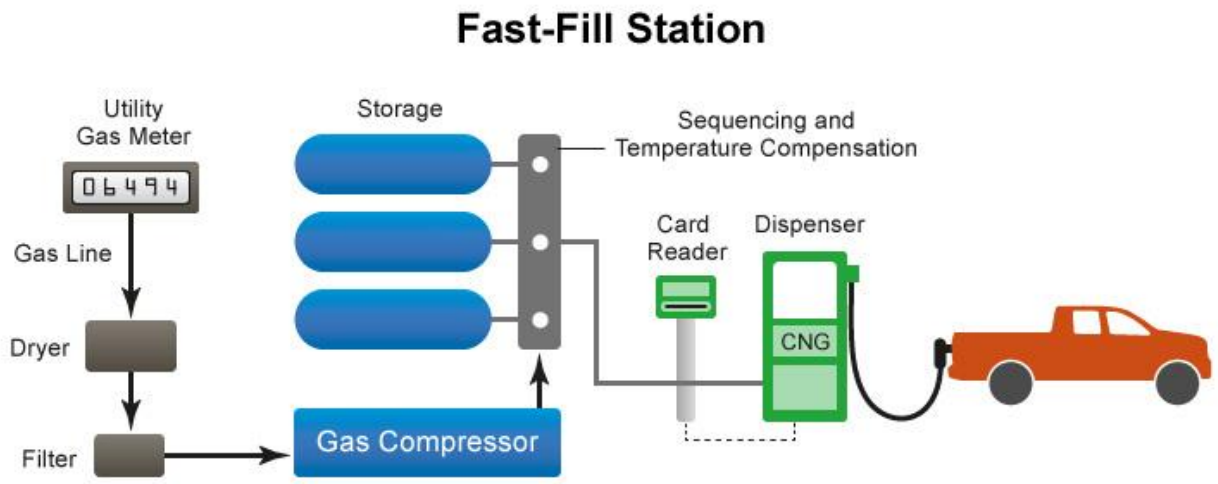

Figure 12. SNG dispensing station schematic, from U.S. Department of Energy [138]

2.1.4.4 Renewable Gasoline and Diesel Dispensing

Renewable gasoline and diesel are both drop-in fuels, and therefore can be sold at existing gasoline and diesel stations. Gasoline for LDVs and diesel for HDVs are the primary fuels today, and their fueling infrastructure is prevalent. In fact, many intersections have multiple gasoline and diesel stations to choose for fueling. Therefore, no significant infrastructure would need to be built for these fuels into the future.

2.1.5 Fuel Emissions

Emissions from fuel for this work are considered only from the feedstock, whether electricity or biomass, and the overall pathway efficiency. However, efficiency of the various steps, including distribution and dispensing is considered and therefore has an effect on the emissions associated with the vehicle fuel.

Not included are leakage emissions from distribution, particularly applicable for gaseous fuels such as hydrogen and SNG. GREET notes that 1.3% of US natural gas throughput is emitted into the air as methane. This methane comes from both leakage from extraction, processing, and distribution, as well as some combustion used for heat for any needed process. GREET also notes that about 0.2% of natural gas is leaked in transmission from the natural gas processing plant to electric generators that run on natural gas. Therefore, the leakage that can be assumed for the distribution of SNG falls somewhere between the above two numbers. Overall, this value is negligible and will not be considered a loss in this work. The same is assumed for hydrogen, which has been shown to be about 1.5 to 3 times faster to escape from an intentionally-manufactured leak [139]. Even at this slightly increased leakage, the rate is still negligible. Similarly, distribution of renewable gasoline and diesel are assumed to be leak-free. Electricity is not leaked, but distribution efficiency will be included.

2.2 Vehicle Powertrains

Vehicles will be separated into two categories for this work: light-duty vehicles (LDVs) and heavy-duty vehicles (HDVs). LDVs include passenger vehicles that most of the public drives for daily transportation needs. Included in this category are sedans, sport utility vehicles (SUVs), minivans, small pick-up trucks, and other similar vehicles. HDVs are classified by their weight. In fact, all such large vehicles are classified into a scheme from Class 1 through Class 8 based on their gross vehicle weight rating (GVWR), which is the total weight of the loaded vehicle including cargo. The present work focuses on only Class 8 HDVs, which are 33,001 pounds and greater. These Class 8 HDVs are responsible for the most vehicle miles traveled (VMT) of any vehicle category [140], as shown in Figure 13. Class 8 HDVs are also responsible for a large

portion of GHG and CAP emissions in the transportation sector [7][141]. For the rest of this dissertation, HDVs will refer only to Class 8 HDVs.

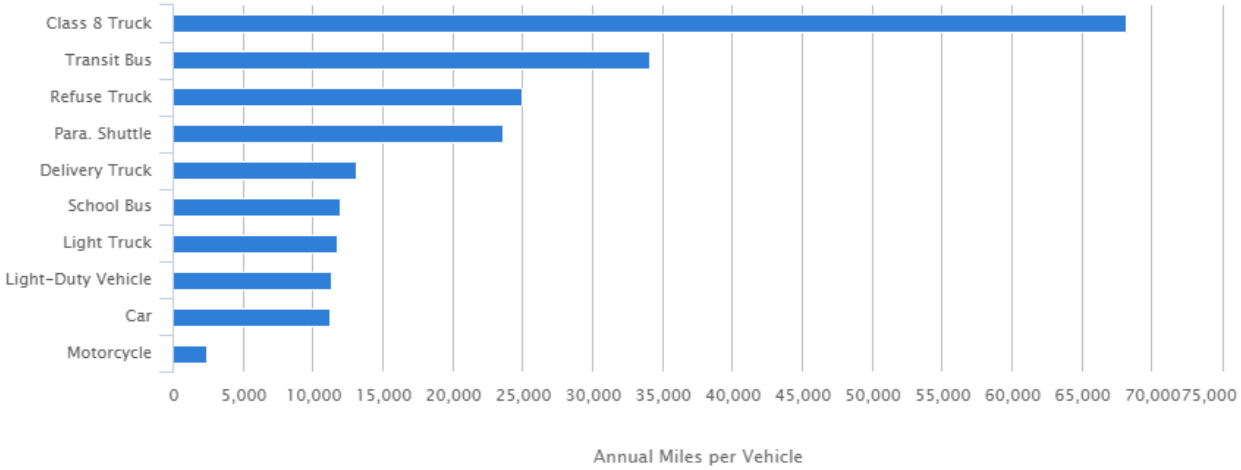

Figure 13. Annual VMT by vehicle category, from U.S. Department of Energy [140]

Six powertrain configurations can be found in the literature for being major contenders in both the current and future market for LDVs and HDVs: internal combustion vehicles (ICVs), hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), battery electric vehicles (BEVs), fuel cell electric vehicles (FCEVs), and plug-in fuel cell electric vehicles (PFCEVs) [26]–[30]. For vehicle types with a combustion engine (ICVs, HEVs, and PHEVs), the specific fuel used is a further consideration. Gasoline is the dominant fuel for the combustion engine of LDVs in the U.S., such as the passenger vehicles that the vast majority of the public drives. This work assumes this long-established trend will continue in the near future, and diesel will not be a significant portion of ICVs in the LDV spectrum. However for HDVs in the U.S., both diesel and natural gas are prevalent depending on the vocation (i.e. type of work, including long haul, refuse collection, etc.); therefore, both of these fuels will be considered for the combustion engine of HDVs in this work.

Alternative passenger vehicles, particularly PEVs, are increasing in popularity in California and worldwide. Figure 14 shows the new California passenger vehicle registrations from the first half of 2018 broken down by powertrain category. The vast majority of these vehicles being purchased is still mostly ICVs, but just over 10% of them have some version of an electric powertrain. This is significant considering the relatively short timeframe that these non-ICV powertrains have been available, and it is a sign that the future may portend a paradigm shift towards electric powertrains for passenger vehicles.

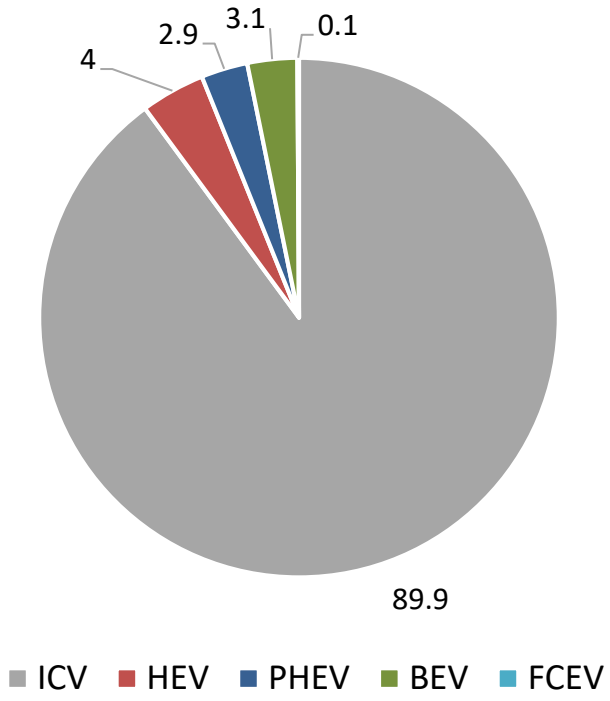

Figure 14. California new vehicle registrations in first half of 2018, data from [142]

The transition of HDVs is not as rapid or as ripe with options as that of LDVs. Currently, about 98% of Class 8 HDVs are diesel-fueled ICVs [141]. However, there is strong encouragement to increase the rate of alternative fuel powertrain adoption for HDVs. The California Energy Commission (CEC) awarded an $8 million grant for a hydrogen refueling station dispensing hydrogen sourced exclusively from biogas at the Port of Long Beach using a

technology known as tri-generation to produce electricity, heat, and hydrogen fuel [140][143]. Grants like this along with the laws, regulations, and goals from Table 1 show the focus on transitioning HDVs to cleaner technology.

Important to note are different vocations for HDVs. While LDVs typically serve only to transport drivers from one location to another, HDVs are specialized in a particular task or set of tasks. These tasks vary from transporting goods from ports to distribution centers, hauling goods long distances, collecting trash from communities and delivering it to landfills, and many others. For this work, four vocations are selected based on total number of miles traveled in California and the relative impact they have on air quality through CAP emissions. The four vocations considered are as follows: (1) linehaul, which transport goods long distances, (2) drayage, which transport goods from ports to distribution centers, (3) refuse, which collect waste from various locations and transport it to processing centers or landfills, and (4) construction, which move construction material or assist in construction of buildings and other built structures.

Vehicle emissions are composed of the emissions from the vehicles tailpipe and also include other emissions such as tire and brake emissions. While tire and brake emissions do depend on vehicle mass (which varies from one vehicle powertrain to another), this factor is not considered in this work. Therefore, all vehicle powertrains are assumed to have the same tire and brake emissions. Due to this assumption, there is no comparative advantage between powertrain configurations in this modelling, so these tire and brake emissions are neglected in this work.

The BEV, FCEV, and PFCEV are all zero-emission vehicles (ZEVs), meaning there are no tailpipe emissions from these vehicles. All other powertrain configurations have tailpipe emissions that must be analyzed.

Regarding HDVs, there has been recent advancement in ICV engines which are referred to as low-nitrogen oxides (low-NO_x) engines. Both diesel and CNG engines have low-NOx variations that are either available now (for CNG) or expected to be on the market in the next few years (for diesel) [144]. These standards set limits of 0.02 grams of NOx emission for each brake horsepower-hour of operation [145], [146]. It is assumed that any HDVs that are fueled by either SNG or renewable diesel in this modelling effort will be low-NO_x engines, once the technology has become available. More information on the availability of low-NO_x diesel engines will be detailed in a later section of this dissertation.

2.2.1 ICV

ICVs have been the primary vehicle type in recent history, after a short stint of BEV popularity when passenger vehicles were first introduced [147]. ICVs use a hydrocarbon fuel (typically gasoline for LDVs and diesel for HDVs). This fuel is combusted in the engine which, through mechanical linking of the powertrain, leads to the spinning of the vehicle's wheels. The combustion process leads to tailpipe GHG and CAP emissions from these vehicles.

For HDVs, SNG is also a fuel for ICVs (as well as any other powertrain with a combustion engine such as HEVs and PHEVs). SNG is a gaseous fuel, so to store any reasonable quantity of fuel on the vehicle, SNG must be stored either at pressure or a liquid after being liquefied. Storing as a gas is more prevalent in vehicles and also more efficient as it does not require the energy intensive and costly step of liquefying. Either option requires a robust tank that is able to withstand significant pressure.

2.2.2 HEV

HEVs add a traction battery and electric motor to the ICV powertrain to gain efficiency in moving the vehicle. The addition of the battery and electric motor offer two main benefits over the ICV. First, the HEV can recharge its battery when braking by running the electric motor in reverse, as a generator. This is known as regenerative braking and is done instead of or in addition to the brakes of the vehicle, which has the additional benefit of extending brake pad life. Regenerative braking reduces the amount of fuel needed because the battery helps accelerate and drive the vehicle instead of using just fuel in the combustion engine. In addition to regenerative braking, HEVs also allow the engine to run at more efficient operating conditions while the battery works on the dynamic portions of the power demand.

HEVs trace back to the end of the 19th century, but their presence soon died out as ICVs became the vehicle type of choice [148]. However, with the ZEV Action Plan of 1990, automakers were to make increasing numbers of ZEVs for California sale staring in 1998 [18]. In later revisions of the plan, cars with very low emissions known as partial ZEVs (PZEVs) were eligible to help meet the goals [149]. The HEV was a method for automakers to work towards complying with the ZEV Action Plan, though they were not clean enough to count as a PZEV.

2.2.3 PHEV

The evolution of the HEV is the PHEV. Quite similar to HEVs, PHEVs have two major benefits stemming from the inclusion of a larger traction battery than the HEV: (1) a modest battery electric range (BER) and (2) recharging of the traction battery from an external electricity supply, which classifies the PHEV as a PEV. This allows for efficient and tailpipe emissions-free

driving for a limited range, but does not limit drivers to only go short distances as a combustion engine works as a range extender.

Note the acronym BER instead of the conventional acronym all electric range (AER). While the battery is the only source of electric power in the PHEV powertrain, this is not always true. Therefore, the conventional acronym AER is not adequate to describe driving range powered by the traction battery of a vehicle. The new acronym BER is used to distinguish between the traction battery and the other power source, whether that other power source is electric or not.

Due to the dramatic emissions reductions of PHEVs compared to HEVs (25-50% for carbon dioxide [150]), PHEVs are classified as PZEVs and so comply with the ZEV Action Plan.

While PHEVs are attractive for the above reasons, they do use combustion engines and therefore have tailpipe GHG and CAP emissions. For this reason, PHEVs may prove to be a transitional vehicle into a future of vehicles that have no tailpipe emissions.

2.2.4 BEV

BEVs are powered by a traction battery, typically significantly larger than that of PHEVs. This increased size is needed as the battery is the sole source of power to move the vehicle. Refueling the BEV is done by connecting the vehicle to some electricity source. Typically, this electricity source is the electric grid, but with the right equipment, it would be possible to recharge the BEV (or any other PEV) from off-grid renewable electricity.

Before Henry Ford's ICV revolution in the early 20th century, BEVs were the vehicle powertrain of choice for some time [147]. Due to the focus on reducing emissions society-wide

as well as improving battery technology, BEVs are regaining popularity and sales are dramatically increasing [151].

Because there is no combustion engine in a BEV, there are no tailpipe emissions. In fact, there is no tailpipe at all. BEVs also have very high efficiency compared to most other vehicle types. However, they typically cannot drive as far or refuel as fast as other vehicle types [152]. In the case of LDVs, even if drivers are able to charge their BEVs at home (given they have access to a charging outlet at home), the inconvenience of a long charge time can dissuade drivers from purchasing BEVs.

Recent improvements in battery technology bring approximately 200 mile driving range to BEVs in a more-affordable price range. Additionally, PEV chargers are increasing their charging rates, allowing for shorter charging times [153]–[155].

While BEVs do not have tailpipe emissions, they can indirectly create emissions depending on the source of the electricity charging them. If a BEV is charged using only renewable sources, it is effectively emission-free (aside from other life-cycle emissions such as manufacturing that is beyond the scope of this work). However, if the BEV is charged from the California electric grid, it has emissions associated with the natural gas power plants that, along with the emissions-free renewables, are part of the electric grid. There is a trend of increasing emission-free electricity, particularly in California, so the emissions of BEVs (and all PEVs) are decreasing accordingly [156].

For HDVs, long charging time and short driving range can severely limit the types of work these vehicles are able to do. Therefore, careful consideration must be given for BEV adoption in the HDV sector. As of 2015, only drayage and refuse trucks had been demonstrated to operate with a BEV powertrain [157]. While improving battery and charging technology may

increase the aptitude of heavy-duty BEVs, current thinking is that BEVs will have a limited role in the heavy-duty sector, particularly with regard to range. Further consideration of this issue will be discussed in a later section.

Note that catenary HDVs, which use external electrified lines to charge the battery of a vehicle (whether BEV or any PEV), are not considered in this work due to the necessity of spatial resolution. Catenary technology is best suited for particular sections of a highway that may cause trouble for a HDV relying on batteries, for example, an extended incline, and that spatial resolution is not within the scope of this work [157]. This does not mean, however, that catenary HDVs will not play a role in helping to electrify some HDV areas. This work assumes that application of catenary HDVs will be done on a case-by-case basis in a limited number of locations.

2.2.5 FCEV

FCEVs are powered by a fuel cell. A fuel cell is an electrochemical device, similar to a battery. The main difference is a battery stores its fuel and oxidant within the housing of the battery itself. A fuel cell stores these two outside, with the fuel in a tank and oxidant often being ambient air. This key difference allows for the power and energy to be scaled independently for fuel cells, unlike batteries. FCEVs use proton exchange membrane fuel cells (PEMFCs) as they are relatively low temperature (below 100 ^{o}C) and handle dynamic operation better than other fuel cell varieties. PEMFCs operate on hydrogen fuel. Because hydrogen is a gas with relatively low volumetric energy density, it must be compressed to very high pressures (typically 70 MPa for LDVs, and roughly half that for HDVs) for vehicular use. A schematic diagram of a PEMFC is shown in Figure 15. One important note is that, despite not being in the name, FCEVs are

typically hybrids with a traction battery installed to allow for regenerative braking and efficient fuel cell operation. FCEVs in this work are assumed to be hybrids.

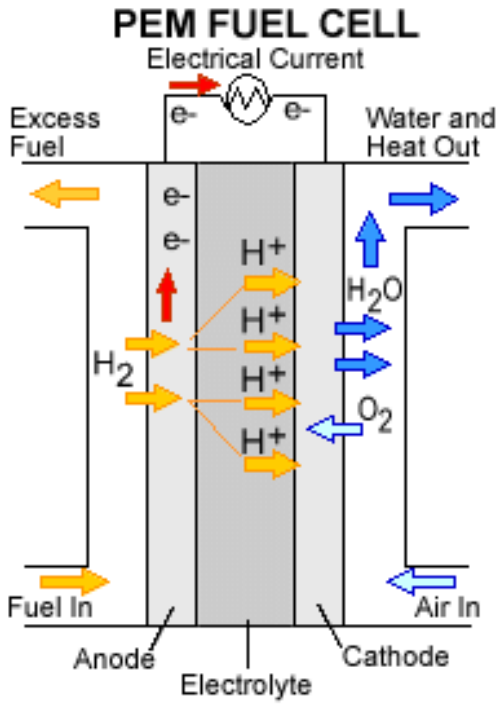

Figure 15. Schematic of PEM Fuel Cell, from U.S. Department of Energy [158]

FCEVs are new to the commercial market, with an introduction in the mid-2010s. Their overall emissions are dependent on the method of fuel production (of which there are many options, as has been detailed). Nearly all of the current production of hydrogen in the U.S. is from natural gas by SMR [53]. This will likely change in future as, already, California requires at least one third of the hydrogen sold at fueling stations has to have a renewable feedstock if that station receives State funds [20]. This requirement will necessarily increase the use of biomass and renewable electricity in hydrogen production.

In practice, FCEVs share similarities to both BEVs and ICVs. Like BEVs, FCEVs have no tailpipe emissions, other than the small amount of water produced by the fuel cell, and

relatively high efficiency, though not as high as that of BEVs [14]. Like ICVs, refueling FCEVs is fast, nearly as fast as refueling a gasoline or diesel vehicle. Additionally, driving range is also comparable to ICVs due to the independent sizing of power and energy, so an adequately-sized hydrogen tank can be incorporated. The former qualities make an environmentally-friendly vehicle. The latter qualities make a vehicle convenient for drivers.

While the above is true in theory, the current lack of hydrogen fueling infrastructure means fueling is not yet very convenient for drivers unless they happen to live and travel near one of the 40 California stations open as of June 2019 [133]. This becomes less of an issue with time as the fueling infrastructure develops. However, the FCEV market is affected by the low number of hydrogen fueling stations, but costly stations are hard to justify without higher FCEV adoption. This is proving to be a challenge for FCEVs that could be overcome by optimism in the market. For example, the California Energy Commission has recently awarded an $8 million grant for a hydrogen station at the Port of Long Beach which will use 100% biogas [159].

2.2.6 PFCEV

The PFCEV shares similarities with the FCEV and PHEV. From a systems level, the PFCEV operates the same as a PHEV; however, instead of a combustion engine, the PFCEV has a fuel cell and it is fueled by hydrogen. A schematic of a PFCEV powertrain can be seen in Figure 16. Note that all of the powertrain components are electric. This increases the efficiency compared to the PHEV as it removes the efficiency loss of converting from mechanical energy of a combustion engine to electrical energy through an electric generator.

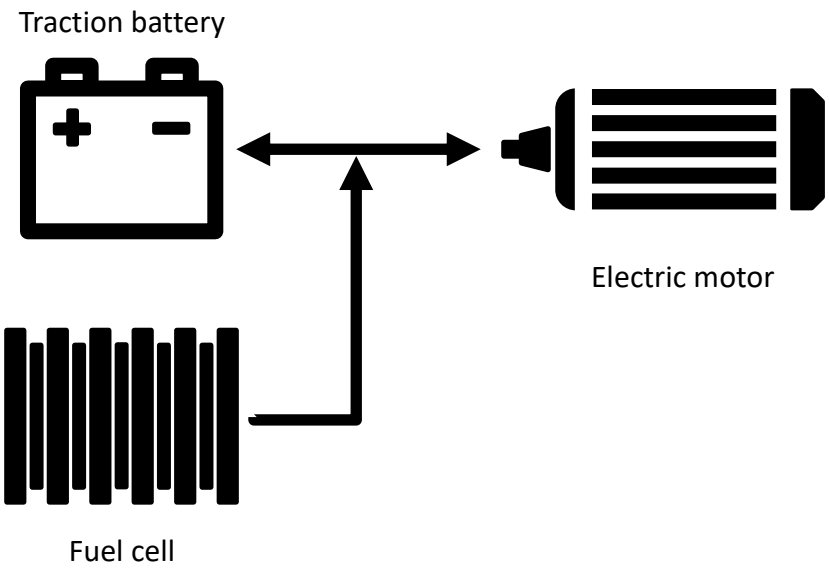

Figure 16. Simplified powertrain schematic of PFCEV

PFCEVs are not yet available for public purchase. Several major automakers have announced both concept and test vehicles, and at least one manufacturer has begun preparing for series production of a PFCEV [160]. Additionally, the literature has many studies analyzing this vehicle powertrain configuration [26], [27], [29], [161]–[166].

Similar to PHEVs, PFCEVs allow for limited driving on the very efficient and potentially clean battery electricity, but have a source of additional range in the fuel cell and hydrogen tank. Unlike PHEVs, the PFCEVs' range extender is also tailpipe emissions-free and more efficient than a combustion engine [26]. The advent of the PFCEV is the reason for the introduction of the BER acronym; both the traction battery and the fuel cell are electric powertrain components, so BER specifies the traction battery as the power source whereas AER would be ambiguous as to which powertrain source is being used.

2.2.7 Vehicle Components

Having described each of the vehicle powertrains considered in this work, it is helpful to now summarize the various components of these vehicles that will be combined to determine an overall vehicle cost in this work. These components are listed in Table 5.

Table 5. Vehicle components considered

COMPONENT	COMPONENT DESCRIPTION
Glider, LDV	The LDV glider includes all of the vehicle components that are not part of the powertrain. This includes parts such as the chassis, wheels, windows, etc.
Glider, HDV	The HDV glider includes all of the vehicle components that are not part of the powertrain. This includes parts such as the chassis, wheels, windows, etc.
IC engine, gasoline	For LDVs, the gasoline IC engine is the sole power plant of ICVs, as well as a co-power plant (along with a battery) of HEVs and PHEVs
IC engine, diesel	For HDVs, the diesel IC engine is one option for the power plant of ICVs, as well as a co-power plant (along with a battery) of HEVs and PHEVs
IC engine, SNG	For HDVs, the SNG IC engine is one option for the power plant of ICVs, as well as a co-power plant (along with a battery) of HEVs and PHEVs
Fuel cell	The fuel cell is the sole power plant of FCEVs and co-power plant of PFCEVs
Traction battery	The traction battery is the sole power plant of BEVs, and co-power plant of HEVs, PHEVs, FCEVs, and PFCEVs
Electric motor / generator	The electric motor is used in all electric powertrains (HEV, PHEV, BEV, FCEV, and PFCEV) to convert electrical energy to motion of the wheels, and it can be run in reverse as a generator to convert wheel motion into electric energy
Liquid fuel tank	The liquid fuel tank holds gasoline or diesel for ICVs fueled by those liquid fuels
SNG tank	The SNG tank is a stronger, more robust tank that holds pressurized SNG (typically around 25 MPa [167]) for HDVs fueled by SNG, which is typically stored as a gaseous fuel
Hydrogen tank	The hydrogen tank is an even stronger and more robust tank that holds pressurized hydrogen (typically at 70MPa) for vehicles fueled by hydrogen, which is typically stored as a gaseous fuel
Hybrid adder, LDV	The LDV hybrid adder accounts for various equipment beyond the traction battery and electric motor (i.e. controls, wiring, etc.) needed to convert a LDV powertrain into its equivalent hybrid one
Hybrid adder, HDV	The HDV hybrid adder accounts for various equipment beyond the traction battery and electric motor (i.e. controls, wiring, etc.) needed to convert a HDV powertrain into its equivalent hybrid one
Plug-in hybrid adder, LDV	The LDV plug-in hybrid adder accounts for various equipment beyond the traction battery and electric motor (i.e. controls, wiring, etc.) needed to convert a LDV powertrain into its equivalent plug-in hybrid one
Plug-in hybrid adder, HDV	The HDV plug-in hybrid adder accounts for various equipment beyond the traction battery and electric motor (i.e. controls, wiring, etc.) needed to convert a HDV powertrain into its equivalent plug-in hybrid one

2.3 Optimization and Linear Programming

So far, many vehicle fuel production pathways have been introduced. Furthermore, several vehicle types that can use those fuels have been introduced. Together, there is a wide range of potential options that can be pursued for the transportation sector. In a problem as complex as this, it is important to have a systematic and objective approach.

Consider the Sankey diagram in Figure 17. Currently, the vast majority of transportation is fueled by petroleum. Additionally, one can see the amount of energy needed for transportation near the bottom-right corner (5.91 quadrillion British thermal units) as well as the various resources that can be utilized to meet that demand on the left side. It is clear that there is no one carbon-free source that can meet the transportation needs, whether that is biomass or some renewable source of electricity. Therefore, some methodology is needed to determine what combination of fuel sources and pathways should be pursued to meet our societal goals at the lowest cost. The proposed methodology of doing so is optimization.

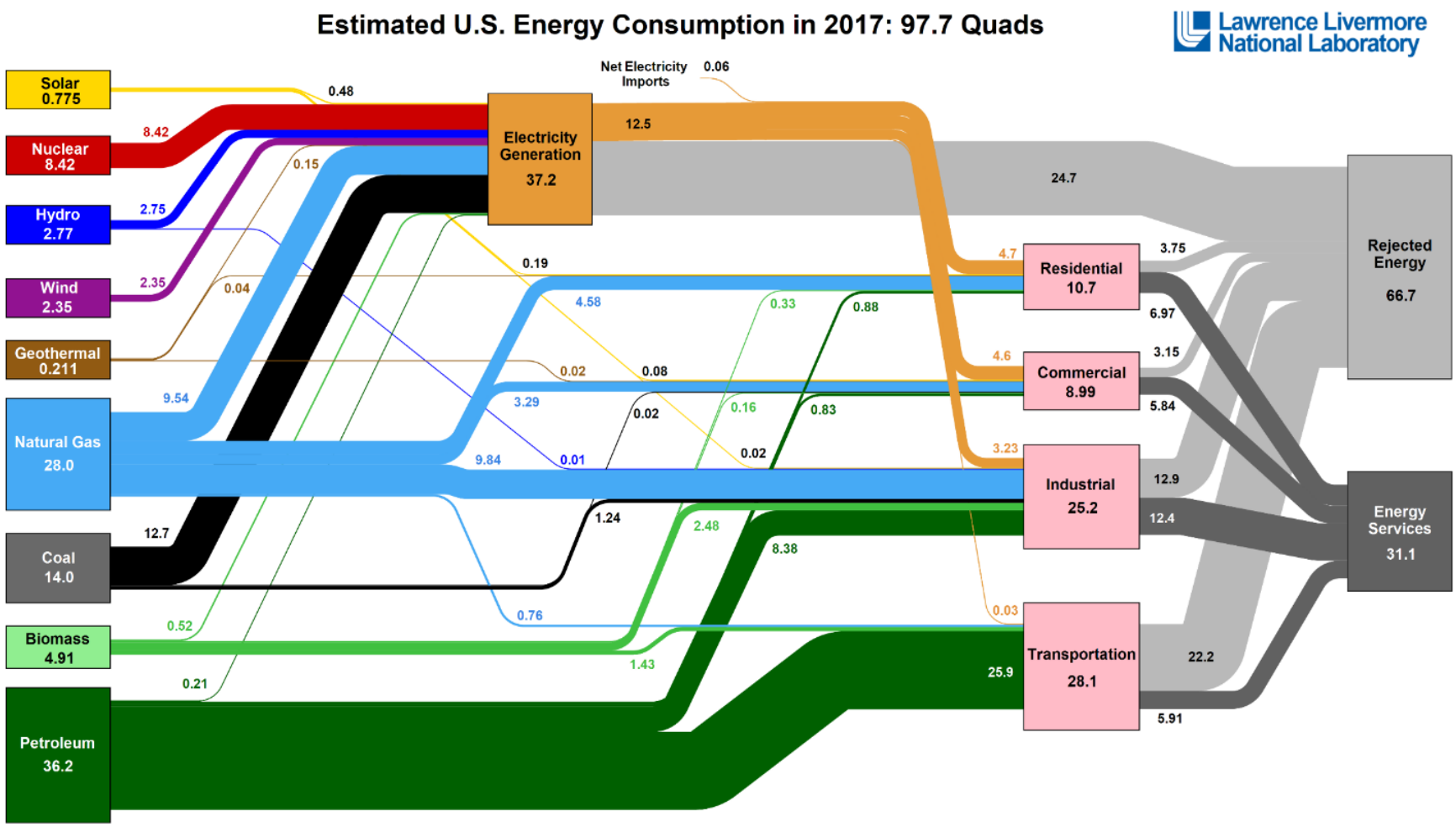

Figure 17. Sankey diagram for US Energy consumption, from U.S. Department of Energy [168]

Optimization is a mathematical methodology which selects the “optimal” option from a given set of possibilities. Here, “optimal” is defined using what is known in the optimization discipline as the cost (or objective) function. Each possible solution has an associated cost which is defined by this cost function. Note that the word “cost” here can be a misnomer in that the cost of an objective function does not necessarily have to be the cost in colloquial terms (though in the optimization problem of this dissertation it is). Optimization problems are typically set up to select from the possible solutions the one with the minimum cost. However, some optimization does attempt to maximize the cost function, which is often done when the cost function is actually reflecting a profit. Converting from a maximizing optimization problem to a minimizing optimization problem can be done by simply multiplying the cost function by negative one.

In addition to the cost function, optimization often includes constraints. These are mathematical representations that prevent certain solutions from being chosen for any desired reason, such as physical impossibility or respecting an existing regulation.

The cost function and constraints are perhaps best explained by a simple example, as follows. Imagine you are in charge of managing how electricity is generated, with multiple electricity generators at your control. Each generator has its own cost associated with producing a given amount of electricity. You must produce the exact amount of electricity that is demanded by those using the electricity in the area (this is due to the fact that there is no significant storage in the electric grid). In this example, the cost function that must be minimized is the total cost of using each of the generators to produce electricity. The constraint is that the total electricity produced by all of the generators is equal to the electricity demand. This minimization problem can be written mathematically with the minimization of the cost function which is the total cost of producing electricity shown in Equation 4, and the constraints which require electricity production must be equal to demand shown in

Equation 5. In Equation 4 and Equation 5, n is the number of electricity generators available, $genCost_i$ is the cost of producing electricity from the ith generator, x_i is the amount of electricity chosen to be generated by the ith generator, and *electricityDemand* is the amount of electricity that must be generated to meet demand.

Equation 4. Example minimization cost function

$$\min \sum_{i=1}^{n} genCost_i * x_i$$

Equation 5. Example minimization constraints

$$\sum_{i=1}^{n} x_i = electricityDemand$$

Note that optimization problems can have a single cost function to minimize (or maximize) or multiple cost functions to minimize (or maximize). In the case of multiple cost functions, a weighting must be established to determine priority of costs in finding the optimal solution. Different costs allow for optimizing with respect to different qualities, such as money spent, emissions output, driving range, or societal happiness. Note that these costs may be somewhat qualitative, but as long as a value can be artificially applied to them, they can be represented as a cost function. This dissertation uses a single cost function, which is money spent. Emissions, another major parameter included in this work, are included as constraints.

Linear programming (LP) is a subset of optimization in which the cost function(s) and each of the constraints is linear. This means that of every term in the cost function(s) and constraints, there is at least one term that is of mathematical order one, and there are no terms of higher order. Linear programming is less computationally intensive than non-linear programming, leading to solutions that converge much faster and consistently. In general, it is advisable to attempt to linearize a non-linear problem using approximations to make solving the programming problems faster and better-behaved (better convergence).

A common subset of LP is mixed integer LP (MILP). This subset allows for some variables to be constrained as integers, which may be appropriate for some problems. Consider

for example, a problem with number of people as a variable. There can be no fraction of people, so a MILP approach is appropriate.

However, this care in keeping certain variables as integers may be relaxed based on the scale of the problem and the desired detail of results. One could imagine that for some work, the difference in knowing there are, hypothetically, 14,500,000 vehicles on the road in California versus 14,500,001 vehicles is so small that the practical difference is often negligible. Furthermore, an estimate of 14,500,000.5 vehicles, while physically nonsensical, could very appropriately be rounded up to 14,500,001 vehicles without issue in most scenarios. Therefore, even some problems which may at first seem appropriate for a MILP approach may be satisfied by a relaxation to a LP without the integer variables constraint. This would improve solving time without practical detriment to the results.

2.4 Literature Review

This section reviews the literature relevant to the scope of this work. There are two sections of literature review: first, analyzing and comparing either a single or multiple fuel pathways, and second, a supply chain optimization that considers multiple fuel pathways and optimizes them according to some cost function.

2.4.1 Literature Review of Individual or Multiple Fuel Pathways Compared

Before attempting to optimize fuel production and vehicle powertrain pathways, it is wise to assess the individual characteristics of each pathway. Much of the literature is split between work on electrolytic fuels and work on biomass-sourced fuels. There is not much work that compares fuels coming from the two different feedstocks.

Bertuccioli et al. is a techno-economic assessment of hydrogen production pathways, with AEC and PEMEC electrolyzer technology improvements. Major contributions of this work are the efficiency and cost of both AEC and PEMEC technology with projections to 2030, as well as distribution and dispensing considerations [169]. Not included in this work are data for SOECs or analysis of vehicles. Also, projections were only made to 2030, not to 2050 as in the present work.

Schmidt et al. is another notable techno-economic work for electrolytic hydrogen pathways, including a ten-expert survey of five academics and five industry representatives. Included electrolyzer technologies are AEC, PEMEC, and SOEC [170]. Only fuel production is considered, and there are no emissions considerations. Like Bertuccioli et al., projections were also only made out to 2030.

Ramsden et al. have evaluated the current state of 10 P2G pathways and determined their associated levelized cost of hydrogen and greenhouse gas emissions. Data used for this analysis are sourced primarily from the H2A Production Model, the Hydrogen Delivery Scenario Analysis Model, GREET, and the Cost-per-Mile Tool. The updated version of the report includes, in addition to up-to-date data, additional P2G pathways that add up to the 10 mentioned as well as more analysis with FCEVs. The pathway with distributed natural gas reforming led to the lowest levelized cost of hydrogen, and the pathway with distributed ethanol reforming led to the highest levelized cost of hydrogen [171]. This work is notable for its comprehensive analysis of all major portions of the fuel pathway, including fuel production, distribution, dispensing, and use in vehicles. This comprehensive framework serves as an example of work to be carried out both into the future as well as for other fuels, neither of which are included in this work.

Eichman et al. have studied the value that hydrogen energy storage, an aspect of P2G, has in California specifically in the electricity market. This study found that hydrogen from P2G is more valuable when selling it as hydrogen, for example as a fuel, than it is as energy storage to be converted back to electricity later. NREL concedes that the conclusions may be different in the future as the energy grid changes [172]. This is important to note because it supports the claim of the present work that hydrogen is a viable fuel for vehicles.

Melaina et al. compare production costs of various hydrogen production pathways, including electrolysis, SMR, and biomass gasification. The report also details the benefits of P2G at various scales, from small scale with fork lifts and backup power, to medium scale with fuel cell electric vehicles, to large scale with more renewable energy interplay [173]. This is one of the few pieces of work that compares hydrogen production costs between electrolytic and biomass gasification methods. However, no vehicle or emissions analysis is included, and neither are any other fuels besides hydrogen.

Zhu et al. did a comprehensive techno-economic assessment of liquid fuel production from biomass feedstocks. Included production methods are gasification-FT, liquefaction, and pyrolysis [120]. This work is valuable due to its comparison of a wide variety of liquid fuel production methods with a biomass feedstock, but it does not include a scenario of hydrolysis, and it also does not include any pathway steps beyond fuel production.

Hanggi et al. compiled a review work detailing the energy efficiency from fuel production to vehicle use for several fuels and LDV powertrains. This work stands out for the inclusion of all major fuel and vehicle pathway steps for passenger vehicles. However, the work does not include any cost or emissions analysis, nor any work on HDVs.

Table 6 summarizes the key literature in this area, including that mentioned above as well as other studies in this field.

Table 6. Individual or Multiple Fuel Pathways Compared Literature Review

Authors and year	Scope	Fuel pathway consideration	LDV/HDV	Fuels	GHG emissions	CAP emissions	Cost	Optimization
Ramsden et al. 2013 [171]	WTW energy and emissions of 10 P2G hydrogen pathways (distributed NG reforming lowest cost, distributed ethanol reforming lowest emissions)	Production, distribution, dispensing, vehicles	LDV (FCEV)	Hydrogen	Yes	No	Yes	Distribution (trucking and pipeline sizing)
Eichman et al. 2016 [172]	Compare cost and price of hydrogen storage vs. hydrogen fuel in CA, and fuel is most economical	Production	LDV (FCEV)	Hydrogen	No	No	Yes	No
Melaina et al. 2015 [173]	Compares production costs of various hydrogen production pathways including electrolysis, SMR, and gasification; assesses various issues and opportunities for hydrogen	Production	No	Hydrogen	No	No	Yes	No
Paakkonen et al. 2017 [66]	Electrolysis and biological methanation with AD for power production or fuel	Production	No	Methane	No	No	Yes	No
Campanari et al. 2009 [174]	BEVs fueled by multiple electric grid compositions and FCEVs fueled by various hydrogen pathways are compared for efficiency and GHGs	Production, distribution, vehicles	LDV (BEV and FCEV)	Electricity, hydrogen	Yes	No	Hydrogen distribution only	Distribution (pipeline sizing), vehicle (FCEV hybrid battery)
Bolat and Thiel 2014 [175]	Bottom-up techno-economic assessment of hydrogen production pathways	Production	No	Hydrogen	Limited	No	Yes	No
Bertuccioli et al. 2014 [169]	Bottom-up techno-economic assessment of hydrogen production pathways, electrolyzer technology improvements	Production, distribution, dispensing	No	Hydrogen	Yes	No	Yes	No

Authors and year	Scope	Fuel pathway consideration	LDV/HDV	Fuels	GHG emissions	CAP emissions	Cost	Optimization
Schmidt et al. 2017 [170]	Bottom-up techno-economic assessment of electrolytic hydrogen production pathways, 10 expert survey (5 academic, 5 industry)	Production	No	Hydrogen	No	No	Yes	No
Krewitt and Schmid 2005 [176]	Techno-economic assessment of hydrogen production from various renewable and non-renewable sources, electrolyzer technology	Production, distribution, dispensing	No	Hydrogen	No	No	Yes	No
Robinius et al. 2018 [177]	Modeled electricity distribution grid with P2G additions compared to electricity grid expansion	Production	No	Electricity, hydrogen	No	No	Yes	No
Wulf et al. 2018 [178]	Characterized GHG impact of hydrogen distribution pathway options, with a sensitivity analysis for each of the components	Production, distribution, dispensing	No	Hydrogen	Yes	No	No	No
Snehesh et al. 2017 [179]	Techno-economic assessment of liquid fuel production from gasification-FT	Production	No	Liquid (gasoline, diesel)	No	No	Yes	No
Zhu et al. 2011 [120]	Techno-economic assessment of liquid fuel production from biomass feedstocks. Included production methods are gasification-FT, liquefaction and pyrolysis.	Production	No	Liquid (gasoline, diesel)	No	No	Yes	No
Hanggi et al. 2019 [180]	Energy efficiency well-to-wheel analysis of various electrolytic fuel production pathways	Production, distribution, dispensing, vehicles	LDV	Electricity, hydrogen, methane, liquid	No	No	No	No

2.4.2 Literature Review of Supply Chain Optimization

Significant work has been done in the area of reducing emissions from transportation. Focusing on the areas closely related to optimization in fuel pathways and powertrains, the work can be narrowed down, and some of the standout work in this field are summarized below.

A study from d'Amore and Bezzo looked at minimizing the cost of carbon dioxide capture, transport, and sequestration in Europe [181]. This work can be thought of as part of a fuel production pathway, as carbon dioxide is needed to make SNG in the electrolytic pathways. Here, an optimization with spatial consideration determines the lowest cost method of capturing carbon dioxide from industrial and combustion processes and then transporting that carbon dioxide to geologic locations to sequester it, or store it indefinitely, in Europe. While the application of the optimization problem does not align too closely with the work of this dissertation at it only considers carbon dioxide, the methodology shares similarities with the present work but with an increased spatial focus.

Work by Angeles et al. looked at optimizing the production, transportation, and use of ammonia as fuel in both ICVs and FCEVs [182]. This study includes both fuel production and fuel use in a powertrain, but it is limited in scope to only one fuel and two powertrains. Moreover, the use of ammonia as a fuel in vehicles is unlikely considering offerings from vehicle manufacturers and general literature consensus. Therefore, the present work does not consider ammonia as a future vehicle fuel. However, the work by Angeles et al. is still relevant due to the methodology detailed within the work.

A study by Ribau et al. details optimization of efficiency, cost, and life cycle carbon dioxide emissions for FCEV and PFCEV buses, particularly focusing on powertrain. This study

uses single- and multi-objective genetic algorithms with ADVISOR, a powertrain modeling tool [162]. This study is noteworthy for including PFCEVs in addition to FCEVs and BEVs in the robust optimization methodology, but it does not include other HDV fuels such as SNG or renewable diesel.

Samsatli and Samsatli optimize considering cost, profit, and emissions various fuel production pathways for electricity, hydrogen, SNG, and syngas in Great Britain. All pathway sections, including feedstock, fuel production, distribution, dispensing, and vehicles are included in the analysis, as well as projections out to 2050. However, vehicle work is minor, only considering light-duty FCEVs. This work's focus is on energy and heating demands, so transportation analysis is a secondary consideration [183]. Drawbacks to this work, in addition to the aforementioned minor vehicle analysis, include no liquid fuels consideration and no CAP emissions analysis.

Table 7 summarizes the key literature in this area, including that mentioned above as well as other studies in this field.

Table 7. Supply Chain Optimization Literature Review

Authors and year	Scope	Fuel pathway consideration	LDV/HDV	Fuels	GHG emissions	CAP emissions	Cost	Optimization
d'Amore and Bezzo 2017 [181]	Techno-economic work to minimize the cost of carbon dioxide capture, transport, and sequestration in Europe	Production, distribution	No	(Carbon dioxide)	Yes	No	Yes	Yes, MILP
Angeles et al. 2017 [182]	Well-to-wheel analysis of fossil- and bio-NH3 as a fuel for ICEVs or FCEVs, minimizing carbon and nitrogen emissions	Production, distribution, vehicles	Unspecified	Ammonia	Yes	Yes	No	Yes, P-graph
Ribau et al. 2014 [162]	Single- and multi-objective optimization of FCEV and PFCEV with comparison to diesel ICV, including cost, efficiency, and lifetime GHG emissions	Vehicles	HDV (ICV, FCEV, and PFCEV)	Hydrogen, electricity	Yes	No	Yes	Yes, genetic
Parker, Tittmann, et al. 2010 [184]	Resource analysis and biorefinery siting to optimize biomass use for transportation fuel given price	Production, distribution	No	Liquid biofuels	No	No	Yes	Yes, MILP
Parker, Fan, et al. 2010 [49]	Analysis of economic potential and infrastructure for H2 from biomass	Production, distribution	No	Hydrogen	No	No	Yes	Yes, MINLP
Parker et al. 2017 [185]	Techno-economic model with renewable CH4 supply curves, up to 2025	Production, distribution	No	Renewable CH4	No	No	Yes	Yes, spatial
Zandi Atashbar et al. 2018 [186]	Review paper of models and methods to optimize biomass supply chains	Production, distribution	No	Biofuels	Yes	Yes	Yes	Yes, mostly MILP
Samsatli and Samsatli 2018 [183]	Multi-objective MILP model with evolution of electricity, H2, natural gas, and syngas networks to 2050; considers technological constraints	Production, distribution, dispensing, vehicles	LDV (FCEV)	Electricity, H2, natural gas, syngas	Yes	No	Yes	Yes, MILP

2.4.3 Background Summary

After introducing the vast number of options for alternative fuel production and powertrain options for both LDVs and HDVs, it is apparent that a comprehensive, objective methodology is needed to account for techno-economic data as well as fuel infrastructure and vehicle use characteristics. The fuel production pathways and vehicle powertrain options detailed in this chapter will serve as the map from which such a methodology will follow, adding to it the necessary data and projections needed to comply with environmental legislation.

The key finding from the preceding literature review is that no work has analyzed and optimized options for the breadth of fuels and vehicle powertrains to the extent of pathway proposed in this work. In particular, the fuels to be included are electricity, hydrogen, SNG, renewable gasoline, and renewable diesel; the vehicle powertrains to be included are ICV, HEV, PHEV, BEV, FCEV, and PFCEV; and the pathway components to be included are fuel production, distribution, dispensing, and use in vehicles.

A second finding is that LP appears to be an appropriate optimization tool for this work. If the cost function and constraints allow for its use, LP will be the chosen optimization tool for this work. For any cost or constraint that is not linear, care will be taken to effectively simplify these non-linear components to linear ones.

This dissertation fills the gap in knowledge by establishing the viable fuel pathways and powertrain configurations noted above for LDVs and HDVs. The fuel pathways and powertrain configurations techno-economic data are projected out to 2050 and options are optimized using LP to minimize the cost of complying with environmental constraints from the transportation sector.

3. APPROACH

The goal of this dissertation is to establish viable fuel pathways and powertrain configurations for LDVs and HDVs that meet environmental constraints at the lowest cost. This work develops a methodology to characterize and project various fuel pathways and powertrain configurations techno-economic data and then determine a fleet to meet transportation needs into 2050. The results of this work will inform the transportation industry and policy makers how society might effectively transform the transportation sector in a future of stricter environmental regulations.

3.1 Tasks

To meet this dissertation goal, the following tasks will be completed.

Task 1. Establish the fuel pathways for LDVs and HDVs.

A literature review of the transportation sector will yield a list what fuels are being considered for LDVs and HDVs as the State works toward cleaner vehicles across all vehicle types and applications. Fuels come in the form of gaseous and liquid fuels, as well as electricity in the case of PEVs.

Once the range of fuels has been selected, each one will be studied to determine its pathway, that is, the steps that are followed from raw feedstock to finished fuel at the appropriate dispensing station. Once each of the fuel pathways has been decomposed into its corresponding individual steps, these steps can be further analyzed in the later Tasks for the techno-economic analysis of this dissertation.

Task 2. Establish the powertrain configurations for LDVs and HDVs.

A literature review will expose the alternative fuel powertrains that should be included in this study. The powertrains may vary based on classification, so each one will be considered individually. Once the powertrains have been selected, each one will be studied to determine the main components to consider, as a simplification of the vehicle as a whole without looking into the various powertrain components may yield unrealistic results, particularly with respect to the vehicle costs.

Note that the results of both Tasks 1 2 have been detailed in the Background of this dissertation.

Task 3. Develop efficiency, cost, and emissions data out to 2050 for the fuel pathways established in Task 1 and the vehicle powertrain configurations established in Task 2.

This Task is a comprehensive literature review to collect data of efficiency, cost, and emissions of the various fuel pathways and powertrains. Additionally, this Task requires the development of a methodology to project those data throughout the time horizon of analysis, up to 2050. These projections will be the inputs to the optimization tool developed and run in later Tasks.

Task 4. Establish the constraints of the optimization problem using California legislation and executive order for emissions, realistic growth scenarios for travel and technology, and feedstock availability.

Four classes of constraints are present in this optimization problem: emissions regulations, VMT, realistic technology deployment, and feedstock availability. California

legislation will be consulted to determine the emissions regulations up to 2050; from these pieces of legislation, constraints will be created for the WTW emissions from vehicles. VMT in California are documented annually, and these will be extrapolated up to 2050 to create constraints that must be met. Realistic technology deployment rates will constrain the problem such that technologies cannot be deployed instantly or at rates that may not be feasible for a number of practical reasons. Lastly, feedstock availability constraints must be considered as there is only a limited amount of biomass and electricity that could be used to make vehicle fuels.

Task 5. Determine optimization tool to use given the results of Tasks 3 and 4, and establish the formal optimization problem.

Many optimization algorithms and software exist. This Task will focus on studying the various algorithms and software, with the goal of determining which combination will be best suited to this study. The method and software must take in the data developed in Task 3 and the constraints developed in Task 4. The formal optimization problem is then established in this Task, including the cost function and the constraints.

Task 6. Solve the optimization problem established in Task 5 to determine the emissions and cost impacts of the optimum cases. Compare these results to the Reference Case.

Solving the optimization problem established in Task 5 will determine the mix of fuel pathways and vehicle powertrain configurations that minimizes total cost of implementation while still meeting California emissions legislation. Task 6 then develops a Reference Case of conventional fuels (mainly gasoline and diesel) and conventional vehicle powertrains

(combustion engines) which is representative of the vehicle fleet today. The costs and emissions associated with these fuels and vehicles will be calculated and serve as a Reference Case with which to compare the alternatives studied in this work. Then, the optimization results will be compared to the Reference Case to see the changes in emissions and the associated costs from two alternative cases, a Non-ZEV Constrained Case and a ZEV-Constrained Case.

Task 7. Systematically assess the results to establish viable fuel pathways and powertrain configurations for LDVs and HDVs that meet the constraints of this problem.

Task 7 uses the results of Task 6 to achieve the goal of this dissertation and provide pathways for potential transportation sector evolution in the context of California's legislation and realistic constraints of adoption.

4. VEHICLE FUEL PATHWAYS

This chapter details the vehicle fuel production, distribution, and dispensing techno-economic projections that are carried out to be inputs to the optimization problem.

Because the timescale of the present work is long (30 years from 2020 to 2050), inflation must be considered. This work assumes a 2% rate of inflation, which is in line with recent historic data from the U.S. [187].

Also needed due to the long timescale and the high capital costs of creating large fuel production plants, the idea of a capital recovery factor (CRF) is introduced. A CRF is a method of capturing various economic data such as interest rates, depreciation, lifetime of equipment, and others to convert a single bulk capital cost into recurring payments. The present work assumes a CRF of 0.12 for all equipment to calculate yearly payments from a single capital cost. The precedent for this value is work from the U.S. Department of Energy using such a CRF for its coal power plants for low-risk scenarios [188]. Inherent in using this CRF is the assumption that the proceeding fuel production plants will be low-risk. This would mean that large entities such as utilities would be the ones creating these plants, a valid assumption for a high-capital plant. Also assumed is a lifetime of 30 years, which is the time of interest for this work. Therefore, when a fuel production plant is built, it will be used until the end of the model run.

4.1 Fuel Feedstocks

Here, the cost of both electricity and biomass feedstocks is detailed. Emissions results are presented at the end of this chapter, at which point both the feedstock emissions as well as the total fuel pathway emissions up to the vehicle will be detailed.

4.1.1 Electricity as a Fuel Feedstock

Electricity cost is sourced from E3's PATHWAYS work that projects demand of electricity and how that demand can be met most cost-effectively while meeting emissions legislation of California [189]. Note that there are different prices associated with different end uses. Fuel production is the lowest, and that is associated with using electricity as a feedstock for other fuels, such as electrolytic hydrogen or SNG. Transportation rates are higher, and these are the rates that would be in place for a driver to charge their PEV with electricity. One could imagine a worst-case scenario of residential rates for PEV charging if there is no special consideration for vehicle charging in the future, an unlikely scenario given that some utilities already have lower PEV charging rates in their contracts [190]. Other electricity rates are projected as well, such as for commercial and industrial sectors, but those are not relevant in the context of fuel production so they are not shown in Figure 18. The present work uses E3's fuel production rates for the electricity feedstock by default.

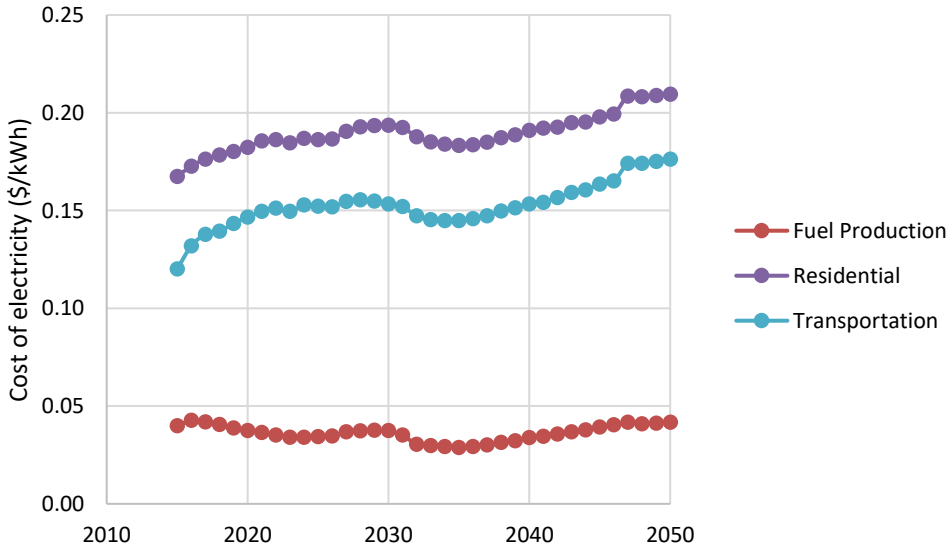

Figure 18. Electricity price projections, current policy reference scenario with SB 100, from [189]

These prices are assumed to be constant over the range of availabilities described in Chapter 6.4, an assumption that is most accurate if the modeled electricity demand of this work is similar to that of E3's. Given the assumptions of Chapter 6.4, these prices should be appropriate.

A co-feedstock one must consider with electrolytic fuels is water, as water is split to produce hydrogen and oxygen. Water can come from various sources, and it is scarcer in Southern California than Northern California. The Metropolitan Water District of Southern California lists water rates for water originating from Northern California at around $300 per acre-foot [191]. Using an average value from electricity costs of $0.0375/kWh, this leads to water accounting for on the order of 0.1% of total electrolytic fuel production (this involves data and calculations that are shortly to be detailed). Even at the extreme case of water produced by desalination, with the highest cost estimates of $5,000 per acre-foot [192], that leads to water costs of about 1.5% of total electrolytic fuel cost. Therefore, it is safe to assume water costs are insignificant for these electrolytic fuels, and water is not analyzed in the proceeding techno-economic work.

4.1.2 Biomass as a Fuel Feedstock

Prices for biomass feedstocks are found in the U.S. Department of Energy's Billion Ton Report [31]. Figure 19 shows the quantity of each of the categories of biomass available at various selling prices. These quantities are given every 5 years from 2020 to 2040. Selling prices start at $30/dry ton and increase by $10/dry ton increments up to $100/dry ton.

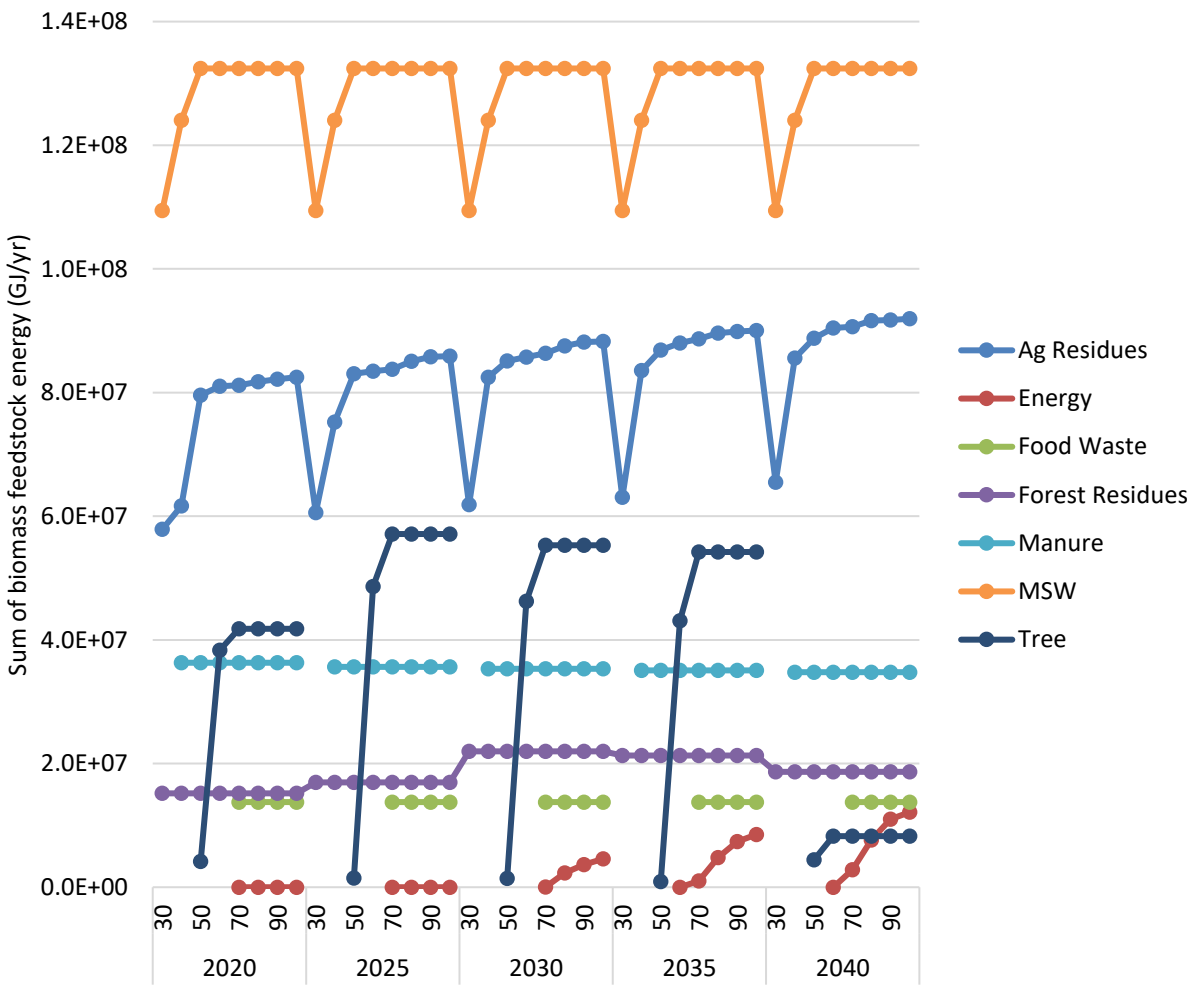

Figure 19. Current and potential biomass production for energy use in California based on medium housing, medium energy use, and base case energy crop growth scenario with non-organic MSW removed, data from [31].

Here, a weighted average of heating value for the categories of food waste, manure, agriculture, waste, forestry, and energy crops is used to convert from dry ton of each individual biomass feedstock to energy content. Weighting is based on the capacity available according to the Billion Ton Report. Using the weighted average is justifiable for this conversion because the relative ratio of the specific biomass feedstocks within the above categories stays relatively similar throughout the years and prices considered, as shown in Figure 20.

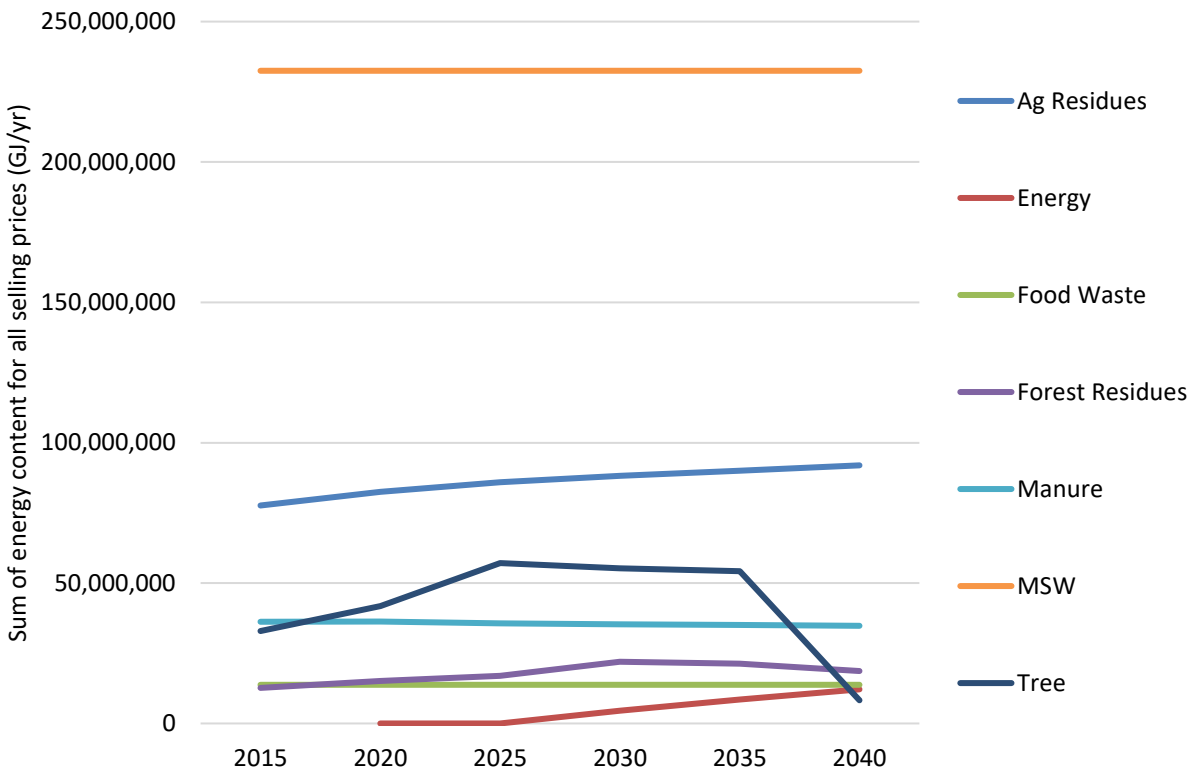

Figure 20. Total biomass energy available by feedstock category, data from [31]

Some important notes from the biomass feedstock data are described below.

MSW is the feedstock with the highest availability, both at the lowest cost of $30/dry ton, as well as for every higher cost. This makes MSW an attractive biomass feedstock for the technologies that can use it, though emissions are another important factor that have yet to be discussed.

Energy crops, which are grown for energy purposes, do not show up as a feedstock option until 2030. Additionally, these energy crops are available only at the higher end of the cost scale, meaning they will not get used until the cheaper feedstocks are all used. Incentives could be introduced, like how corn is subsidized, but these incentives are outside the scope of the present work.

Tree biomass reaches a peak in 2025, slightly declines until 2035, and then dramatically reduces in 2040. One possible explanation for this is over-using this biomass in the earlier years and reduced forestation in future years, leading to less dead and fallen trees for use as a feedstock. This is an issue that should be further investigated to ensure sustainable use of this biomass feedstock.

Lastly, some feedstocks have similar availabilities at all selling prices, while others have increasing availability as selling price increases. Crop types that do not increase in availability with selling price are food waste, forest residues, and manure. Crop types that do increase in availability with selling price are agriculture residues, energy crops, MSW, and trees. This behavior of increasing availability with selling price is indicative of the fact that increasing selling price opens the opportunity for more involved and costly extraction or collection procedures. For energy crops, which are expressly grown for energy uses, there is the additional factor that increasing selling price increases the number of market players willing to grow energy crops for profit. For the crop types that exhibit increased availability at increased selling price, all but energy crops increase in availability for the first two selling price increases, but thereafter stay constant in availability (or nearly constant in the case of agriculture residues). Energy crops have a more consistent increase in availability at increasing selling price, likely due to the above-mentioned factor of increasing market players.

Simplifications are made to reduce the number of separate cost brackets for each of the feedstocks. For example, agriculture residues are available at $30/dry ton up to $100/dry ton at different quantities for each $10/dry ton increment. However, looking at Figure 19, a reasonable simplification is to consider in 2020 that 5.8e7 GJ/yr of agriculture residues available for $30/dry ton, and 8e7 GJ/yr available for $50/dry ton. This is neglecting the slight increase in availability

at $40/dry ton compared to $30/dry ton, and the slight increase in availability at prices higher than $50/dry ton. This same methodology is carried out for the rest of the years analyzed as well as the other feedstocks with varying availabilities at different costs.

4.2 Fuel Production

This section details the efficiency and cost of fuel production for the five fuels considered in this work (electricity, hydrogen, SNG, renewable gasoline, and renewable diesel). Note that the electrolysis pathways for both hydrogen and SNG include the most detail as this was the area with least information and agreement in the literature. The methodology developed for these electrolytic fuels is then applied to the other fuel production methods.

Many methods have been proposed for estimating technological progress and the effects on cost. These include Moore's law [193], Wright's law [194], and various other variants [195]. Nagy et al. tested these different methods for estimating technological progress based on a database of 62 different technologies and showed that Wright's law and Moore's law perform essentially the same with a slightly better performance by Wright's law [195].

Wright's law projects future capital costs based on the cumulative capacity produced (rather than using time as in the case of Moore's law). The equation for Wright's law can be written as shown in Equation 6 according to [196].

Equation 6. Wright's law

$$\mathrm{C}(\mathrm{p_t}) = \mathrm{C}(\mathrm{p_i})\left(\frac{\mathrm{p_t}}{\mathrm{p_i}}\right)^{-\mathrm{b}}$$

Here, p_i is the initial production volume, p_t is the production volume at time t, $C(p_t)$ is the cost at production volume at time t, $C(p_i)$ is the cost at the initial production volume, and b is an exponential learning parameter related to the learning rate (LR) by the equation.

Equation 7. Learning rate

$$LR = 1 - 2^{-b}$$

Figure 21 shows the probability distribution of learning rates for various industrial technologies collected from 108 studies [196].

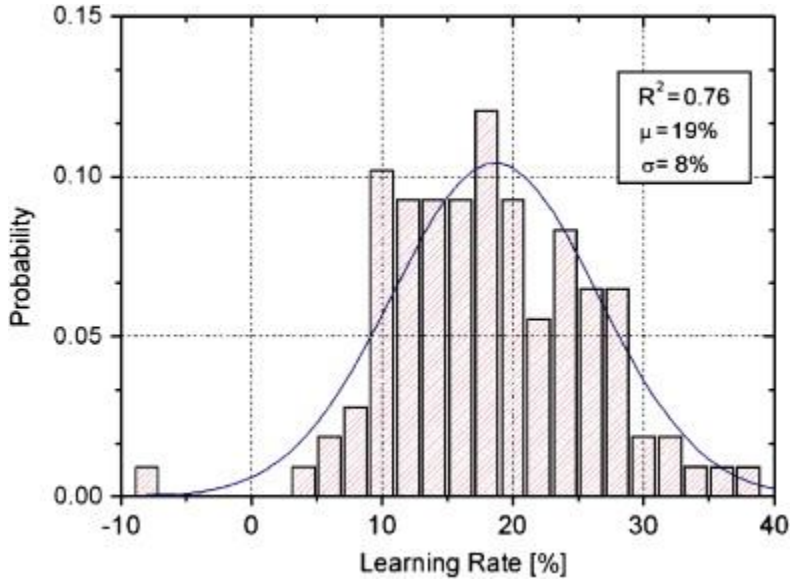

Figure 21. Probability distribution of 108 studies that report learning rates in 22 industrial sectors from [196]

In the coming sections, it will be shown that there is a wide range of current costs and cost projections for electrolyzer technologies. Therefore, a conservative and an optimistic scenario are proposed in this work for the cost projections of P2G equipment. The conservative scenario assumes a constant 14% learning rate for electrolyzers and 10% for the remaining P2G equipment throughout the timeframe considered. The optimistic scenario assumes a 25% learning rate until 2030, 15% learning rate until 2035, and then 10% learning rate until 2050 for the electrolyzers and a constant 14% learning rate for remaining P2G equipment. The rest of the equipment considered in this work are less technologically-complicated and therefore have lower

associated learning rates because costs should not be expected to decrease as drastically. Therefore, a learning rate of 10% is applied for non-P2G fuel production equipment.

Fuel production equipment has a dependence on scale for both efficiency and cost. Therefore, for each type of equipment, the scale of plant used for the techno-economic data presented is noted. Significant deviation in plant size from that scale could result in inaccuracies. Generally, electrolyzers are less affected by scale than other fuel production equipment [197].

Note that while the following sections include cumulative installed capacities for each of the fuel production technologies (in cumulative GW in the corresponding years shown), these numbers should only be considered hypothetical examples at this point to give an idea of how cumulative installed capacities of these technologies affect cost. The capacities shown will be further detailed in Chapter 6, and the actual projected cumulative installed capacities of the modeling will be determined by a methodology explained in Chapter 7.

4.2.1 Hydrogen Fuel Production

Hydrogen can be produced by electrolysis or gasification in the context of this work. Both the electrolyzers and gasifiers are taken to be 50 MW in size.

4.2.1.1 Electrolytic Hydrogen Fuel Production

Electrolytic hydrogen uses electricity as its feedstock and electrolyzers as the fuel production equipment. As noted before, water costs are negligible and will therefore not be considered in the proceeding work.

a) Efficiency of Electrolytic Hydrogen Fuel Production

Literature values for electrolyzer efficiency give a range of efficiencies both now and into the coming decades. Table 8 and Figure 22 show recent and current values for electrolyzer efficiency from the literature sources as cited.

Table 8. Information on efficiency for SOEC, PEMEC, and AEC from literature

EC TYPE	AUTHOR	YEAR	SOURCE INFO	STACK LHV EFFICIENCY (%)
SOEC	Tang et al.	2016	[198]	83.9
	Ouweltjes et al.	2007	[199]	79-95
	Pan et al.	2017	[64]	73
	Paakkonen et al.	2018	[66]	95
PEMEC	Millet et al.	2010	[200]	71-72.5
	Gibson and Kelly	2008	[201]	75-77
	Siracusano et al.	2010	[202]	70
	Paakkonen et al.	2018	[66]	70
AEC	Campanari et al.	2009	[174]	60-90%
	Bolat and Thiel	2014	[175]	61-79%
	Paakkonen et al.	2018	[66]	70%

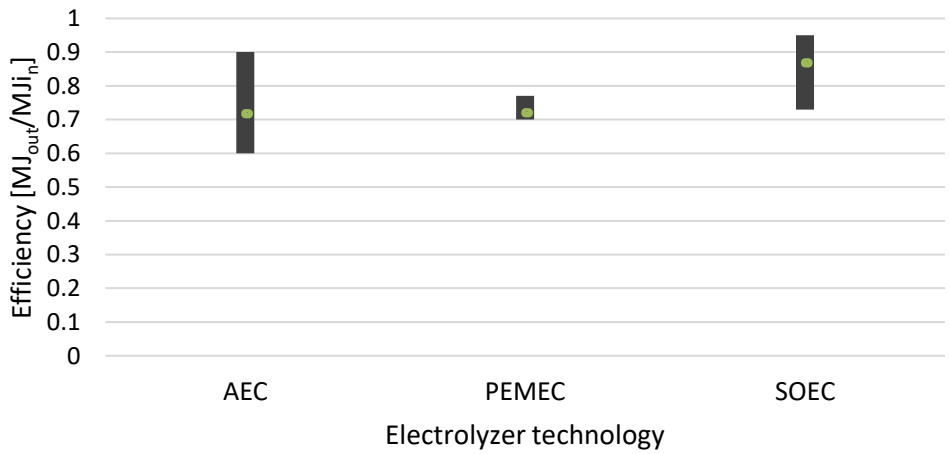

Figure 22. Range of electrolyzer efficiencies found in the literature, from sources of Table 8

Also necessary is determining the evolution of electrolyzer efficiency with time. According to Schmidt et al. [170], efficiency projections are not as important as others due to manufacturers stating they are focusing on cost reduction and overall P2G efficiency instead of

simply electrolyzer efficiency. See Figure 23 for projections of various electrolyzer efficiency projections from standout studies in the literature.

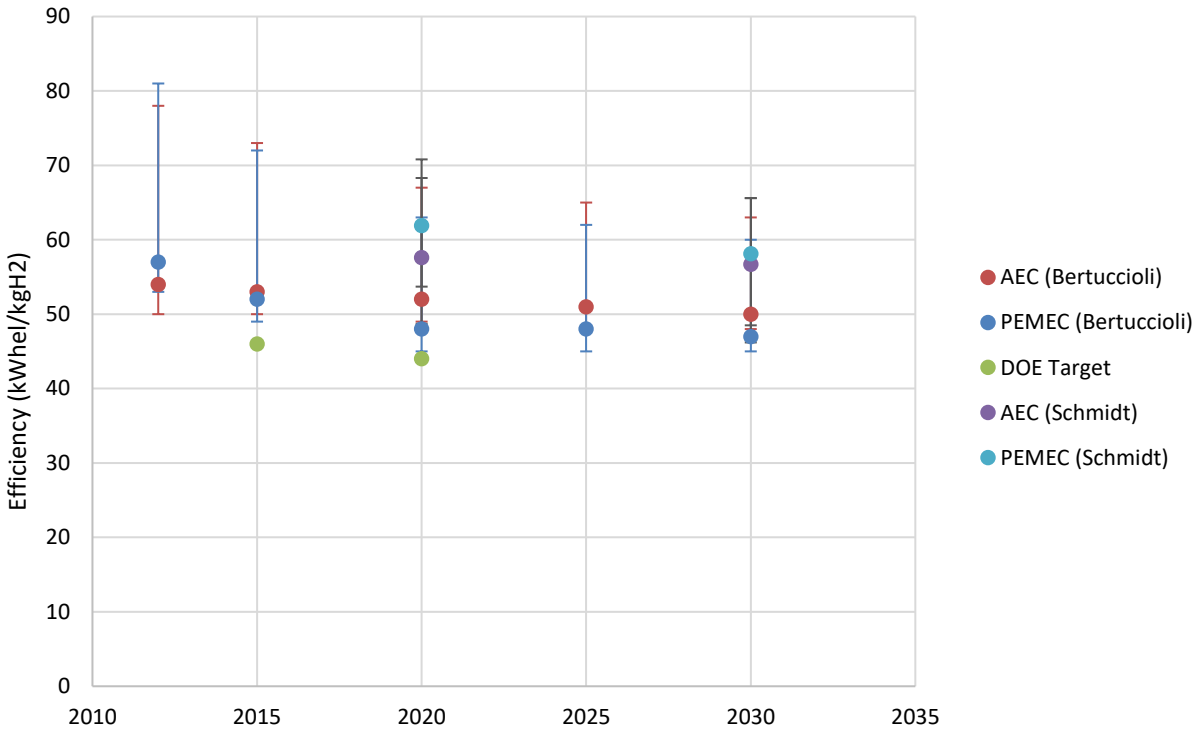

Figure 23. Electrolyzer system efficiency projections from [37], [170], [203]

There is clearly a wide range of values in this set, so some work must be done to simplify the data into more usable values. To distill efficiency information from the literature into values to use for this analysis, two efficiency scenarios are introduced. The first is the conservative scenario, which uses efficiency numbers on the lower end of the spectrum of the literature data. The second is the optimistic scenario, which uses efficiency numbers on the higher end of the literature data. Note that these efficiency projections are to align with the conservative and optimistic learning rate scenarios introduced previously.

In addition to the initial values used for efficiency, as well as some long-term efficiency estimates from the literature, intuition, and an understanding of general technology learning assisted in creating curves for the evolution of electrolyzer efficiency. One detail that stands out

for the efficiency evolution is for SOECs. SOECs are unique among the electrolyzer technologies selected in that they are high temperature and get more efficient as their temperature increases. This means that they are able to use the waste heat of methanation, which is an exothermic reaction, to increase their efficiency instead of any other potential use of heat. Therefore, two SOEC scenarios are considered: (1) lower efficiency SOECs without methanation where the end product is hydrogen, and (2) higher efficiency SOECs with methanation where the end product is SNG.

Plots for the efficiencies of the three electrolyzer technologies for the conservative scenario and the optimistic scenario are found below in Figure 24 and Figure 25, respectively.

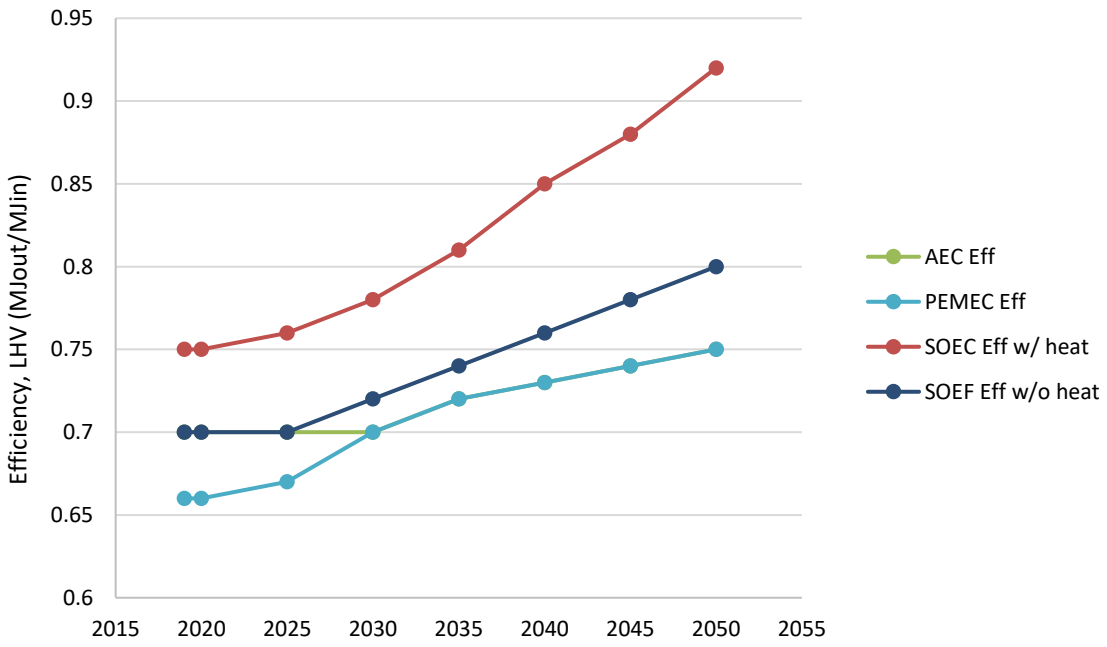

Figure 24. Conservative estimate on electrolyzer efficiency projection

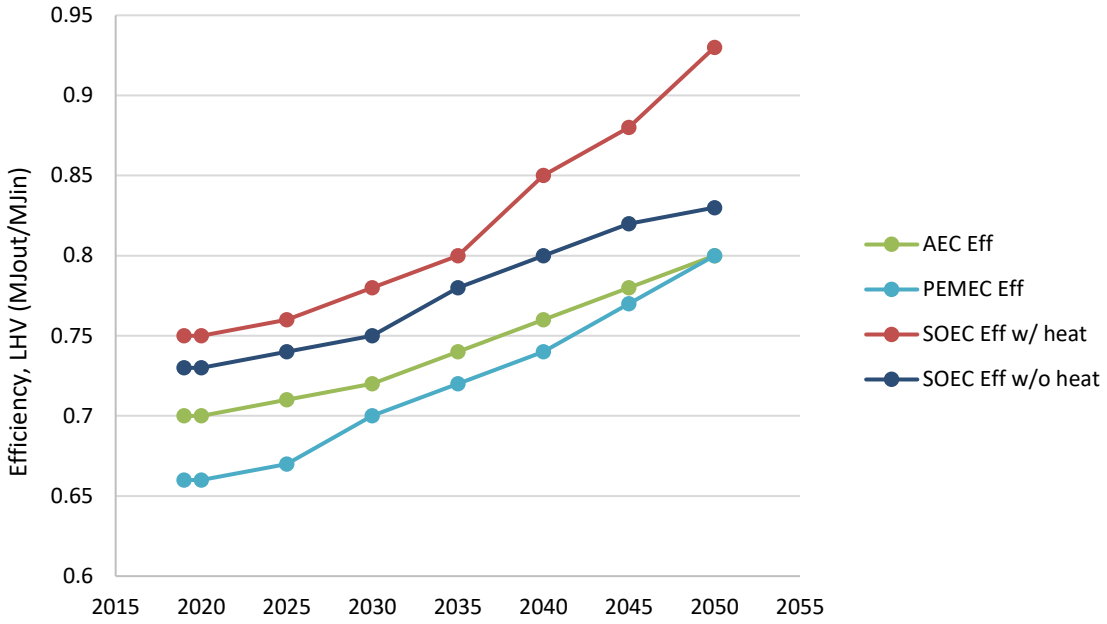

Figure 25. Optimistic estimate on electrolyzer efficiency projection

b) Cost of Electrolytic Hydrogen Fuel Production

Two areas are important here for cost: the first is current cost estimation, and the second is future cost projection. Literature was again consulted for these two areas, and the findings for current cost estimations are presented in Figure 26 and Figure 27, with the various sources shown in Table 9.

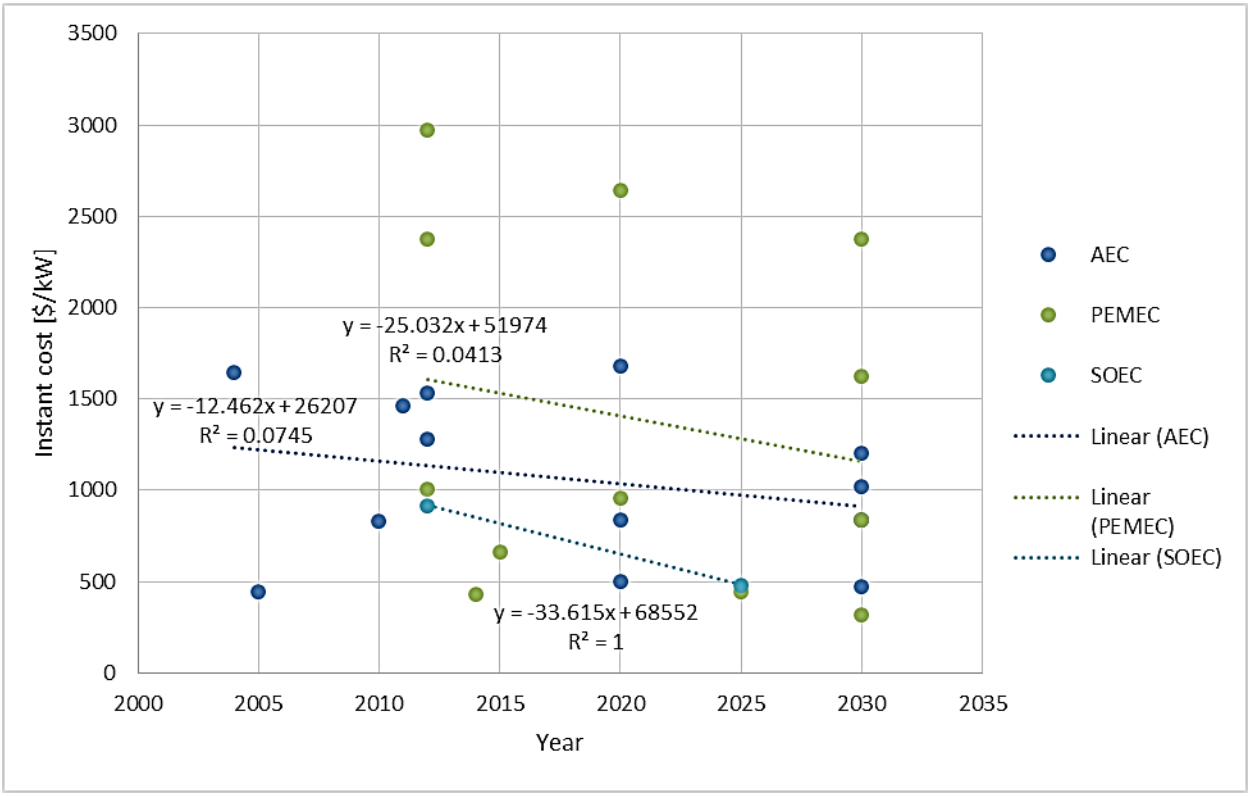

Figure 26. Information on cost for PEMEC and AEC versus time for references listed in Table 9

Table 9. Information on cost for PEMEC, SOEC, and AEC from literature

EC TYPE	AUTHOR	YEAR	SOURCE INFO	INSTALLED COST ($/KW)
SOEC	US DOE	2012	[204]	918
	US DOE	2025	[204]	481
PEMEC	Bertuccioli et al.	2012	[37]	2376-2970
	Bertuccioli et al.	2030	[37]	320-1626
	Godula-Jopek et al.	2015	[205]	665
	Schmidt et al.	2020	[206]	960-2640
	Schmidt et al.	2030	[206]	840-2376
	James (DOE, SAI)	2013	[207]	1008
	James (DOE, SAI)	2025	[207]	448
AEC	Mansilla et al.	2011	[208]	1464.
	Krewitt and Schmid	2005	[209]	445
	National Research Council	2004	[210]	1643
	Bertuccioli et al.	2012	[37]	1280-1536
	Bertuccioli et al.	2030	[37]	469-1024

	Schmidt et al.	2020	[206]	840-1680
	Schmidt et al.	2030	[206]	840-1200
	NEL/H2V Agreement	2020	[211]	~500

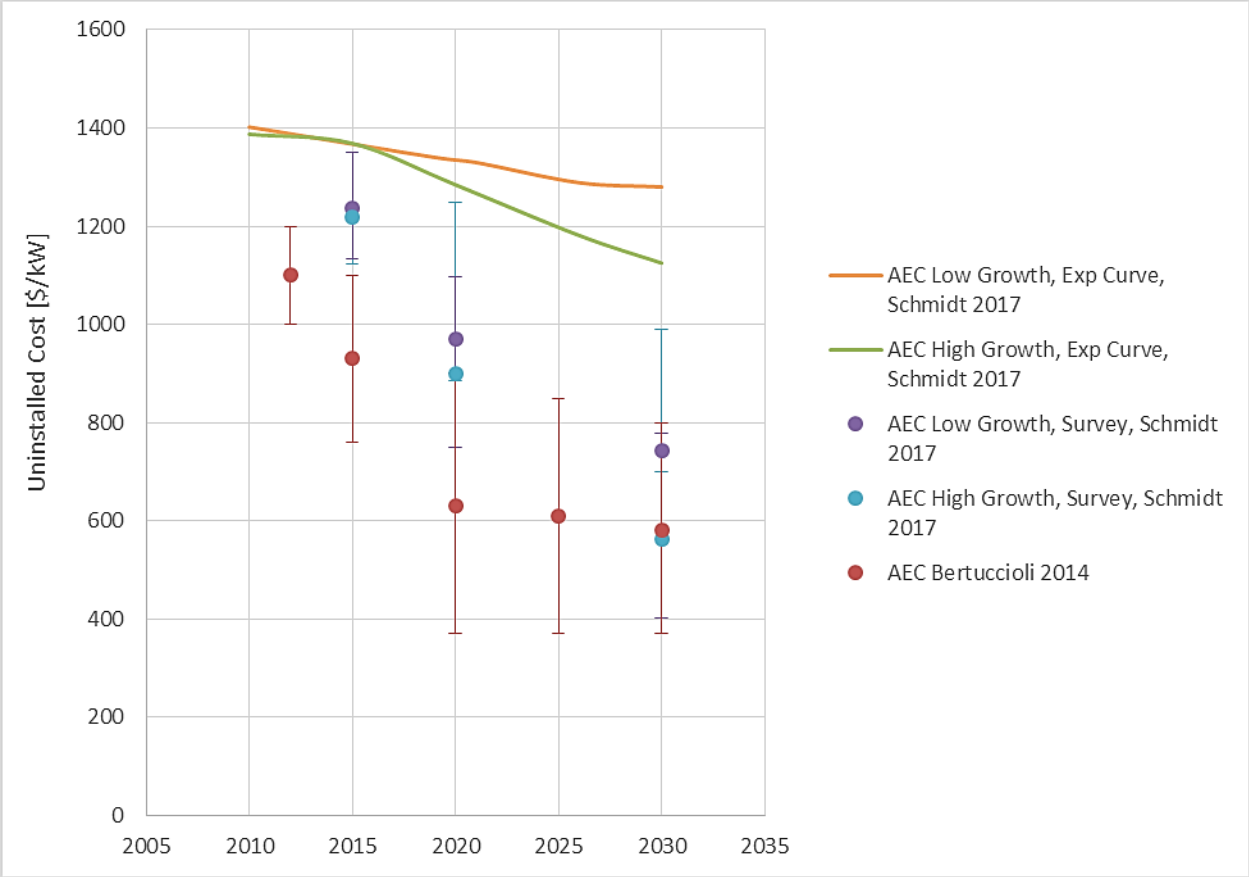

Figure 27. More detailed information on cost for AEC versus time for [206] and [37] to show difference between survey information and experience curve calculations

Given the literature data gathered, the following starting costs are taken for three electrolyzer technologies as they represent a middle-ground of the most comprehensive work from the literature: $1,000/kW for AEC, $1,320/kW for PEMEC, and $9,324/kW for SOEC. Note that economies of scale are a factor in electrolyzer technology, and even more so for the other fuel production methods, so it is important to also include a reference to scale when noting the efficiency and cost. For electrolyzer technologies, a 50 MW scale is used as it is projected to be the P2G plant size.

Note that the cost for SOECs in the optimistic projection using the above learning rate methodology leads to very low future cost if production quantities are high enough. This is due to the learning rate methodology used and the projected cumulative SOEC production. Even early on, the SOEC costs decrease markedly due to early projected market size growth rates. To prevent SOEC costs from becoming unreasonably low, literature was consulted to determine the cost of an electrolyzer from a ground-up methodology, which would give end-game costs of the technology. Work from [212] determined the above for a solid oxide fuel cell, so the final cost per power capacity was divided by two to account for the same stack being able to operate at twice the power in electrolyzer mode compared to fuel cell mode. This is due to the fact that when a solid oxide cell is operated at a given current density, its voltage is approximately twice as high in electrolysis mode than in fuel cell mode, leading to twice the power for the same stack in electrolysis mode compared to fuel cell mode [213]. This methodology leads to a price floor for SOECs of $191/kW.

Combining the starting values for electrolyzer cost, projections for electrolyzer cumulative production capacity, and Wright's law gives a method for projecting the cost of electrolyzer technology into the future. Figure 28 and Table 10 show the conservative projection with representative lower electrolyzer production growth and constant 14% learning rate. Figure 29 and Table 11 show the optimistic projection with higher representative electrolyzer production growth and varying learning rate starting at 25% and lowering to 10% with time.

A reminder that the representative electrolyzer production growth numbers (in cumulative GW in the corresponding years shown) are merely to give an idea of how cumulative installed capacities of these technologies affect cost.

Figure 28. Conservative projection of cost and representative electrolyzer market size

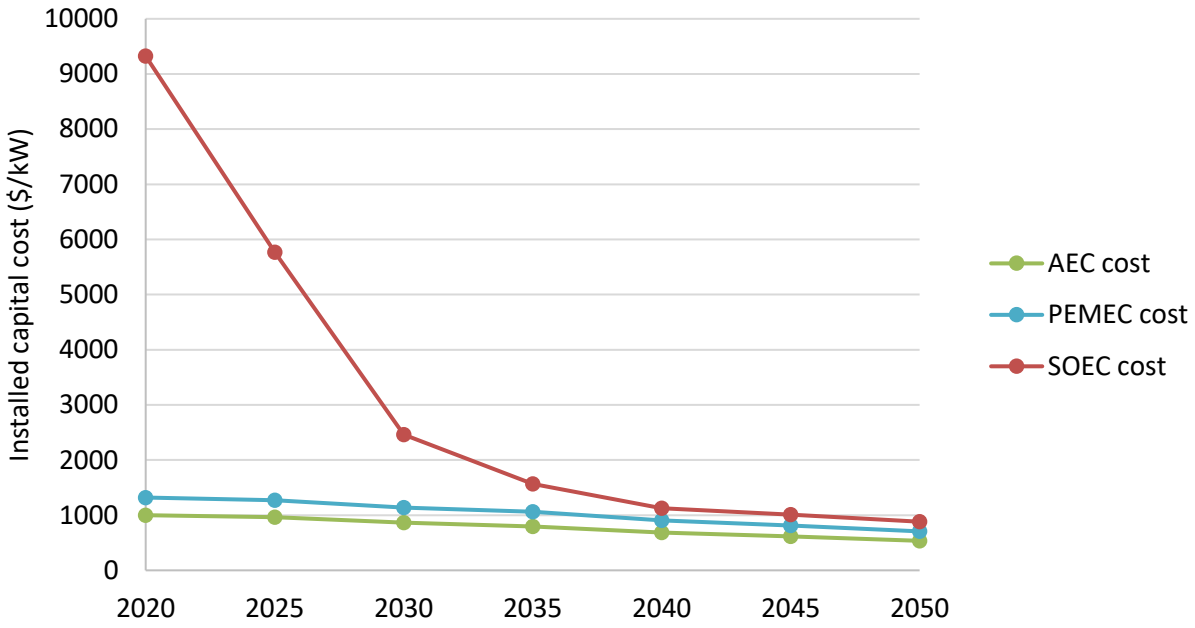

Table 10. Conservative projection of installed cost and representative electrolyzer market size

	AEC			PEMEC			SOEC		
	Pt [GW]	Ct [$/kW]	LR [%]	Pt [GW]	Ct [$/kW]	LR [%]	Pt [GW]	Ct [$/kW]	LR [%]
2020	7.6	1000	14%	5.1	1320	14%	0.0011	9324	14%
2025	9	964	14%	6	1274	14%	0.01	5768	14%
2030	15	862	14%	10	1140	14%	0.5	2462	14%
2035	22	794	14%	14	1060	14%	4	1566	14%
2040	43	686	14%	29	904	14%	18	1129	14%
2045	72	613	14%	48	810	14%	30	1010	14%
2050	134	536	14%	90	707	14%	56	882	14%

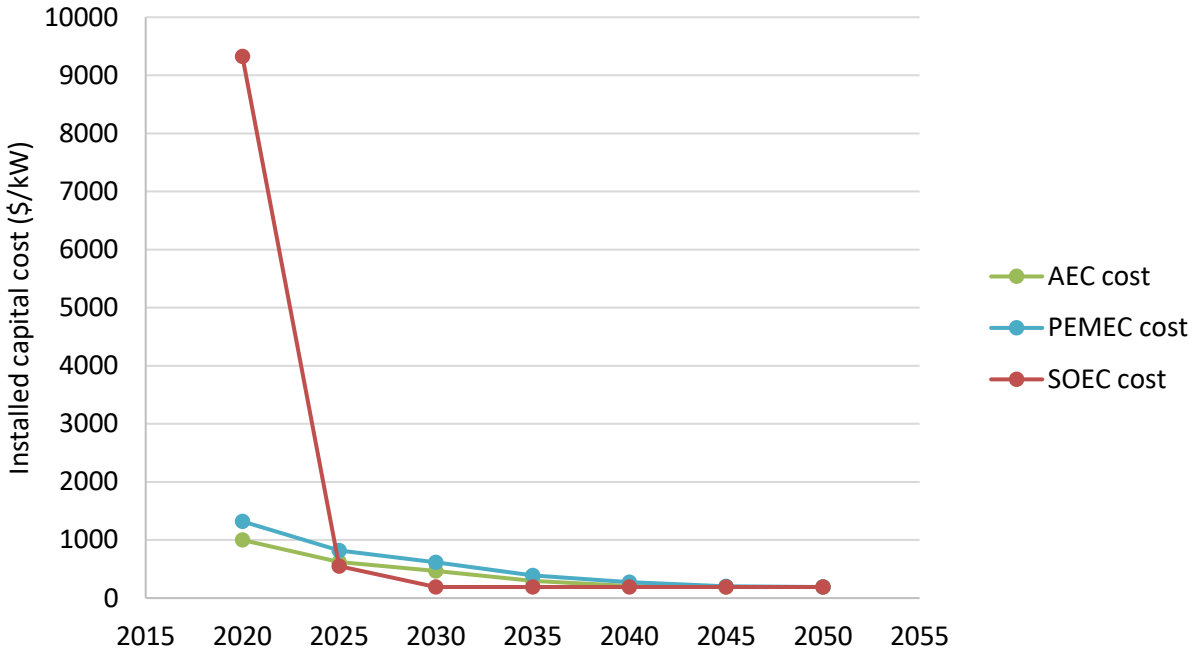

Figure 29. Optimistic projection of installed cost and representative electrolyzer market size

Table 11. Optimistic projection of installed cost and representative electrolyzer market size

	AEC			PEMEC			SOEC		
	Pt [GW]	Ct [$/kW]	LR [%]	Pt [GW]	Ct [$/kW]	LR [%]	Pt [GW]	Ct [$/kW]	LR [%]
2020	7.6	1000	25%	5.1	1320	25%	0.0011	9324	25%
2025	24	620	25%	16	821	25%	1	552	25%
2030	47.5	467	25%	31.68	619	25%	19.8	191	25%
2035	144	295	15%	96	390	15%	60	191	15%
2040	336	208	10%	223.68	275	10%	139.8	191	10%
2045	720	191	10%	480	200	10%	300	191	10%
2050	1313	191	10%	875.52	191	10%	547.2	191	10%

The costs in both the conservative and optimistic scenarios group around similar values relative to the starting costs for each of the three technologies, so it is helpful to include a chart focused on the costs in later parts of the analysis. Such a detailed view can be seen in Figure 30.

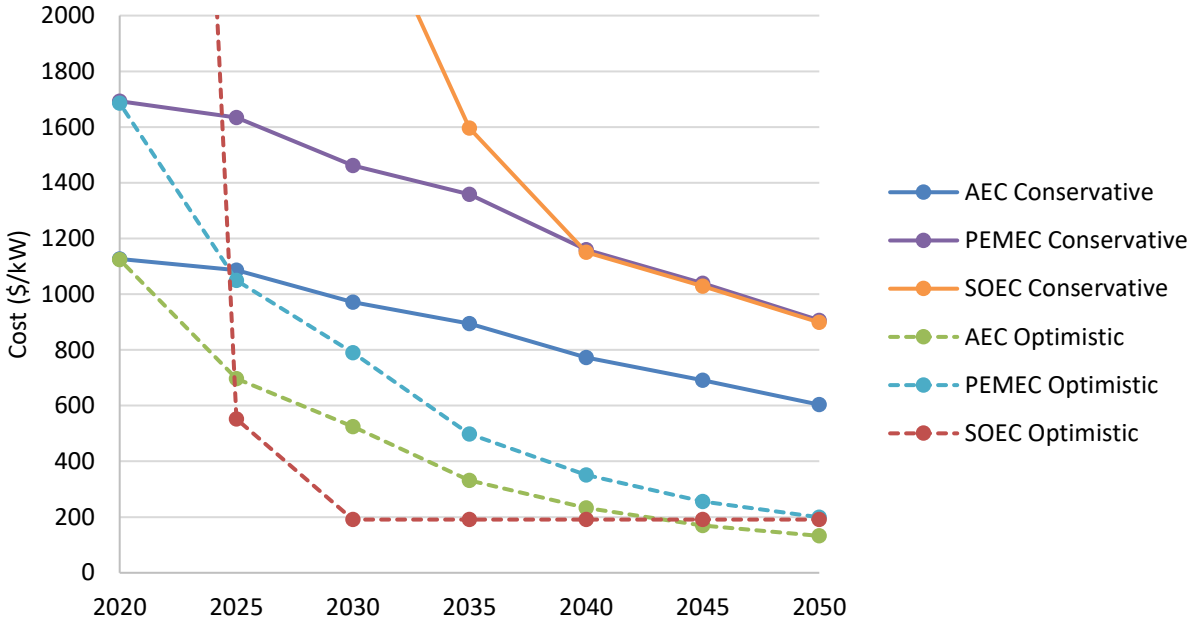

Figure 30. Detailed view of electrolyzer cost projections

The projections are also shown alongside cost data from the literature as cited in Figure 31 for the conservative scenario and Figure 32 for the optimistic scenario. Note that the starting cost for SOECs is cropped out of frame to provide better perspective on the rest of the data.

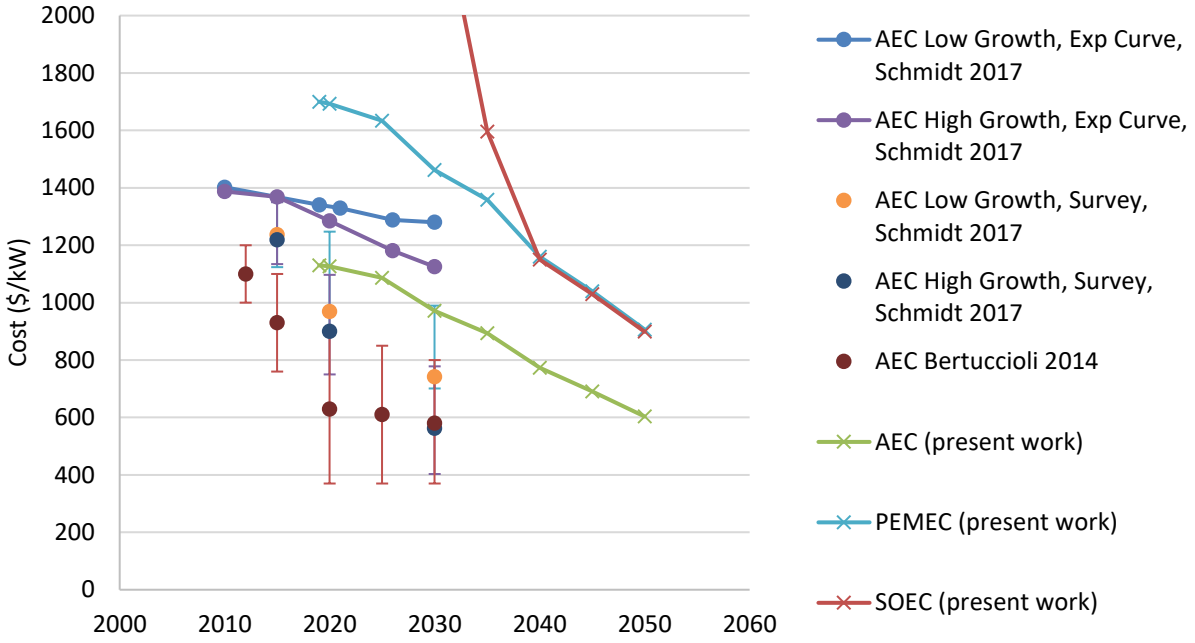

Figure 31. Conservative projection of installed cost compared with literature projections

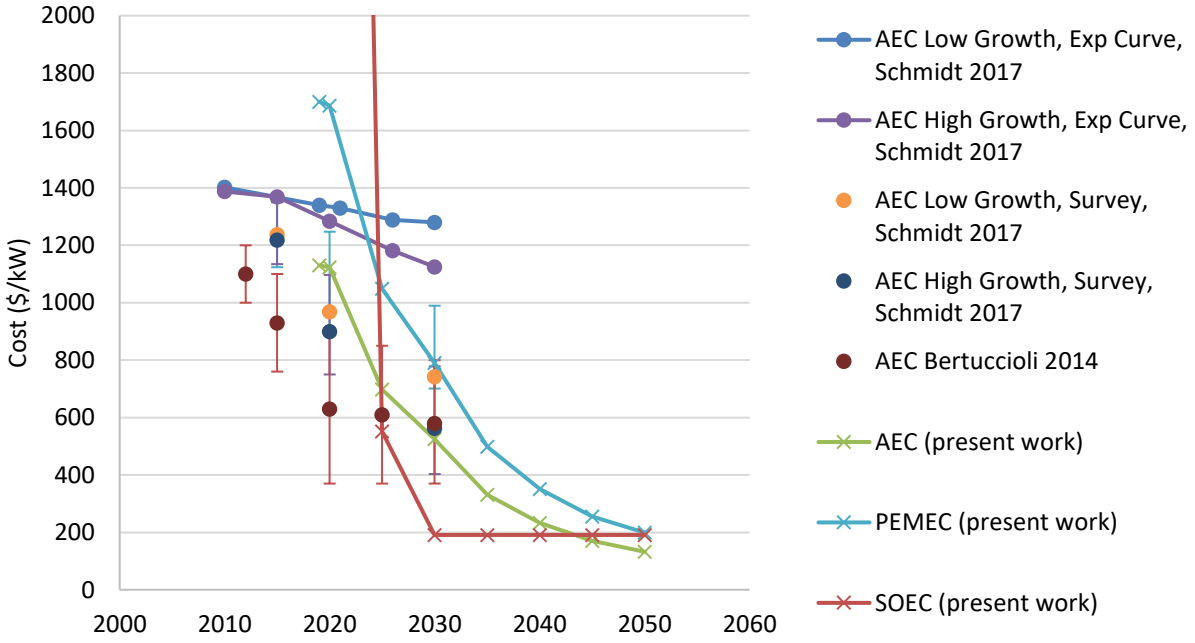

Figure 32. Optimistic projection of installed cost compared with literature projections

Comparing the above projections to values from Schmidt et al. [170], the cost for AECs, PEMECs, and SOECs align well for 2020, with the conservative scenario yielding a value at the upper end of the ranges provided and the optimistic scenario yielding a value at the lower end of the ranges. For 2030, similar is true except for the optimistic SOEC scenario. In that scenario, the present work predicts a value that is slightly below the low range of values from Schmidt et al. [170]. Overall agreement between costs is encouraging here. Furthermore, the two scenarios (conservative and optimistic) bound the literature values well as originally intended.

Operations and maintenance (OM) costs for electrolyzers are taken to be 1.75% of the capital costs [169], [170][214][215] [216]–[219]. This is a fixed OM (FOM) cost, as it depends solely on the size of the plant. There is also variable OM (VOM) which depends on the quantity of fuel being produced, and some of the technologies that will be detailed shortly have associated VOM, but no VOM is modeled in the present work. Note that Wrights Law is not applied to these OM costs as they are typically composed of labor, fuel, and workplace requirements such as lighting, and these do not lend themselves to improvements over time like the capital costs do.

4.2.1.2 Gasification Hydrogen Fuel Production

Having developed a methodology for projecting efficiency and cost for electrolyzer technologies, those same methodologies are carried out for gasification to produce hydrogen.

a) Efficiency of Gasification Hydrogen Fuel Production

Shown in Figure 33 are the range of values and the average for energetic efficiency of gasification technology for hydrogen production from the literature. Sources for the range of values are the following: [41], [42], [51], [52], [43]–[50].

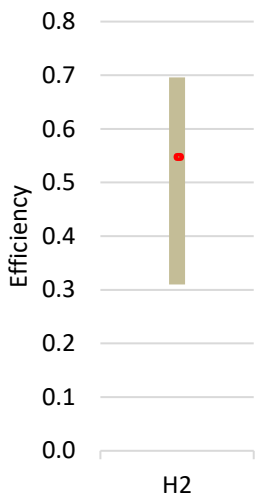

Figure 33. Gasification efficiency ranges and average for hydrogen production, data from [41], [42], [51], [52], [43]–[50]

The method used for projecting gasification efficiency for hydrogen production is to start with the average literature value of 0.54 in 2020 and reach the high efficiency estimates by 2050. Progress is assumed to be about half by 2035. The modeled efficiency projections are shown in Figure 34.

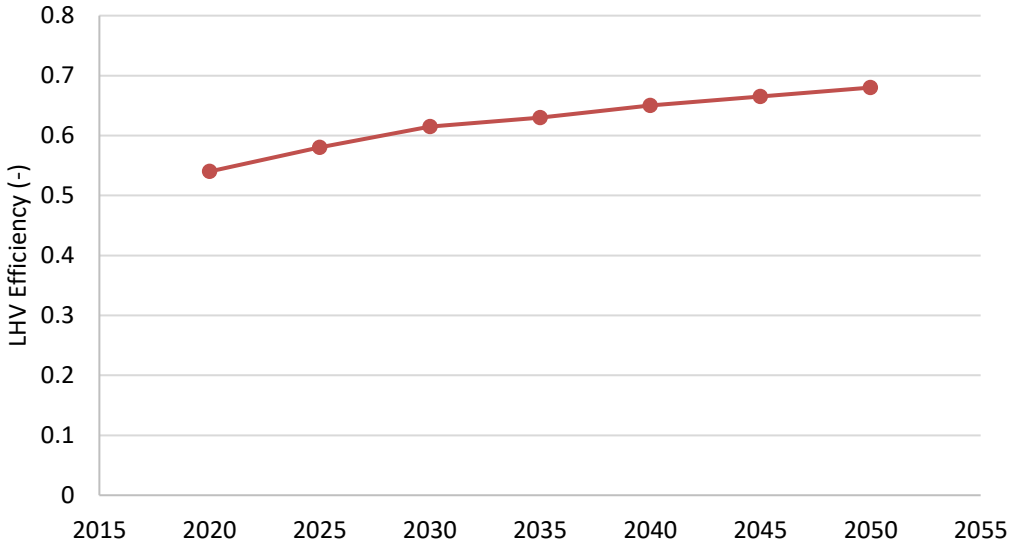

Figure 34. Efficiency projections of gasification for hydrogen production

b) Cost of Gasification Hydrogen Fuel Production

The cost range from the same literature cited for efficiency are shown in Figure 35, with the following sources: [41], [42], [51], [52], [43]–[50].

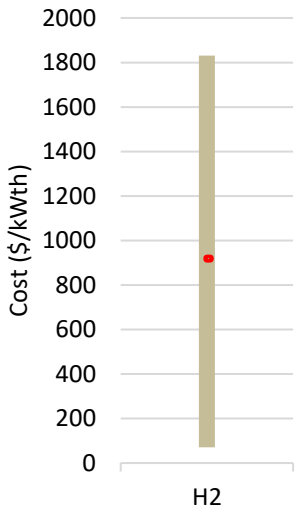

Figure 35. Gasification cost ranges and average for hydrogen production, data from [41][42][43], [44][45]–[52]

The value used in modeling as the starting cost in 2020 is $1200/kW as some of the stronger references are around that value. Projections for the capital cost are calculated using the same learning rate methodology used for electrolytic technology described previously, using a learning rate of 10% due to the technology being a simpler and more mature and less likely to decrease drastically in cost compared to electrolyzer technologies. Representative cost projections are shown in Figure 36. As with the electrolyzers, the production capacities and the years in which those are achieved are shown merely for illustrative purposes to display how installed cost is affected by cumulative installed capacity. Again, the modeling methodology introduced in Chapter 7 will dictate the actual capacities of this work.

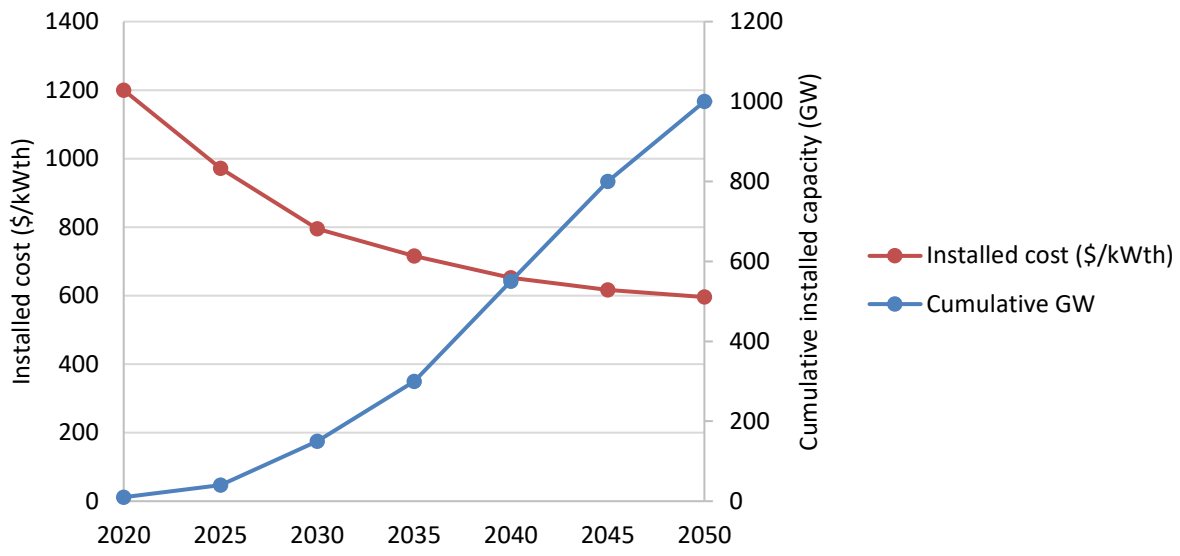

Figure 36. Cost projection for gasification production of hydrogen

FOM is estimated as $40/kW-yr and VOM is estimated as $6/kWh, using the same literature sources from which the capital costs are sourced [41][42][43], [44][45]–[52].

4.2.2 SNG Fuel Production

SNG can start much in the same way as hydrogen, but with the additional step of methanation. The required data for hydrogen are the same as electrolytic hydrogen production as previously detailed. The following is for the methanation requirement, which would be added on top of the electrolytic hydrogen production. SNG can also be made through AD and gasification.

SNG produced by electrolyzers (and the accompanying methanation equipment) and gasifiers are by plants of the scale of 50 MW. The AD plant is smaller, on the order of 500 kW.

4.2.2.1 Electrolytic SNG Fuel Production

a) Efficiency of Electrolytic SNG Fuel Production

Methanation efficiency is 79% as calculated previously in the Electrolytic SNG section of the Background. The efficiency drop for the carbon capture technology is neglected as the power requirement is small compared to that of the electrolyzer. Therefore, the overall efficiency of converting the electrolytic hydrogen to SNG is 79%.

b) Cost of Electrolytic SNG Fuel Production

Previous work has shown that due to the production costs, electrolytic SNG is not economical for plants with low capacity factors, or utilization compared to nameplate capacity [63]. The present work will provide more insight into this area with a detailed techno-economic analysis as an input to the overall optimization.

The supporting P2G equipment cost is determined using the same learning rate methodology as for the electrolyzers. For these technologies, the learning rate is assumed to be 10% for the conservative scenario and 14% for the optimistic scenario as previously noted.

<u>Methanator</u>

In Table 12, the installed methanator capacities shown are determined by the capacity required for methane production corresponding to the installed electrolyzer capacity (which again is merely a hypothetical example to illustrate the dependence of cost on production). Capacities are given as GW of SNG output.

Table 12. Methanator cost projections by market size

	METHANATOR, CONSERVATIVE		METHANATOR, OPTIMISTIC	
	Pt [GW]	Ct [$/kW]	Pt [GW]	Ct [$/kW]
2020	7.60	339.18	7.60	338.83
2025	8.99	330.68	24.55	262.56
2030	15.27	305.08	59.27	216.74
2035	23.95	284.90	179.61	170.28
2040	53.88	251.86	418.48	141.65
2045	89.803	233.05	898.03	119.97
2050	167.63	211.95	1638.00	105.26

Carbon Capture

For carbon capture technologies, which capture the carbon dioxide needed for the methanation reaction, the average electricity input required for the three carbon capture technologies is used to get a fleet-wide installed capacity. In Table 13 and Table 14, the installed carbon capture capacities shown are determined by the capacity required for methane production corresponding to the installed electrolyzer capacity. Capacities are given as GW of electricity input. Carbon capture cost is determined using the same learning rate methodology as for the electrolyzers, with a learning rate of 10% for the conservative scenario and 14% for the optimistic scenario. Two different costs are used at the initial year of 2020. For the conservative scenario of Table 13, a high cost value from the literature is used. For the optimistic scenario of Table 14, an average cost value from the literature is used. Note that E-CEM, which is a low TRL technology, has only one initial cost associated with it as literature data is scarce.

Table 13. Conservative projection of carbon capture technology cost by market size

	E-CEM, CONSERVATIVE		PCC, CONSERVATIVE		DAC, CONSERVATIVE	
	Pt [GW]	Ct [$/tonCO2/d]	Pt [GW]	Ct [$/tonCO2/d]	Pt [GW]	Ct [$/tonCO2/d]
2020	0.2238	1.82E+06	0.2238	6.35E+04	0.2238	4.55E+05
2025	0.2645	1.77E+06	0.2645	6.19E+04	0.2645	4.44E+05
2030	0.4493	1.63E+06	0.4493	5.71E+04	0.4493	4.09E+05
2035	0.7048	1.53E+06	0.7048	5.33E+04	0.7048	3.82E+05
2040	1.5859	1.35E+06	1.5859	4.71E+04	1.5859	3.38E+05
2045	2.6432	1.25E+06	2.6432	4.36E+04	2.6432	3.13E+05
2050	4.9339	1.13E+06	4.9339	3.97E+04	4.9339	2.84E+05

Table 14. Optimistic projection of carbon capture technology cost by market size

	E-CEM, OPTIMISTIC		PCC, OPTIMISTIC		DAC, OPTIMISTIC	
	Pt [GW]	Ct [$/tonCO2/d]	Pt [GW]	Ct [$/tonCO2/d]	Pt [GW]	Ct [$/tonCO2/d]
2020	0.2238	1.81E+06	0.2238	4.36E+04	0.2238	3.15E+05
2025	0.7225	1.41E+06	0.7225	3.38E+04	0.7225	2.44E+05
2030	1.7445	1.16E+06	1.7445	2.79E+04	1.7445	2.01E+05
2035	5.2864	9.12E+05	5.2864	2.19E+04	5.2864	1.58E+05
2040	12.3173	7.58E+05	12.3173	1.82E+04	12.3173	1.32E+05
2045	26.4319	6.42E+05	26.4319	1.54E+04	26.4319	1.11E+05
2050	48.2117	5.64E+05	48.2117	1.35E+04	48.2117	9.77E+04

VOM for all scenarios, including the methanator, carbon capture source, and heat sink, is $0.01/kWh. FOM is estimated as $200/kW-yr for E-CEM scenarios, $10/kW-yr for PCC scenarios, and $8/kW-yr for DAC scenarios [72], [216], [220].

Co-locating a P2G plant with a biorefinery producing biofuels can be a particularly attractive option both economically and environmentally. Economically, this concept would use PCC technology, which is the lowest cost carbon capture technology as seen in Table 13 and Table 14. Environmentally, this concept would use biomass feedstocks to produce either a gaseous or liquid fuel in a bioconversion plant, in addition to carbon dioxide that can be added to

hydrogen to produce SNG. This would maximize the fuel potential and therefore energy extraction of carbon that is stored in biomass.

While this co-location is attractive for the reasons stated above, it is important to note that there are practical limitations that may hinder widespread adoption. A P2G plant must be fed by off-grid solar or wind to economically make fuel in a carbon-free manner. Additionally, electrolysis requires water input, so this P2G plant must also be at or near a large source of water for economic and logistic reasons. Lastly, this P2G plant must also be located adjacent to a biorefinery to get the carbon dioxide from that plant. This biorefinery would be best located near a large source of biomass to improve efficiency, economics, and logistics of the biorefinery. One can now see the many factors that must be aligned for a P2G plant co-located with a biorefinery to come to fruition. Therefore, these combined plants should be considered an optimistic option that should be pursued when possible, but not be assumed to be widely existent in the future.

Heat Sink

Steam turbine installed capacity is determined as the power output of the turbines that would be required by the heat output of the methanator for the given scenario's power input. Costs are again determined using the learning rate methodology, with a learning rate of 10% for the conservative scenario and 14% for the optimistic scenario.

Here, it is important to determine the size of steam turbine that would be expected to be at a P2G plant. This is because the cost and efficiency of steam turbines vary based on scale. Estimating P2G plants to be approximately 50 MW of electricity input [221] and using the heat rejected from the methanator, we arrive at a steam turbine on the order of 3 MW, which is a

medium-sized turbine. This sets the unit cost of the steam turbines, which can be used along with the installed capacity to determine the overall cost of steam turbines in a given scenario.

Table 15. Projection of steam turbine cost by market size

	STEAM TURBINE, CONSERVATIVE		STEAM TURBINE, OPTIMISTIC	
	Pt [GW]	Ct [$/kW]	Pt [GW]	Ct [$/kW]
2020	5.717	680.36	5.717	679.65
2025	6.757	663.30	18.456	526.67
2030	11.478	611.96	44.563	434.75
2035	18.005	571.49	135.041	341.56
2040	40.512	505.21	314.645	284.14
2045	67.520	467.47	675.203	240.65
2050	126.038	425.16	1231.571	211.15

Boiler installed capacity is determined as the power output of the turbines that would be required by the heat output of the methanator for the given scenario's power input. Costs are again determined using the learning rate methodology, with a learning rate of 10% for the conservative scenario and 14% for the optimistic scenario.

Table 16. Projection of boiler cost by market size

	BOILER, CONSERVATIVE		BOILER, OPTIMISTIC	
	Pt [GW]	Ct [$/kW]	Pt [GW]	Ct [$/kW]
2020	1.422	399.04	1.422	398.62
2025	1.681	389.03	4.591	308.90
2030	2.855	358.92	11.085	254.98
2035	4.479	335.18	33.592	200.33
2040	10.078	296.31	78.270	166.65
2045	16.796	274.17	167.961	141.14
2050	31.353	249.36	306.361	123.84

4.2.2.2 Anaerobic Digestion SNG Production

a) Efficiency of Anaerobic Digestion SNG Production

The eficiency of AD to produce SNG depends on the feedstock. Generally, the feedstocks are broken into two categories: (1) manure and (2) organic material. Efficiency estimates from the literature for each of these categories are shown in Figure 37, using data from [84], [222], [231]–[236], [223]–[230]. Note that swine and cattle both refer to types of manure, while food waste and yard trimmings are both organic material.

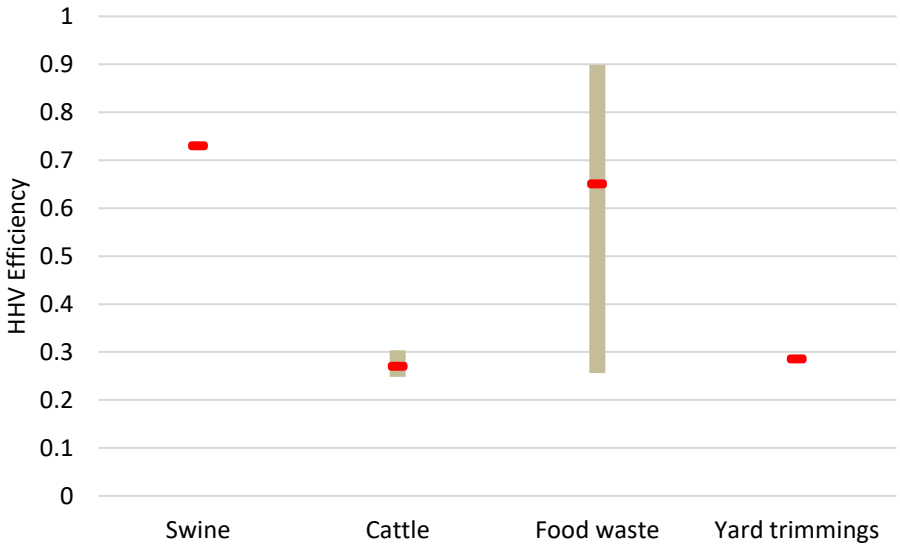

Figure 37. Efficiency of anaerobic digestion, categorized by feedstock, with data from [84], [222], [231]–[236], [223]–[230]

The method used for projecting AD efficiency is to start with an average literature value in 2020 and reach the reasonable high efficiency estimates by 2050. Progress is assumed to be about half by 2035.

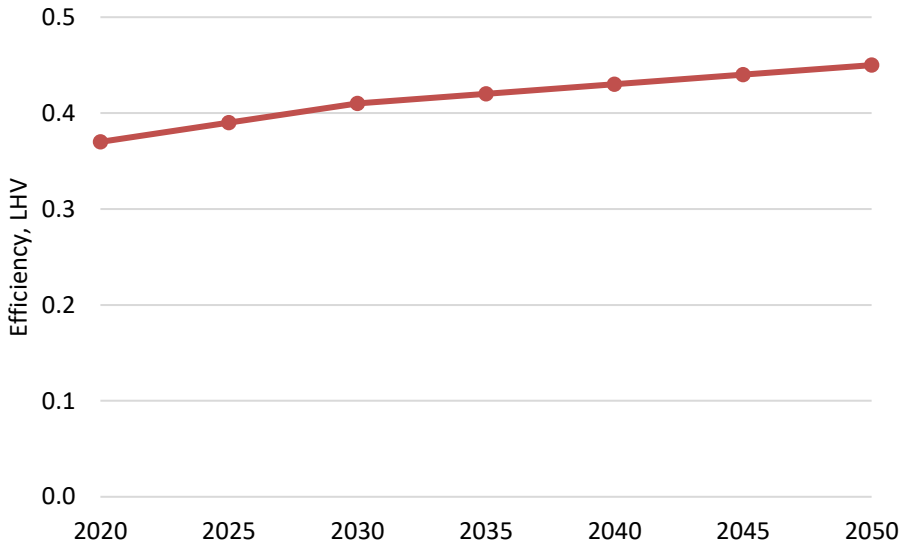

Figure 38. Efficiency projections for anaerobic digestion of manure feedstocks

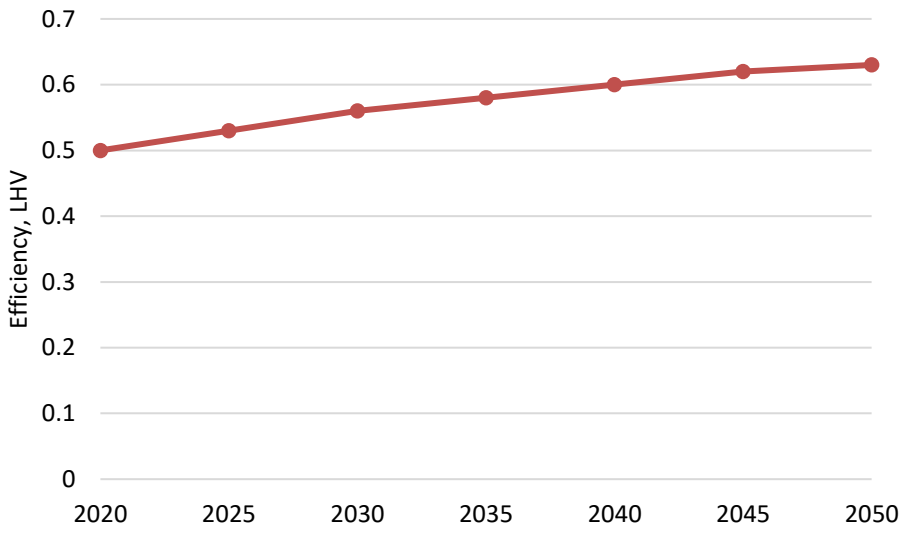

Figure 39. Efficiency projections for anaerobic digestion of organic feedstocks

b) Cost of Anaerobic Digestion SNG Production

The cost data from the literature, also with distinction between feedstocks, are taken from [84], [222]–[225], [237]–[241]. Note the very wide range of organic material AD cost in the literature.

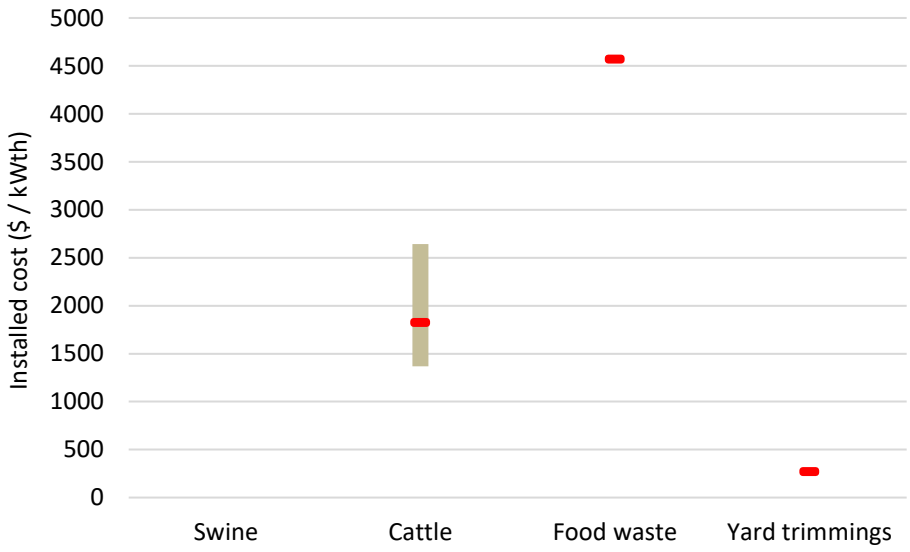

Figure 40. Installed cost of anaerobic digestion, categorized by feedstock, data from [84], [222]–[225], [237]–[241]

Projections for AD costs take an average value of $2,000 per kW as the starting cost in 2020 for both manure and organic feedstocks. Again, the learning rate is modeled as 10%, and the cumulative installed capacities are merely examples to show how cost depends on capacity.

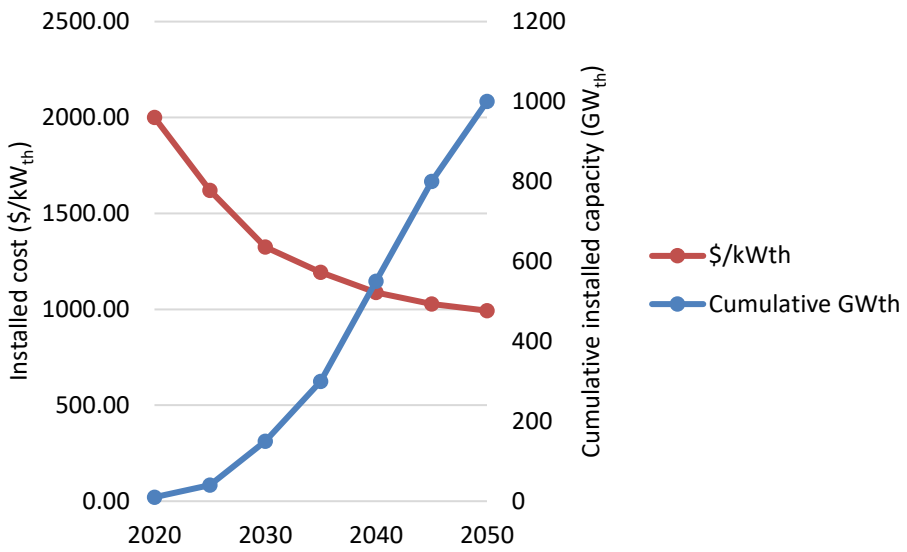

Figure 41. Cost projections for anaerobic digestion

FOM for AD is modeled as $60/kW-yr and $0.01/kWh [84], [222]–[225], [237]–[241].

4.2.2.3 Gasification SNG Production

a) Efficiency of Gasification SNG Production

Shown in Figure 42 are the range of values and the average for energetic efficiency of gasification technology from the literature, specified by the fuel being produced. Sources for the SNG production data are the following: [86], [87], [96]–[104], [88]–[95][105], [106], [115], [116], [107]–[114]. The value used in modeling is 0.67. Again, a 50MW plant is used for design.

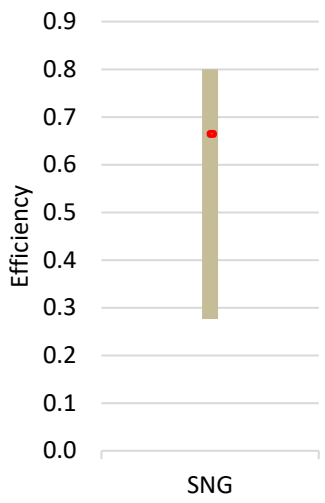

Figure 42. Gasification efficiency ranges and average for SNG production, data from [86], [87], [96]–[104], [88]–[95][105], [106], [115], [116], [107]–[114].

The method used for projecting gasification efficiency for SNG production is to start with the average literature value in 2020 and reach the reasonable high efficiency estimates by 2050. Progress is assumed to be about half by 2035.

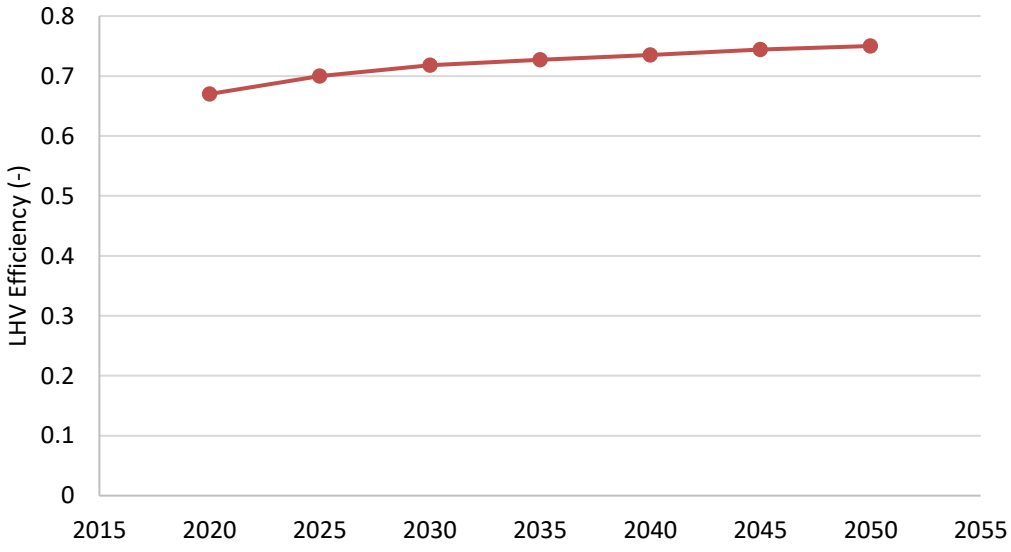

Figure 43. Efficiency projections for gasification for SNG production

b) Cost of Gasification SNG Production

The cost range from the same literature cited for efficiency are shown in Figure 44, with sources being the following literature: [84], [222]–[225], [237]–[241].

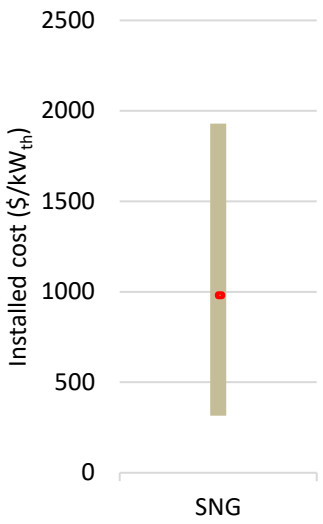

Figure 44. Gasification cost ranges and average for SNG production, data from [84], [222]–[225], [237]–[241]

The value used in modeling is $1400/kW. The learning rate is taken to be 10% as for gasification with hydrogen as a product and hypothetical installed capacity growth for illustrative purposes.

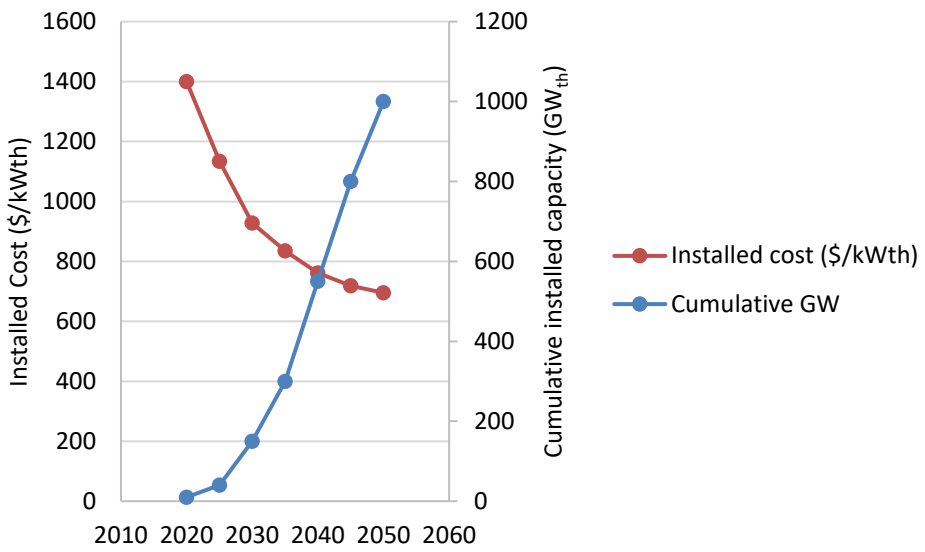

Figure 45. Cost projections for gasification for SNG production

FOM is estimated as $60/kW-yr and VOM is estimated as $0.013/kWh, using the same literature sources.

4.2.3 Renewable Gasoline and Diesel Production

The figures stated for efficiency and cost of the following renewable gasoline and diesel production methods are for plants on the order of 50 MW. There are limited data for efficiency projections into the future, so it is assumed there is a 2% efficiency improvement every 5 years for each of these production technologies, which is comparable to the improvements of the electrolyzer, gasifier, and AD equipment.

Note the brevity of the proceeding sections is due to the use of the same methodologies introduced in detail in the preceding sections, so there is no need to repeat.

4.2.3.1 Liquefaction Renewable Gasoline and Diesel Production

a) Efficiency of Liquefaction Renewable Gasoline and Diesel Production

The starting efficiency of liquefaction is modeled as 60% from Laser et al. [46], and a 2% efficiency improvement every 5 years is assumed.

b) Cost of Liquefaction Renewable Gasoline and Diesel Production

The starting cost for liquefaction is modeled as $1440.25 per kW input from Zhu et al. [120], and the learning rate is taken to be 10%.

4.2.3.2 Gasification and Fischer-Tropsch Renewable Gasoline and Diesel Production

a) Efficiency of Gasification and Fischer-Tropsch Renewable Gasoline and Diesel Production

The starting efficiency of gasification followed by FT is modeled as 55% from Laser et al. [46], and a 2% efficiency improvement every 5 years is assumed.

b) Cost of Gasification and Fischer-Tropsch Renewable Gasoline and Diesel Production

The starting cost for liquefaction is modeled as $1,440.25 per kW input from Zhu et al. [120], and the learning rate is taken to be 10%.

4.2.3.3 Pyrolysis Renewable Gasoline and Diesel Production

a) Efficiency of Pyrolysis Renewable Gasoline and Diesel Production

The starting efficiency of pyrolysis modeled as 0.6 from Laser et al. and Jahirul et al.[46], [242], and a 2% efficiency improvement every 5 years is assumed.

b) Cost of Pyrolysis Renewable Gasoline and Diesel Production

The starting cost for pyrolysis is modeled as $817.43 per kW input from Vasalos et al. [243], and the learning rate is taken to be 10%.

4.2.3.4 Hydrolysis Renewable Gasoline and Diesel Production

a) Efficiency of Hydrolysis Renewable Gasoline and Diesel Production

The starting efficiency of hydrolysis is modeled as 55% from Laser et al. [46], and a 2% efficiency improvement every 5 years is assumed.

b) Cost of Hydrolysis Renewable Gasoline and Diesel Production

The starting cost for pyrolysis is modeled as $4,680 per kW input from Zhao et al.[244], and the learning rate is taken to be 10%.

4.3 Fuel Distribution

Having detailed the techno-economics of the production of the five fuels included in the present work, it is now the proper time to move to the distribution of each of those fuels.

4.3.1 Electricity Distribution

4.3.1.1 Efficiency of Electricity Distribution

Electricity distribution efficiency comes from losses in the electricity lines. The efficiency modeled is 95% [245] and is held constant throughout the time of analysis.

4.3.1.2 Cost of Electricity Distribution

Cost of electricity distribution depends on the level of charging required. For light-duty PHEVs and PFCEVs, which have both batteries and range extenders to power the vehicle, only level 1 charging is needed [246][247][248]. For light-duty BEVs and all HDVs using electricity as a fuel, some electric grid upgrades will be required to support the additional throughput.

Prior work by Lane [248] calculates the infrastructure costs for the electric grid upgrades needed to support level 1 and level 2 charging of vehicles throughout California. Dividing those costs by the amount of electricity the infrastructure supports as fuel for vehicles and using a CRF of 0.12 again to annualize costs, this leads to a cost of $2.21 per GJ of electricity distributed when using charging greater than level 1. Level 1 charging is assumed to have no distribution cost as it uses significantly less power than an electric oven or stove [249], and therefore should not require electric grid upgrades.

4.3.2 Hydrogen Distribution

As introduced previously, hydrogen distribution can be categorized into two segments: from production facility to a terminal and delivery from the terminal to the dispensing station.

4.3.2.1 Efficiency of Hydrogen Distribution

The efficiency of hydrogen distribution is calculated from three components: liquefying the hydrogen, trucking the hydrogen to the dispensing station, and any leakage that occurs during the distribution. Liquefying is taken to be 82% energy efficient [250]. Hydrogen leakage is assumed to be negligible as previously mentioned. Prior work shows distribution of hydrogen by

a hydrogen-powered HDV requires under 0.2% of the amount of hydrogen that is being distributed [248], so the trucking portion of distribution is assumed to have negligible impact on the efficiency of the process. Therefore, hydrogen distribution is modeled as 82% efficient overall.

4.3.2.2 Cost of Hydrogen Distribution

Previous work shows that there is only a very slight dependency on hydrogen production plant size for the cost of distributing hydrogen from production plant to dispensing site. The maximum change in distribution cost was about $0.02 per kilogram of hydrogen [251]. The range of plant considered in this work is from 21.4 MW to 500 MW. Perhaps if the range was extended, there could be some impact of production plant scale on distribution cost, but it is assumed in the present work that distribution cost is independent of scale of production plant.

Working with the U.S. Department of Energy's H2A Delivery Analysis model yields costs for the distribution and dispensing of hydrogen. Due to the way the results are displayed, the aggregate cost of both distribution and dispensing are given here. Figure 46 shows the sum cost of hydrogen terminals, delivery to hydrogen dispensing station, and hydrogen dispensing station cost. The plot shows insight into factors that affect the cost of hydrogen distribution. One is that terminal size has a significant impact on the cost of hydrogen. Increasing terminal size decreases the cost of hydrogen. Second, the impact of terminal size diminishes as the size continues increasing. At low terminal size (up to about 30,000 kg/day), increasing terminal size has a dramatic decrease in cost. After about 50,000 kg/day terminal size, the effect becomes nearly negligible.

Figure 46 also shows the difference in cost between gaseous hydrogen and liquid hydrogen. At lower terminal sizes, liquid hydrogen is significantly more expensive than gaseous hydrogen. This trend stays true for low-capacity stations no matter the terminal size. However, mid- and high-capacity hydrogen stations, liquid hydrogen becomes cheaper than gaseous hydrogen for larger terminal size. Recall that the present work assumes liquid hydrogen distribution.

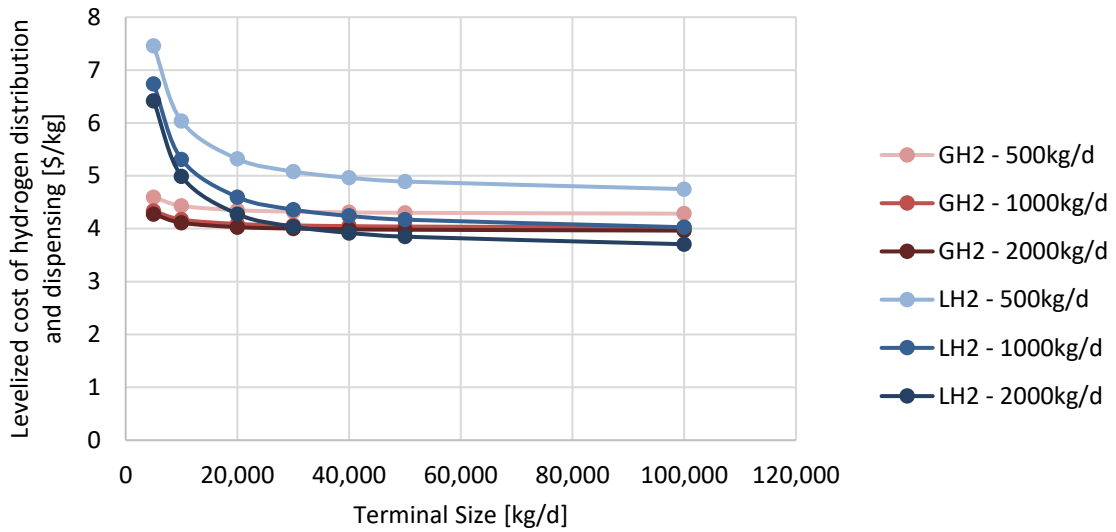

Figure 46. Levelized cost of hydrogen distribution and dispensing, data from [252]

A representative distribution and dispensing cost of $4.50 per kilogram of hydrogen is used to account for variability of station cost with size.

4.3.3 SNG Distribution

SNG distribution is assumed to take the form of pipeline distribution, making use of the prevalent pipeline infrastructure that natural gas uses today.

4.3.3.1 Efficiency of SNG Distribution

SNG distribution using the natural gas pipeline is 99% efficient from a primary energy input basis [180]. This slight efficiency loss is assumed negligible in the present work, and therefore SNG distribution is modeled as 100% efficient.

4.3.3.2 Cost of SNG Distribution

SNG distribution costs are from Southern California Gas Company and San Diego Gas & Electric Company, which have a customer charge of $65 each month and $0.20 per British thermal unit (BTU) of natural gas delivered [253][254]. Even if a high estimate of 1,000 SNG stations would be created to support HDVs in the future (a number that is one-tenth the number of gasoline stations in California), this would yield a customer charge of $780,000 for distribution spread among all stations. This cost is significantly less than the cost of a single SNG station, which will be detailed shortly. Therefore, the customer charge will be neglected and only the per-BTU charge of $0.20 will be considered in this analysis.

4.3.4 Renewable Gasoline and Diesel Distribution

Distributing renewable gasoline and diesel is assumed to be carried out in the same manner as fossil gasoline and diesel, which is by trucking.

4.3.4.1 Efficiency of Renewable Gasoline and Diesel Distribution

Renewable liquid fuels have negligible energy losses in distribution, so they are assumed to be 100% efficiency in the present work [180].

4.3.4.2 Cost of Renewable Gasoline and Diesel Distribution

According to the U.S. Energy Information Administration, approximately $0.40 to $0.60 of every gallon of gasoline and diesel sold goes to distribution and marketing [255]. It is assumed for the present work that $0.20 of each gallon goes to distribution of the gasoline and diesel, after removing the marketing costs included in the reference.

4.4 Fuel Dispensing

4.4.1 Electricity Dispensing

Electricity dispensing is categorized by the power output as mentioned previously. For LDVs, PHEVs and PFCEVs use level 1 charging, and BEVs use level 2 charging [246][247][248]. HDVs have larger battery capacities due to their lower efficiencies; therefore, higher charging powers are needed to meet driving demands. For HDVs, the present modeling assumes PHEVs and PFCEVs use level 2 charging and BEVs use level 3 charging.

4.4.1.1 Efficiency of Electricity Dispensing

The efficiency of electric chargers does very somewhat depending on what level the charger is. An average value of 92% from Apostolaki-Iosifidou et al. [256] and Sears et al. [257] is used for the present modeling .

4.4.1.2 Cost of Electricity Dispensing

Just as for efficiency, the cost of electric chargers depends on the level of charging as well. Additionally, the amount of chargers that are to be added depend on the level of charging.

For example, level 1 charging can be assumed to be already installed in single-unit dwellings and office spaces; the only major place in need of level 1 charging for vehicles is multi-unit dwellings, which typically do not have infrastructure to support any sort of vehicle charging. Using prior work by Lane [248] which determined level 1 and level 2 charging costs for California and dividing by electricity dispensed by those chargers as well as using a CRF of 0.12 to annualize payments, the cost of level 1 and level 2 charging is determined. For level 3 charging, the same methodology of Lane [248] is used with the updated cost for the level 3 chargers found in [258]. The costs used for chargers as well as the levelized cost of the various levels of chargers is shown in Table 17.

Table 17. Electricity dispensing levels and costs

Level of charging	**Vehicles using**	**Charger cost ($)**	**Levelized cost of dispensing ($/GJ)**
1	LDV: PHEV, PFCEV	1,000	0.13
2	LDV: BEV HDV: PHEV, PHEV	10,000	15.01
3	HDV: BEV	50,000	72.27

4.4.2 Hydrogen Dispensing

Hydrogen dispensing infrastructure is in a nascent state in California as of the time of this writing, so any significant adoption of hydrogen-fueled vehicles would require further buildout and therefore capital investment.

4.4.1.1 Efficiency of Hydrogen Dispensing

Efficiencies for liquid hydrogen dispensing stations are quite high, with values ranging from 96% from U.S. Department of Energy [252] to 97% from Hänggi et al. [180]. The average of 96.5% efficiency is used in the present work.

4.4.1.2 Cost of Hydrogen Dispensing

A reminder here that the cost of hydrogen dispensing was incorporated with the cost of hydrogen distribution previously. The present work is not spatially resolved, so detailed station size for individual locations is beyond the scope of this work. Therefore, a representative distribution and dispensing cost of $4.50 per kilogram of hydrogen are used to account for variability of station cost with size [252].

4.4.3 SNG Dispensing

SNG is a drop-in fuel, so it can be used in existing natural gas infrastructure. However, as previously noted in Chapter 2.1.4.3, any significant adoption of SNG-fueled HDVs would require building out the SNG dispensing infrastructure [136][137].

4.4.1.1 Efficiency of SNG Dispensing

SNG dispensing efficiency losses are negligible according to Hänggi et al. [180], so it is modeled as 100% efficient.

4.4.1.2 Cost of SNG Dispensing

Just as for hydrogen dispensing, SNG dispensing costs depend on the size of dispensing station. For this work, assume a large station size of 1,500-2,000 GGE per day capacity, which costs $1.8 million [259]. This large station assumption is made as the present modeling is not spatially resolved, so a larger station size is most economical. Again using a CRF of 0.12 to annualize payments, this. leads to $0.32 per GGE for SNG dispensing.

4.4.4 Renewable Gasoline and Diesel Dispensing

Renewable gasoline and diesel are drop-in fuels, so they can use the existing and prevalent gasoline and diesel infrastructure.

4.4.1.1 Efficiency of Renewable Gasoline and Diesel Dispensing

Renewable liquid fuels have negligible energy losses in dispensing [180], so they are assumed to be 100% efficiency in the present work.

4.4.1.2 Cost of Renewable Gasoline and Diesel Dispensing

Cost is negligible because gasoline and diesel stations have already been built in abundance, so no new stations will need to be built if renewable gasoline or diesel vehicles are projected. While in reality there is still some cost to run the stations, these costs are assumed negligible compared to the capital of creating new stations and compared to the dispensing costs of other fuels such as foe electric chargers or constructing SNG stations.

4.5 Total Fuel Pathway Efficiency and Emissions

Emissions associated with the fuel pathway are dependent on the feedstock, production equipment, distribution, and dispensing. The method proposed for calculating the overall emissions is using the feedstock emissions and applying efficiencies at each step of the above-detailed pathway chain. The efficiencies associated with each of the pathway steps have been detailed. Multiplying the total pathway efficiency with the feedstock emissions will result in the total fuel emissions.

4.5.1 Total Fuel Pathway Efficiency

Efficiencies of production equipment have projected improvements as detailed previously. For brevity, only the starting year efficiencies will be shown in the following calculations for total pathway efficiency. The same methodology is applied throughout this analysis, with the further years having efficiency improvements to the production only. Similarly, only the conservative electrolyzer efficiencies are shown, but the optimistic ones are used in the modeling as well. See a summary of each pathway step efficiency as well as the total pathway efficiency for the year 2020 in Table 18. The fuel production efficiencies improve with time, so the total pathway efficiencies improve as well. Note also that while references are not repeated here for simplicity, they are given in the corresponding sections of this chapter.

Table 18. Summary of fuel pathway efficiencies in 2020

Fuel	Production method	Production efficiency (%)	Distribution efficiency (%)	Dispensing efficiency (%)	Total pathway efficiency (%)
Electricity	Electricity	-	95	92	87.4
Hydrogen	AEC	70	82	96.5	55.4
	PEMEC	66	82	96.5	52.2
	SOEC	70	82	96.5	55.4

	Gasifier	54	82	96.5	44.3
SNG	AEC - methanator	55.3	100	100	55.3
	PEMEC - methanator	52.2	100	100	52.2
	SOEC - methanator	59.3	100	100	59.3
	Gasifier	67	100	100	67
	AD (manure)	37	100	100	37
	AD (organics)	50	100	100	50
Renewable gasoline / diesel	Liquefaction	64	100	100	64
	Gasifier - FT	55	100	100	55
	Hydrolysis	55	100	100	55
	Pyrolysis	60	100	100	60

4.5.2 Feedstock Emissions

A common method of comparing the environmental impacts of various processes and equipment is by comparing emission factors. Emission factors give the emission intensity by the ratio of the quantity of emissions released per the amount of activity. The amount of activity can be number of units, miles driven, or the amount of energy associated with a process. In this work, emission factors generally take the form of quantity of emissions released per the amount of associated energy.

Emission factors in this work are separated into two categories: (1) fuel emission factors and (2) vehicle emission factors. Fuel emission factors consider farming, land use change by removing the biomass to harvest for fuel, and transporting the biomass to a fuel production facility. Note that these emissions are held constant independent of this work's results of how many fuel production facilities should be made and how large they should be. There is no spatial consideration to affect the amount of biomass transportation emissions for fuel production. Vehicle emission factors will be discussed in the following chapter.

Fuel emissions can be separated into two categories: electricity and biomass. In general, the emissions associated with the fuel portion of the transportation pathway are dependent on the feedstock (electricity or a type of biomass) and the efficiency of that pathway. While this may be obvious for the electricity feedstock, it may not be as obvious for the biomass feedstocks. For pathways using biomass as a feedstock, the main inputs to the fuel production processes for the various equipment are the feedstock itself, heat, and pressure. Both heat and pressure can be produced by simply burning some of the biomass feedstock used for fuel production. Because the efficiencies cited in previous sections are in terms of primary energy input, this efficiency along with the emission factor of the biomass feedstock are all that are necessary for calculating the emissions associated with fuel production.

The present modeling assumes other emissions from the various pathway processes (for example, the partial oxidation of pyrolysis) are negligible compared to the feedstock itself. Also important to note is that for a given fuel production method, emissions are the same whether producing renewable gasoline or diesel. This is due to the use of only feedstock and pathway efficiency to calculate emissions, and efficiencies for renewable gasoline and diesel production are modeled to be the same.

The majority of the feedstock emission factors used in this work are from Argonne National Laboratory's GREET 2016 [33]. More up-to-date data for electricity GHG emission factors that account for SB 100 goals of zero-carbon electricity by 2045 are sourced from E3's PATHWAYS work and in particular their reference scenario [189], which projects lower GHG emissions in later years compared to GREET; however, the CAP emission factors are sourced from GREET as that has the most detailed CAP emissions data for electricity.

Due to a lack of emission factors for some biomass feedstocks, some assumptions are made for the feedstocks that do not have data available to link them to types of biomass that they are most similar to which do have emission factor data available. All straw biomass (barley straw, rice hulls, rice straw, and wheat straw) are assumed to have the same emission factors as corn stover. Residues (cotton gin trash, cotton residue, noncitrus residues, primary mill residue, secondary mill residue, paper, paperboard, plastics, rubber, leather, textiles, yard trimmings, and other) are all assumed to have the same emission factors as citrus residues. Both hardwood and softwood variations are assumed to have the same emission factors as forestry. Lastly, MSW wood is assumed to have the same emission factors as construction and demolition waste.

Two biomass categories are not present in GREET and therefore other sources were consulted. For citrus residues (and the other biomass types that are approximated to have the same emission factors), emission factors are sourced from Pourbafrani et al. [260]. Food waste emission factors are taken from the California Air Resources Board [261].

Note also that GREET emissions factors are projected into 2040. For the present work, these projections are carried out to 2050, assuming emissions factors stay the same after 2040. For the emission factors sourced from Pourbafrani et al. [260] and the California Air Resources Board [261], they are assumed constant throughout the timeframe of this work as there is no indication of changing values. It should be noted that this is a valid assumption as most emission factors are nearly constant, as will be shown shortly.

CAP emission factors for electricity are specifically for California from the “Fuel” category of the “Electric” tab of GREET. Emission factors for the various biomass feedstocks found in GREET are sourced from the feedstock emissions section of the various production pathways detailed using each of the included feedstocks.

GHG emission factors, also known as carbon intensities (CIs), for the feedstocks are shown in Figure 47. There are a wide range of biomass varieties with a wide range of CI values. Note that both manure and food waste biomass feedstocks have negative CIs. This is because both of these categories of biomass naturally release methane into the atmosphere, which has a greater GHG impact than carbon dioxide. Turning these feedstocks into fuels stops them from emitting methane into the atmosphere and converts most of that methane into carbon dioxide (depending on the method of conversion). Important to note is that the CIs for electricity and manure are on the secondary y-axis on the right side, which has a much greater magnitude of values. The rest of the feedstocks have CIs detailed by the primary y-axis on the left side.

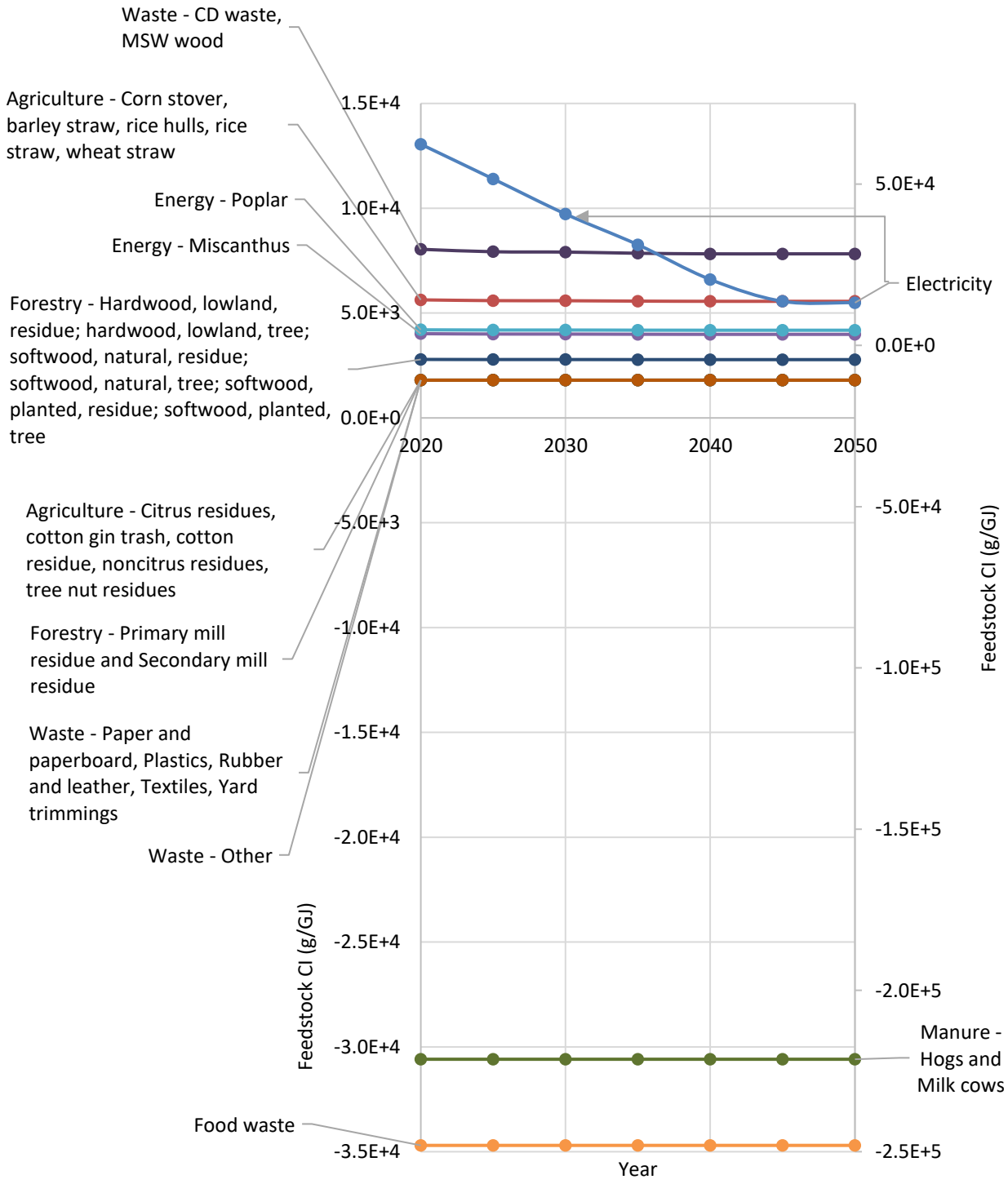

Figure 47. Feedstock carbon intensities

The highest CI is for electricity, which is close to ten times higher than the next-highest CI in early years of modeling. It should be noted that electricity is the only fuel feedstock with a CI that decreases significantly with time. This is due to an increasing amount of carbon-free renewable electricity generation being installed on the electric grid, more-efficient fossil generation, and, perhaps most importantly, legislation such as SB 100 which require cleaner electricity production into the future. By 2045, the CI of electricity is much more comparable to some of the biomass feedstocks. The lowest CI is for manure, which has a very negative value. Compared to these two extremes, all other feedstocks considered (besides food waste) have a relatively low spread between their CIs.

Biomass feedstocks' emission factors stay relatively constant as the emission factors come from farming, land use change by removing the biomass to harvest for fuel, and transporting the biomass to a fuel production facility. Both farming and land use change emissions do not change much with time. Additionally, GREET likely assumes conventional transport of the biomass feedstock to fuel production facilities (which will likely change). While vehicles are assumed to be more efficient as time progresses, there is not a drastic difference in these transportation emissions. Therefore, the overall feedstock emission factors are nearly constant for most biomass feedstocks.

An important concept to keep in mind is that the feedstock emission factors are not the only data that matter when determining the climate change and air quality impacts of a fuel. Also important are the efficiency of the fuel production pathway as well as the emissions from the vehicles themselves. Consider the following: if one feedstock has particularly low emission factors, but it must be made using in an inefficient process and it must be used in an inefficient vehicle, the overall emissions associated with that process may be much higher than using a

feedstock with higher emission factors but that can be made into a fuel more efficiently and used in a more efficient vehicle.

However, there is a situation where the above is not true. Consider now a focus on GHG emissions and CIs. For feedstocks with negative CIs, by definition, using more of the feedstock to produce fuel would effectively be decreasing the climate change-inducing species in the air. Therefore, a less-efficient fuel production process and less-efficient vehicle could be considered better for the environment from a climate change perspective because more of the negative CI feedstock is being used. However, consider the fact that a less-efficient process would be using more of the feedstock. So while lower efficiency would mean a single vehicle could be helping the environment more, this also means fewer vehicles can be fueled by that feedstock. And of course there is only a limited amount of every feedstock available on this planet (while the biomass feedstocks considered will replenish with time, that amount of time is not negligible). Therefore, while negative CI feedstocks may seem to promote lower efficiency to help the environment, that pursuit would not be a wise use of resources.

GHG and CAP emission factors for electricity are shown in Figure 48. The GHG and CAP emission factors for the biomass feedstocks are shown in 11. APPENDIX A.

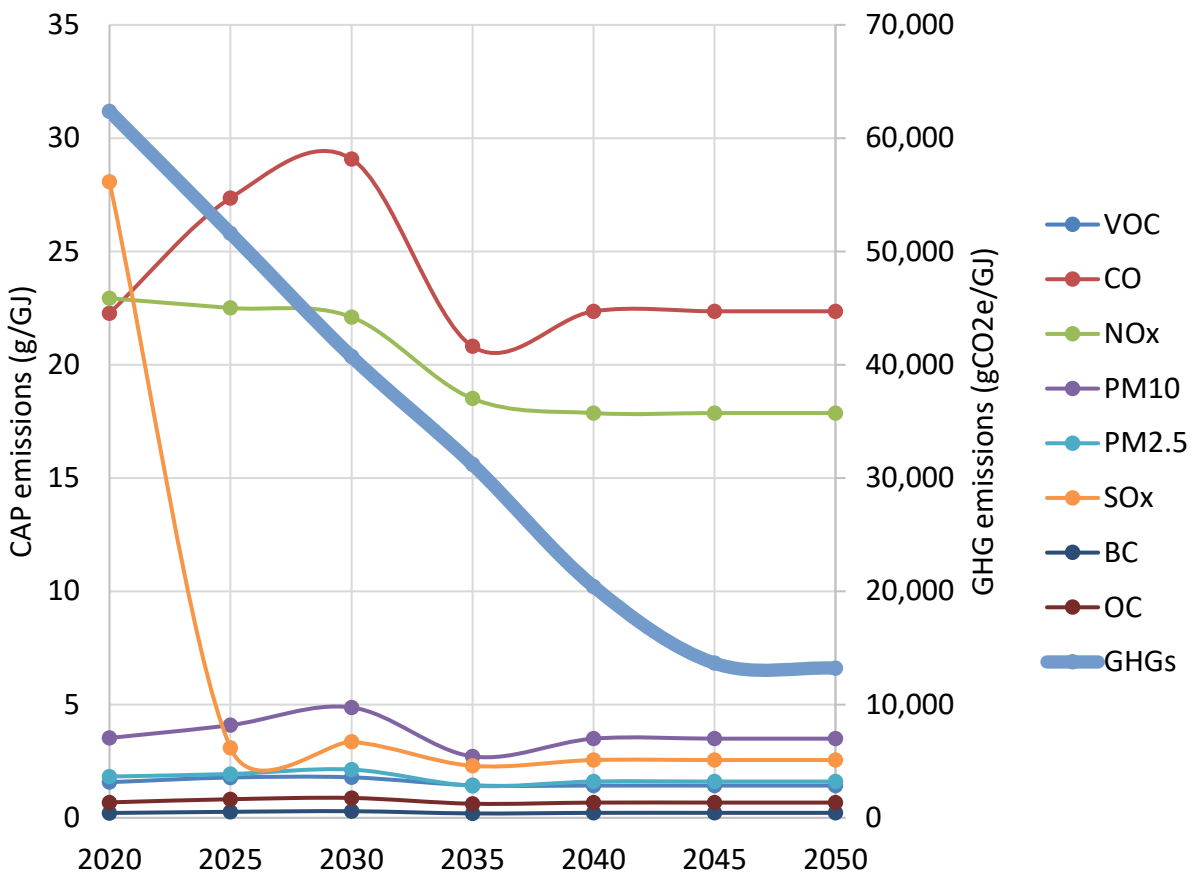

Figure 48. Electricity GHG and CAP emissions, data from [31], [189]

Next it is necessary to determine a representative set of emission factors for each of the main biomass feedstock categories using the emission factors of the individual feedstocks and the relative quantity of each feedstock. It is assumed that the relative quantities of each individual feedstock within a category stay constant. For agriculture residue, there is a relatively homogenous mixture of each individual feedstock, so the average is used. For energy crops, poplar vastly outweighs miscanthus in the energy crops availability, so emission factors for poplar are used. For food waste, there is only one feedstock. For forestry and tree, there is a mixture of each individual feedstock, so the average is used. For manure, there is only one feedstock. For MSW, there is a mixture of each individual feedstock, so the average is used.

For feedstocks that do not have CAP emission factor data from the literature, those of the closest resembling feedstock are used. For example, only half of the agriculture residues have CAP emission factor data gathered from the literature, so the other half are assumed to have the same as those in the same category for which there are data available. For food waste, the CAP emission factors are taken from manure as that is the closest data that could be found.

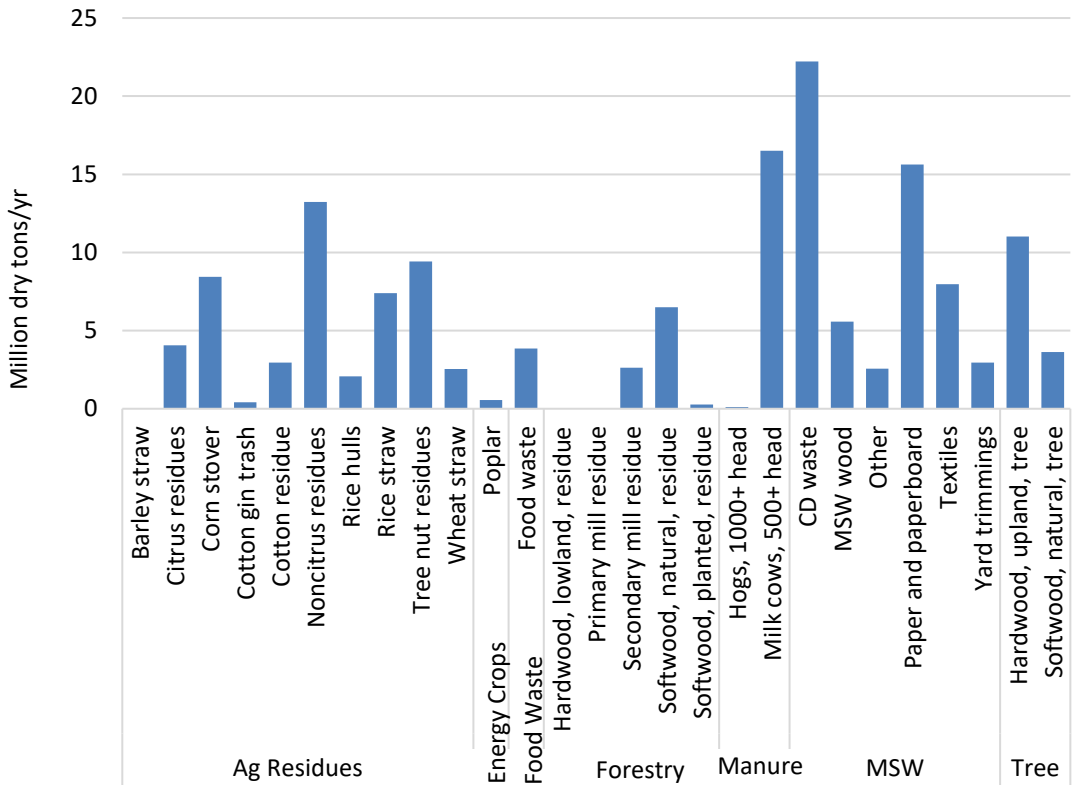

Figure 49. Biomass feedstock availability by individual feedstock, data from [31]

With the feedstock emissions as detailed and the total fuel pathway efficiencies from Table 18, the emission factors associated with fuel feedstock, production, distribution, and dispensing can be calculated for each of the feedstocks by simply multiplying the two (total fuel pathway efficiency and emission factors) together.

5. VEHICLE POWERTRAIN CONFIGURATIONS

Both LDVs and HDVs are modeled in this work, and their powertrain configuration options are largely the same (except for the fact that LDVs with combustion engines are fueled by gasoline while HDVs with combustion engines are fueled by either diesel or SNG). Four main HDV class 8 categories are used in this work: long-haul, drayage, refuse, and construction. These categories were selected based on the number of miles traveled and the amount of GHG and CAP emissions from them. Four were selected to have a balance between adequately representing the wide range of HDVs (each with their own powertrain specifications) without going beyond the scope of this work and getting lost in the vast amount of work that must be done to characterize every single HDV category.

As for the fuel production work, again a 2% rate of inflation is assumed [187] and a CRF of 0.12 is used to annualize costs of vehicles [188].

5.1 Vehicle Efficiencies

Efficiencies for the various powertrain configurations for LDVs are taken from current popular vehicles in their respective categories. The ICV is represented by the Toyota Corolla, the HEV by the Toyota Prius, the PHEV by the Toyota Prius Prime, the BEV by the Chevrolet Bolt, and the FCEV by the Toyota Mirai. One exception to this methodology is the PFCEV, which currently does not have a publically available option. Instead the literature is consulted, and the efficiency data are taken from Lane et al. [26].

Shown in Table 19 are the efficiencies of each of the LDV powertrains mentioned above for the simulation year 2020, and Table 20 shows the same for HDVs. Efficiency projections into the future will be detailed shortly. The “vehicle efficiency” number is the typical miles per gallon

(MPG) or miles per gallon of gasoline equivalent (MPGGE) that one typically sees for LDVs. For vehicles that have both battery and a range extender, this efficiency is known as the charge sustaining (CS) efficiency as it is the efficiency of the vehicle when not using the battery. The "charge depleting (CD) efficiency" is applicable only for PEVs, and it is the efficiency of the vehicle when driven on the battery alone, depleting its charge. In comparison, for PEVs, the former "vehicle efficiency" could be considered the charge sustaining (CS) efficiency, meaning the electric charge of the vehicle is held constant and only the range extender is used, if one is available. The CD efficiency is shown in kilowatt-hours per mile. Note that the BEV efficiency is not shown as the CD efficiency as the battery is the only source of power for BEVs and efficiency is easier to compare using the MPGGE value. The sources of data are given in the table.

Table 20 shows the HDV efficiencies for the year 2020. The efficiencies are shown in miles per gallon of diesel equivalent (MPGDE) to make comparisons with conventional HDVs easier. The CD efficiency is again shown in kilowatt-hours per mile. Determining these efficiencies for HDVs is more involved than for LDVs because not all of the powertrains are available purchase or have much public information at the time of this work.

First is a focus on linehaul HDVs. The efficiencies for the ICV, HEV, PHEV, BEV, and FCEV linehaul vehicles are from Zhao et al. [262]. The CS efficiency for the HDV PHEV is determined by taking the ratio of the LDV PHEV CS efficiency compared to the LDV HEV efficiency and multiplying that ratio to the efficiency of the corresponding HDV HEV. The methodology is captured in Equation 8.

Equation 8. CS efficiency of HDV PHEV

$$\eta_{CS,HDV\ PHEV} = \frac{\eta_{CS,LDV\ PHEV}}{\eta_{LDV\ HEV}} * \eta_{HDV\ HEV}$$

The CD efficiency of the HDV PHEV is obtained by multiplying the above CS efficiency for the vehicle by the ratio of CD efficiency to CS efficiency of the LDV PHEV. The methodology is captured in Equation 9.

Equation 9. CD efficiency of HDV PHEV

$$\eta_{CD,HDV\ PHEV} = \frac{\eta_{CD,LDV\ PHEV}}{\eta_{CS,LDV\ PHEV}} * \eta_{CS,HDV\ PHEV}$$

The CS efficiency for the PFCEV is determined by taking the ratio of LDV PFCEV compared to the FCEV and multiplying that ratio by the efficiency of the HDV FCEV, as shown in Equation 10.

Equation 10. CS efficiency of HDV PFCEV

$$\eta_{CS,HDV\ PFCEV} = \frac{\eta_{CS,LDV\ PFCEV}}{\eta_{LDV\ FCEV}} * \eta_{HDV\ FCEV}$$

The CD efficiency of the HDV PFCEV is obtained by multiplying the above efficiency by the ratio of the CD efficiency of the LDV PFCEV to the efficiency of the LDV PFCEV, as shown in Equation 11.

Equation 11. CD efficiency of HDV PFCEV

$$\eta_{CD,HDV\ PFCEV} = \frac{\eta_{CD,LDV\ PFCEV}}{\eta_{CS,LDV\ PFCEV}} * \eta_{CS,HDV\ PFCEV}$$

The sources for all of the LDV efficiencies used in these processes are given in Table 19. Next is to determine the efficiencies of the other vocations for the HDVs. Work by Kast et al. [263] is used to extrapolate the linehaul efficiencies to the three other HDV vocations of the present work. Kast et al. details the differences in efficiency for FCEVs by vocation using an appropriate duty cycle for the simulation of the vehicles. While the work only details the efficiencies for FCEVs, the present work assumes those efficiency differences will carry across

all powertrain types. The efficiencies for LDVs and all HDV vocations have now been determined and are presented in Table 19 and Table 20.

Table 19. LDV efficiencies for the year 2020

Powertrain	**Representative Vehicle**	**Vehicle efficiency (MPGGE)**	**CD efficiency (mi/kWh)**
ICV	Toyota Corolla [264]	35	-
HEV	Toyota Prius [265]	52	-
PHEV	Toyota Prius Prime [266]	54	3.45
BEV	Chevrolet Bolt [153]	119	-
FCEV	Toyota Mirai [267]	66	-
PFCEV	Custom from Lane et al. [26]	82	3.70

Table 20. HDV efficiencies for the year 2020

Powertrain		**Vehicle efficiency (MPGDE)**				**CD efficiency (mi/kWh)**			
		Linehaul	Drayage	Refuse	Const-ruction	Linehaul	Drayage	Refuse	Const-ruction
ICV	Diesel	5.59	6.30	6.50	9.35	-	-	-	-
	SNG	4.37	4.93	5.09	7.31	-	-	-	-
HEV	Diesel	5.81	6.55	6.76	9.72	-	-	-	-
	SNG	4.62	5.21	5.38	7.73	-	-	-	-
PHEV	Diesel	6.03	6.80	7.02	10.09	0.36	0.32	0.31	0.21
	SNG	4.80	5.41	5.58	8.03	0.28	0.25	0.24	0.17
BEV		12.23	10.85	10.51	7.31	-	-	-	-
FCEV		7.15	8.06	8.32	11.96	-	-	-	-
PFCEV		9.82	11.07	11.43	16.43	0.58	0.52	0.50	0.35

Vehicle efficiency projections into the future are based on historical vehicle efficiency improvements. The U.S. Environmental Protection Agency shows that LDVs have historically improved in efficiency by about 1.0 MPG every 5 years since 1985 [268]. Sival and Schoettle show HDVs have improved in efficiency by about 1.15 MPG every 5 years from 1982 until 2015 [269]. While it is possible that the advanced alternative vehicles, such as FCEVs or PFCEVs, may have different efficiency improvements over time compared to the historical powertrains included in the referenced work, these vehicles have not been on the market long enough to

determine if there will be any significant difference in efficiency evolution. Therefore, the assumption of using the same projection is used due to the lack of more-detailed information.

5.2 Vehicle Costs

The approach for determining vehicle costs is two-fold. First, similar to the methodology of the LDV efficiency, LDV cost is also gathered from popular vehicles currently available for purchase. The manufacturer's suggested retail price (MSRP) is used as proxy for the cost. Again, the PFCEV is an exception due to its lack of current availability. For the PFCEV cost, a ratio of PHEV to HEV cost was multiplied to the cost of the FCEV, which is itself a hybrid. This approximation attempts to determine costs that are not yet well-understood, at least outside of a vehicle manufacturer, but this method should account for the difference in cost of the PFCEV compared to the FCEV due to a larger battery, smaller fuel cell, and the accompanying electronics upgrades. The values from this approach are not used in the present modeling, but are instead used to gauge the results of the following method to ensure reasonable starting values.

The second approach is to categorize vehicle cost by components, categorizing vehicles into powertrain components such as internal combustion engine (ICE), battery, etc., and everything else which is known as the vehicle glider, such as the chassis and wheels. The reason for this is that each vehicle component will have different learning rates (LRs) associated with them. For example, the vehicle glider which is a very mature technology, will have a lower LR compared to a fuel cell, which is a much less mature technology. Note that the default LRs used are reminiscent of those for some of the fuel production technologies. A LR of 0.1 is used for more mature technologies, and a LR of 0.14 is used for less mature technologies. Both the costs and LRs for each of the major vehicle components is listed in Table 21. Note the hybrid and

plug-in hybrid cost adders. These adders consider the additional cost beyond just the battery addition of a hybrid, such as control equipment, wiring, and additional engineering work that go into creating these vehicle types. The cost values in Table 21 are sourced primarily from Zhao, Burke, et al. [262] and Zhao, Wang, et al. [270], with some changes to better match MSRP values.

Table 21. Vehicle Component Starting Costs and Learning Rates

Component	Cost	Units	Component LR
Glider, LDV	15,000.00	$	0.1
Glider, HDV	95,539.00	$	0.1
ICE, gasoline	27.78	$/kW	0.1
ICE, diesel	27.78	$/kW	0.1
ICE, SNG	30.86	$/kW	0.1
Fuel cell	300.00	$/kW	0.14
Traction battery	300.00	$/kWh	0.14
Electric motor and inverter	50.00	$/kW	0.1
Liquid fuel tank	79.31	$/GJ	0.1
SNG tank	2,207.23	$/GJ	0.1
Hydrogen tank	4,166.67	$/GJ	0.14
Hybrid cost, LDV	2,500.00	$	0.1
Hybrid cost, HDV	15,000.00	$	0.1
Plug-in hybrid cost, LDV	5,000.00	$	0.1
Plug-in hybrid cost, HDV	25,000.00	$	0.1

In addition to the component costs, the component specifications for each vehicle are also needed to determine the total vehicle cost. These vehicle specifications are shown in 12. APPENDIX B. Note that the values listed there are from a variety of sources [26], [262], [263], [266], [270]. Some modifications are made to some of the HDVs to ensure that vehicle powers and driving ranges are adequate to meet the needs of different vocations, particularly with power requirements of drayage trucks (400 horsepower) [271], [272] and range requirements of linehaul and drayage trucks (roughly 500 miles and 200 miles, respectively) [272]. BEVs are expected to have difficulty in meeting range requirements of some HDV vocations, but those issues will be addressed later in the model constraints.

Total costs for the various vehicle powertrain configurations can be seen in Table 22 for LDVs and Table 23 for HDVs. Note that these costs are the starting costs, used initially at year 2020 in the model runs. The costs of these vehicles will come down as more are selected to be produced by the modeling, according to the cost and LR of the individual powertrain components listed in Table 21.

Table 22. LDV starting costs and MSRP by powertrain configuration

Powertrain	**Starting cost ($)**	**MSRP ($)**
ICV [264]	17,872.21	18,700
HEV [265]	22,883.93	23,770
PHEV [266]	27,376.98	27,300
BEV [153]	43,000.00	36,620
FCEV [267]	60,357.50	59,295
PFCEV	54,000.00	68,100

Table 23. HDV starting costs by powertrain configuration and vocation

Powertrain		**Starting cost ($)**			
		Linehaul	**Drayage**	**Refuse**	**Construction**
ICV	Diesel	105,539.02	102,874.55	102,426.44	100,732.75
	SNG	140,539.32	133,801.51	112,874.33	114,769.74
HEV	Diesel	128,516.30	129,461.18	128,977.10	123,043.41
	SNG	163,236.29	160,187.34	139,219.39	136,931.01
PHEV	Diesel	160,451.91	179,784.33	164,619.80	153,218.30
	SNG	192,601.58	207,613.50	173,688.97	164,701.03
BEV		265,539.00	242,844.37	238,780.92	195,958.66
FCEV		285,572.67	240,731.64	219,544.14	179,068.41
PFCEV		247,429.04	219,414.46	203,889.99	174,194.07

5.3 Vehicle Tailpipe Emissions Factors

Emissions factors for BEVs, FCEVs, and PFCEVs are quite simple as they are all ZEVs, so they all have emissions factors of zero for the vehicles themselves. It is important to remember, however, that this does not mean there are no emissions associated with using these vehicles. There are still potentially emissions associated with the fuel production, depending on

which fuel feedstock is used. The ICVs, HEVs, and PHEVs have tailpipe emissions and therefore it is necessary to characterize these vehicles' emissions factors.

The total effective GHG emissions can be calculated from the three main GHG emissions using what is known as global warming potential (GWP) of the individual emissions. The GWP relates the strength of a GHG to carbon dioxide. For example, a GHG that has ten times the heating effect per quantity of emission compared to carbon dioxide has a GWP of 10. The sum of GHG emissions is often given in the units of some mass of carbon dioxide equivalent (CO_{2e}). Equation 12 shows the total GHG emissions given the three primary GHG emissions, which are carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O).

Equation 12. GHG emissions from individual components

$$\text{mass of GHG}, \mathrm{CO_{2e}} = 1 * (mass\ of\ CO_2) + 25 * (mass\ of\ CH_4) + 298 * (mass\ of\ N_2O)$$

5.3.1 LDV Tailpipe Emission Factors

GHG tailpipe emission factors for LDVs are calculated using GREET 2018 Well-to-Wheel Calculator, which gives GHG emissions on a per-gallon of gasoline basis. The GHG emission factor for gasoline-fueled vehicles is 10,785 $gCO2_e$/GGE [33]. CAP tailpipe emission factors for LDVs are taken from the 2020 EMFAC projections for model year 2020 LDVs, which include passenger cars and light-duty trucks [141]. Note that the LDV fleet modeled by EMAC has an average of 34 MPG efficiency. With the emissions in terms of fuel input, differences in powertrain efficiencies will have an effect on emissions, whether those efficiency differences are due to a different powertrain configuration or due to technology improvements with time. The LDV tailpipe emission factors are shown in Table 24.

Table 24. LDV tailpipe emission factors

Powertrain	Emission factor (g/GGE)						
	GHG ($CO2_e$)	**VOC**	**CO**	**NO_x**	**PM10**	**PM2.5**	**SO_x**
ICV, HEV, and PHEV	10,785	0.552	22.4	0.920	0.0602	0.0553	0.0851
BEV, FCEV, and PFCEV	0	0	0	0	0	0	0

Combining the above emission factors with the efficiencies of each of the powertrain configurations yields the emissions in terms of grams per mile. This along with the VMT yields the total emissions of these vehicles. Vehicle emission factors are assumed to be constant through time, but the efficiency improvements yield lower emissions per mile traveled as time progresses.

5.3.2 HDV Tailpipe Emission Factors

GHG tailpipe emission factors for HDVs are calculated using GREET 2018 Well-to-Wheel Calculator, just the same as for LDVs. The GHG emission factor for diesel-fueled vehicles is 10,951 $gCO2_e$/GGE and for SNG-fueled vehicles it is 8,767 $gCO2_e$/GGE [33]. Values for the VOC, CO, NO_x, and PM are California Air Resources Board levels for the federal test procedure. The SNG engine is based on a Cummins 11.9 L CNG engine from 2019 [273], which is a low-NOx engine as it meets the standard of 0.02 grams of NOx emission for each brake horsepower-hour of operation (g/bhp-h) [145], [146]. The diesel engine is based on a Cummins 11.8 L diesel engine from 2019, with the NO_x emissions artificially lowered to the low-NOx standard [274]. This assumption for low-NO_x diesel engines is made to the lack of test data for these vehicles. Values for HDV tailpipe emission factors are shown in Table 25. Units have been

converted to match those of Table 24 to allow for easier comparison, despite being somewhat inappropriate for HDVs (as HDVs do not typically take gasoline as a fuel).

Table 25. Low-NOx HDV tailpipe emission factors

Powertrain	**Emission factor (g/GGE)**				
	GHG ($CO2_e$)	**VOC**	**CO**	**NO_x**	**PM_{10}**
Low-NO_x SNG – ICV, HEV, and PHEV	8,767	0.20	74	0.49	0.49
Low-NO_x diesel – ICV, HEV, and PHEV	10,951	0.49	20	0.98	0.20
BEV, FCEV, and PFCEV	0	0	0	0	0

As with the LDVs, these HDV emission factors combined with vehicle efficiencies and annual VMT yields the total emissions of these vehicles. These emission factors are again assumed to be constant through time.

6. MODEL CONSTRAINTS

Four major constraints are modeled in this problem: (1) GHG emissions, (2) VMT for each of the vehicle classes and vocations chosen, (3) technology deployment rates, and (4) feedstock availability.

6.1 California GHG Emissions Goals

California laws and an Executive Order set limits on GHG emissions from the State. AB 32 requires GHG emissions in 2020 to be reduced to 1990 levels [8]. SB 32 requires GHG emissions in 2030 to be 40% below 1990 levels [9]. Lastly, California Executive Order S-3-05 requires GHG emissions in 2050 to be 80% below 1990 levels [10]. Note that only AB 32 and SB 32 have been signed into law. The Executive Order is, at this point, only a goal. However, the State has been acting and planning to achieve this goal, so it is considered a constraint of this work.

These regulations and goals are plotted in Figure 50. Noted that the most recent available emissions data from 2016 [275] are within the necessary limits of 2020, showing that attainment of the law in 2020 is feasible.

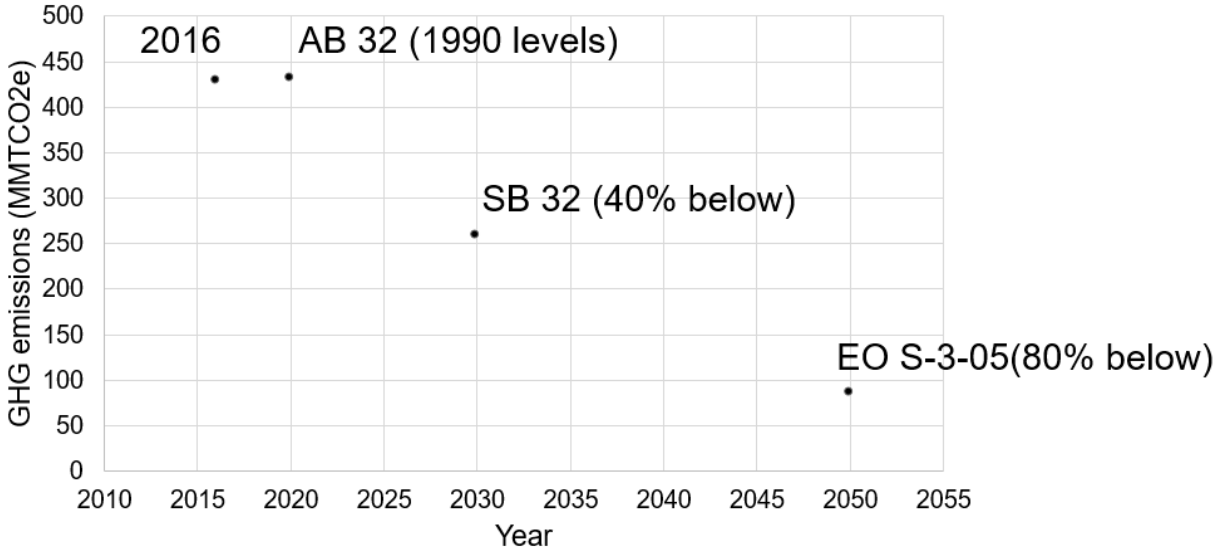

Figure 50. California GHG emissions regulations and the current state, from [275][7], [9], [10]

Note that the above emissions goals are economy-wide. The present work focuses on transportation. To determine the GHG emissions constraints that should be used in the present modeling, it is assumed that the relative proportion of GHG emissions from transportation, which is 41% [7], is held constant out to 2050. Furthermore, 70.3% of GHG emissions are from vehicles modeled in this working according to a 2018 scenario from California Air Resources Board's Mobile Emissions Inventory EMFAC [141]. In total, 28.8% of California GHGs are modeled in this work. Therefore, the GHG emissions constraint used are 28.8% of the limits shown in Figure 50. Additionally, to account for the fact that there are no explicit pieces of legislation or goals for years other than 2020, 2030, and 2050, linear interpolation is used for the GHG emissions constraint for the other years within the timeframe of this modeling.

6.2 Vehicle Miles Traveled

VMT constraints are essential to model as they are what determine how much fuel should be produced at each time step. Additionally, VMT can be used along with average number of

miles traveled by a given type of vehicle to determine how many of those vehicles are on the road or projected to be on the road.

VMT for LDVs with projections out to 2050 are sourced from EMFAC 2017 Web Database [141]. The EMFAC VMT projections are the culmination of a variety of studies from academia and government work, and further details can be found in their Technical Documentation report [276]. As an alternative, VMT for LDV personal vehicles can be found in the National Household Travel Survey (NHTS) data [277]. The most recent NHTS data are from 2009. Projections into the future can be set by scaling VMT by population data, which is recommended by the California Air Resources Board [278]. Both of these LDV VMT projections are depicted in Figure 51. Note that both projections have the same general trend, but EMFAC data are higher number of miles. This could be due to a host of reasons. One hypothesis is the poor economy of 2009, which would depress the number of miles traveled. EMFAC data are more recent, and therefore reflect an improving economy and increased traveling. For the present work, the VMT from EMFAC will be used as they are the most current data.

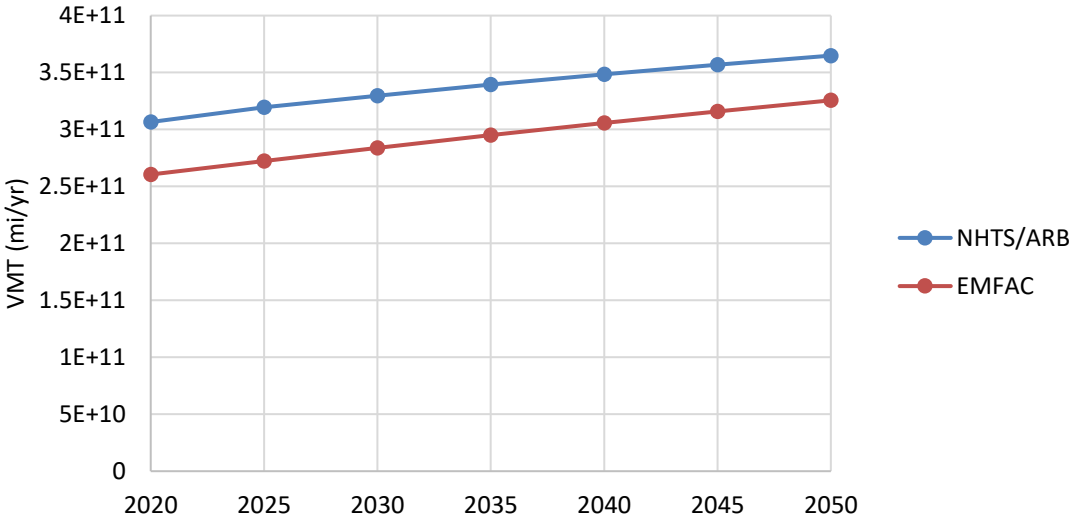

Figure 51. LDV VMT projections with NHTS/ARB data from [277] [278] and EMFAC data from [141]

VMT projections for HDV vocations shown in Figure 52 are from EMFAC as well [141]. The vocations listed are a composite of various EMFAC vehicle classifications. The linehaul category includes EMFAC's 2011 vehicle classification of T7 Tractor. Drayage includes T7 Other Port, T7 POAK, and T7 POLA. Refuse includes T7 SWCV and T7 SWCV-NG, which distinguishes between diesel- and natural gas-powered vehicles. Construction includes T7 CAIRP Construction, T7 Single Construction, and T7 Tractor Construction.

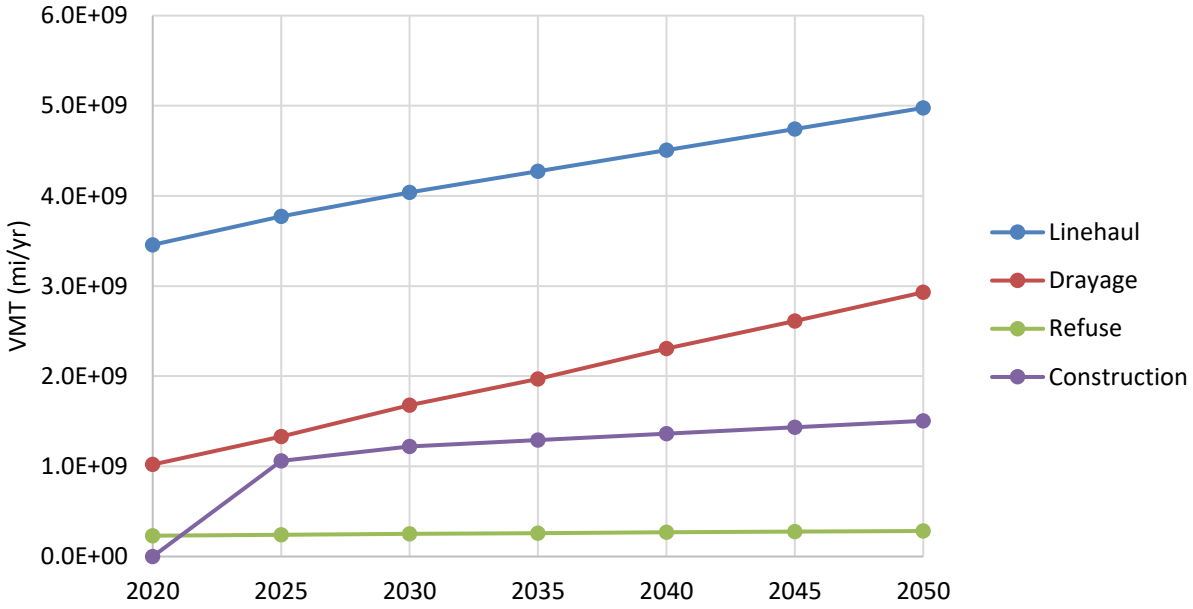

Figure 52. HDV VMT projection by vocation, data from [141]

For both LDVs and HDVs of the various vocations, an average annual VMT is used to convert from the number of miles that must be traveled to the number of vehicles that must be purchased at each timestep to meet that travel demand. Each LDV travels an average of 11,346 miles annually [140]. Linehaul trucks average 72,000 miles per year [141]. Drayage trucks average 44,100 miles per year [141]. Refuse trucks average 14,900 miles per year [141]. Lastly, construction trucks average 44,300 miles per year [141]. Implicit in this is an assumption that the average number of miles traveled by each vehicle in each vehicle category will stay constant with time. If perhaps average VMT per vehicle increased, the number of vehicles purchased would decrease proportionally, decreasing the money spent on vehicles but keeping money spent on fuel constant. If VMT per vehicle decreased, the number of vehicles purchased would increase and money spent on vehicles would increase while money spent on fuel would be constant.

One additional constraint concerning the VMT constraints is the BEV's relatively low driving range and long fueling time compared to other vehicle powertrain configurations.

The BEV modeled for LDVs has a range of 200 miles given its efficiency and traction battery size. This range is similar to that of modern-day BEVs like the Tesla Model 3 and the Chevrolet Bolt, among many others that are coming onto the market. While this range is significantly higher than that of BEVs from years past, it is noticeably less than ICVs and all other alternative powertrain configurations with ranges above 300 miles. As previously noted in Chapter 2.2.4, BEVs also have charging times much longer than drivers are accustomed to at gasoline stations. Karlsson notes that 79% of households with a BEV have more than one car, compared to 48% for those with conventional vehicles [279]. One may hypothesize that this is simply due to the fact that BEVs owners are simply more wealthy and have more vehicles. This is not so. The 79% figure increases when removing the Tesla Model S, an expensive and longer-range BEV. Therefore, the proclivity of BEV owners having multiple cars is significantly related to the short driving range and long fueling times of BEVs.

With 21% of BEV owners having only one vehicle, and the rest having at least two vehicles (meaning at most half of the remaining 79% of vehicles are BEVs), this means at most a total of 61% of LDVs could conceivably be BEVs, due to driving range and fueling time limitations. Assuming this 61% of vehicles translates to 61% of VMT, the light-duty VMT is herein modeled to be composed of at most 61% BEV VMT.

As previously mentioned for HDVs, as of 2015, only drayage and refuse trucks had been demonstrated to operate with a BEV powertrain due to range limitations [157]. Some literature predict low class 8 BEV feasibility of up to about 20% unless higher charging rates or battery

swaps are implemented [280]. The distribution of trip length of Class 8 HDVs can be seen in Table 26, with data from the California Vehicle Inventory and Use Survey. According to this survey, 40% of Class 8 HDVs have trips greater than 150 miles [281]. Considering the state of BEV technology, it would be optimistic to assume a range much higher than 150 miles for HDVs in the near future. Furthermore, the other HDV powertrain technologies lend themselves much better to longer range driving and faster refueling. Therefore, this work assumes that at most 60% of HDV linehaul VMT could be met by BEVs, which would be 150 miles or less in trip length, and the rest of the HDV linehaul VMT must be met by powertrains other than BEVs.

Table 26. Class 8 HDV trip length distribution, data from [281]

Trip length (mi)	**CA-VIUS (% population)**
0-50	27%
>50-100	20%
>100-150	14%
>150-500	26%
>500	14%
Total	101%

Similar to linehaul, drayage trucks also have driving range requirements. In 2013, Papson and Ippoliti surveyed over 1,000 drayage truck operators in the Los Angeles area and found that about 20% of operators would be satisfied with a 100 mile range before refueling, and 46% would be satisfied by a 200 mile range [272]. In 2018, Tetra Tech and Gladstein, Neandross & Associates did additional survey work and found average shift distance for drayage trucks to be 160 miles [271]. The present work projects a future heavy-duty BEV driving range of 150 miles, the same as the range of linehaul BEVs, and a maximum drayage VMT satisfaction of 25%, which falls between the 20% and 46% satisfaction rates of 100 mile and 200 mile ranges, respectively.

The refuse and construction HDV vocations are assumed able to be met fully by BEVs as their trip lengths are not as high as linehaul or drayage.

6.2.1 Utility Factor

The utility factor (UF) of a vehicle specifies how many of the miles that vehicle travels using the battery as the power source compared to the total number of miles traveled. An ICV has a UF of 0 because it has no battery to supply driving power, a BEV has a UF of 1 because it has only a battery to supply driving power, and a PHEV or PFCEV can have a UF anywhere from 0 to 1, depending on how the vehicle is driven and fueled. For example, a PFCEV that travels 30 miles on its battery charge and 70 miles using hydrogen in the fuel cell has a UF of 0.3 for that trip. UFs vary greatly by vehicle specification (BER, CD efficiency, CS efficiency), trip composition (length, grade, etc.), fueling habits (whether one charges the vehicle at home or not), driving personalities (speed, acceleration, etc.), and other factors. Therefore, it is most practical to use an average UF that represents the spectrum of possibilities.

The Society of Automotive Engineers (SAE) International defines a particular UF as a fleet UF (FUF). SAE International suggests using the FUF to determine the electricity and other fuel use for a fleet of vehicles, which is the intended use in the present work. The FUF is calculated using a distribution of vehicle trips and dividing the miles of CD travel by the total number of trip miles [282].

Using the SAE International J2841 specification along with BER specifications with a vehicle yields the FUF. The FUF for LDVs and each vocation of HDVs are shown in Table 27, using the BER and FUF correlation from SAE International J2841 [282]. LDVs for this work are designed with a BER of approximately 40 miles [26][283][284]. The BER for the various HDV

vocations are calculated using the battery capacity and CD efficiency of each of the plug-in hybrid options (diesel and SNG PHEV as well as PFCEV) and then taking the average of those results to get a representative vocation-wide BER. It should be noted that the FUFs listed in Table 27 are from a methodology that uses National Household Travel Survey data to determine trip length distribution. There has been no work detailing the FUF of HDVs by vocation or in general as heavy-duty PHEVs are a new technology. Due to the long trip length of linehaul vehicles, the FUF is artificially lowered from what is specified as 0.512 to half of that value which is 0.256 to fall in line with reasonable expectations of a vehicle traveling such long distances.

Table 27. FUF for analyzed vehicle types and vocations

	LDV	HDV			
		Linehaul	Drayage	Refuse	Construction
BER (mi)	40	29	47	36	37
FUF	0.617	0.256[1]	0.669	0.583	0.592

[1] The linehaul FUF is half of the SAE International specification of 0.512 due to long trip lengths

6.2.2 Vehicle Fleet Turnover Rate

Vehicle fleet turnover rates show the amount of time that vehicles spend on the road. It is not realistic to expect all vehicles on the road to immediately be recycled and replaced with ZEVs. Additionally, considering the emissions associated with manufacturing and recycling the vehicles, that approach may not even be the best on an environmental basis even if it were possible. Therefore, it is necessary to impose some sort of constraint on how quickly the current vehicles on the road will be replaced by new vehicles suggested by the present modeling.

Fleet turnover rates are determined by EMFAC projections of vehicle use [141]. These EMFAC data project VMT by vehicle year for each of the vehicle classes included in the present work. Gathering data every five years from 2020 to 2050 shows how the VMT from vehicles of

prior years decreases as time goes on. Germane to the present work are the VMT from vehicles made prior to 2020, as vehicles made in 2020 and beyond to 2050 will be dictated by the optimization.

Also available in this data set from EMFAC are emissions from the vehicles from different years. Again, emissions from vehicles made prior to 2020 are gathered, and taken to be baseline emissions that will occur regardless of what the optimization suggests for new vehicle purchases. It will later be determined if the EMFAC projected fleet turnover is adequate to meet environmental legislation, or if perhaps turnover must occur at a faster rate.

Figure 53 through Figure 57 show the EMFAC projections for total VMT, VMT met by vehicles manufactured prior to 2020, and VMT met by vehicles manufactured in 2020 and beyond. The reason for the split in vehicle manufacture year is to account for the modeling of the present work. Any vehicles made prior to 2020 will be considered in the analysis as legacy vehicles, whose powertrain configuration and corresponding tailpipe emissions have been set. However, any vehicle made starting in 2020 will have its powertrain and associated emissions determined by the modeling of the present work.

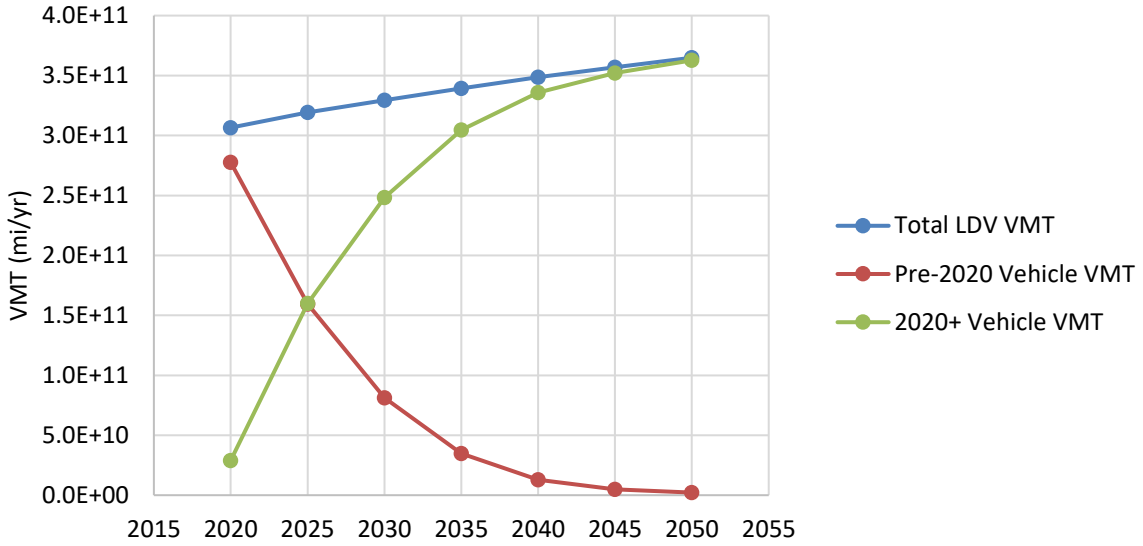

Figure 53. LDV fleet turnover by VMT, data from [141]

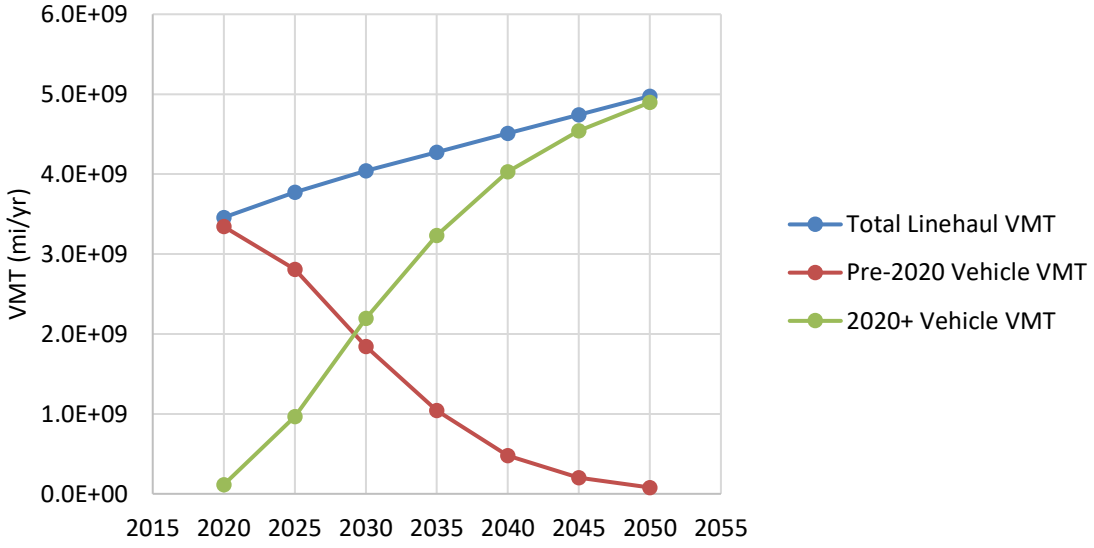

Figure 54. Linehaul HDV fleet turnover by VMT, data from [141]

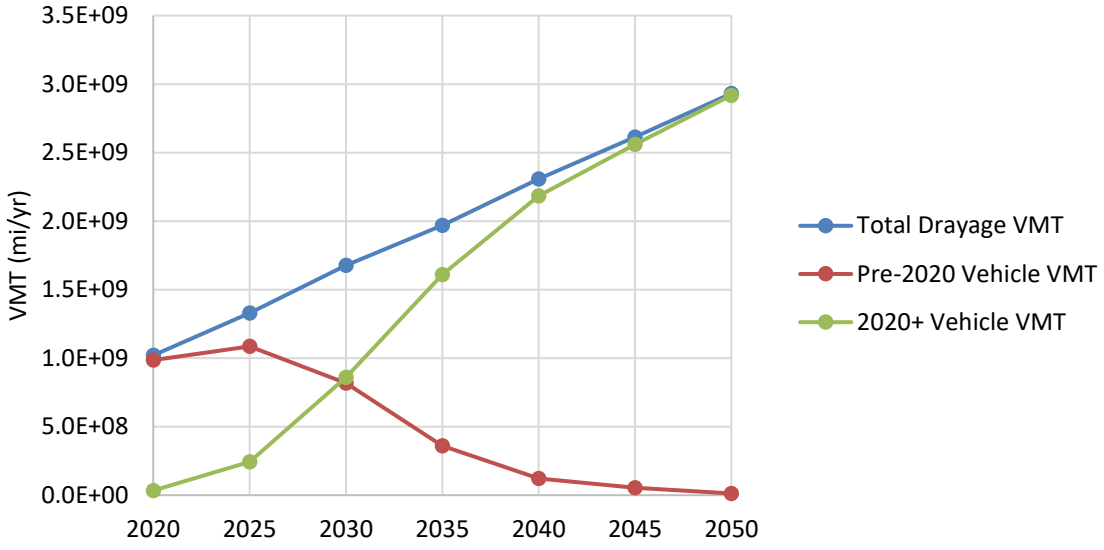

Figure 55. Drayage HDV fleet turnover by VMT, data from [141]

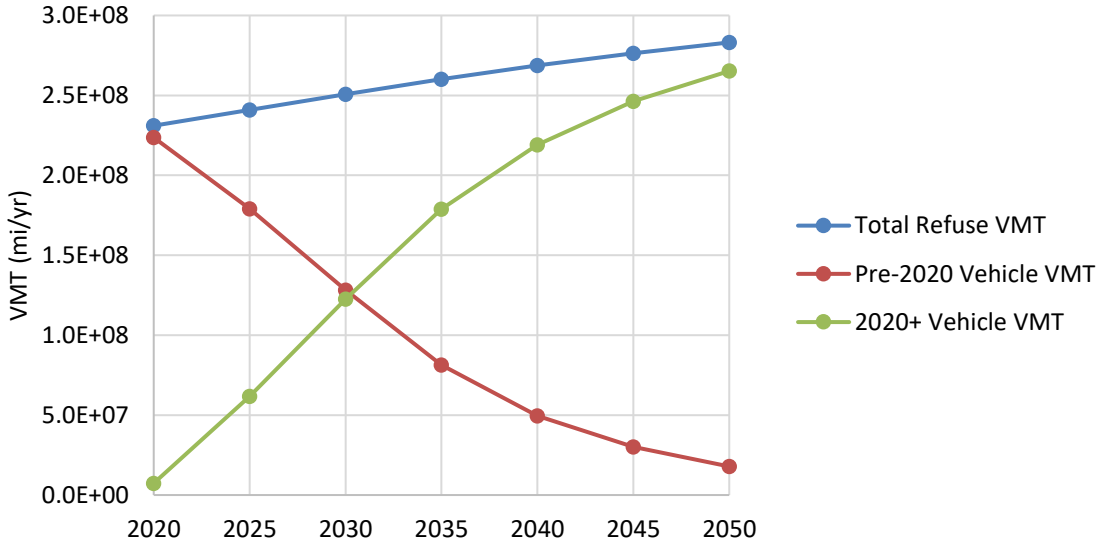

Figure 56. Refuse HDV fleet turnover by VMT, data from [141]

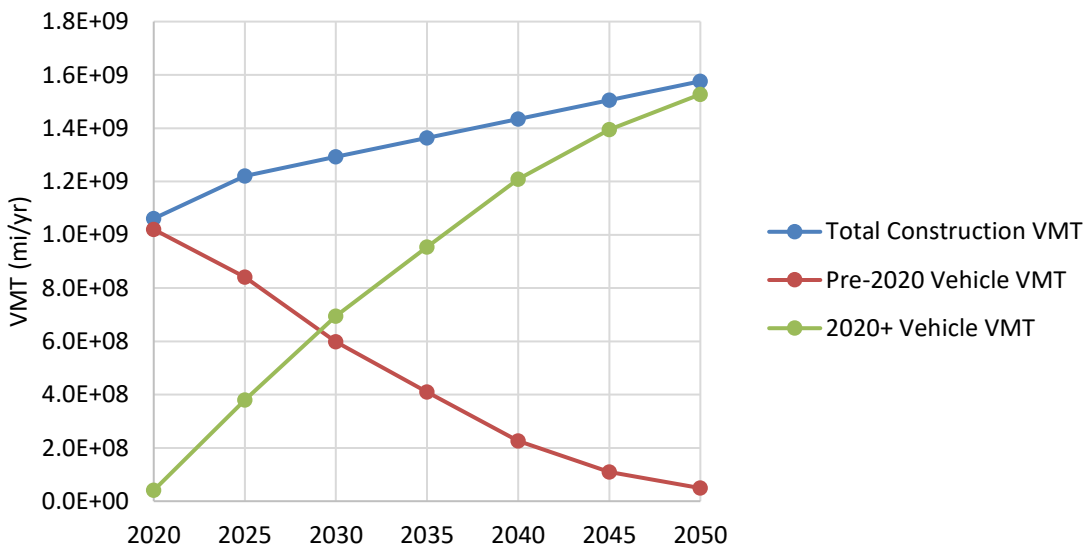

Figure 57. Construction HDV fleet turnover by VMT, data from [141]

6.3 Technology Deployment

Realistic technology deployment rates are needed to ensure results are meaningful. One could imagine a scenario in which a single technology happens to be the cheapest and most efficient at producing fuel, but perhaps it would not be feasible to produce fuel using only that equipment because production takes time. Therefore, these technology deployment constraints are conceived to protect against unreasonable adoption of any given technology.

There are three categories of technologies detailed in the following sections regarding the rate at which the technologies can be adopted. The first is electrolyzer production limits, which constrains the three distinct electrolyzer technologies for fuel production. The second is a limit on biomass fuel production, which includes equipment such as gasifiers and liquefaction. The third category are future vehicle powertrain availabilities, which estimate when currently-unavailable powertrains might come to the market. There are no constraints placed on vehicle

technology deployment rates. Instead, the constraints on the fuel production methods secondarily limit the deployment of the corresponding vehicles that use those fuels.

6.3.1 Electrolyzer Cumulative Production Limits

Growth scenarios for technologies are bounded by current capacity and market size. Current capacity for electrolyzers is sourced from Schoots et al. [285], with a split of 60% AEC technology and 40% PEMEC technology, based on the fact that AEC technology is more mature and deployed than PEMEC technology. Future projections for electrolyzer production scale are by IEA and DOE projections for hydrogen usage and then back-calculating the required installed capacity of electrolyzers [286], [287]. Growth for electrolytic SNG technologies is bounded by natural gas utilization in the U.S. and worldwide, which are 1 TW and 4 TW, respectively. This is due to the market size cap of SNG being the amount of natural gas used, and this is a reasonable limit to the amount of SNG produced by 2050. These natural gas usage data are sourced from the U.S. Energy Information Administration (EIA) [288]. Two scenarios, one with a more conservative, lower electrolyzer capacity in Figure 58 and one with a more optimistic, higher electrolyzer capacity in Figure 59.

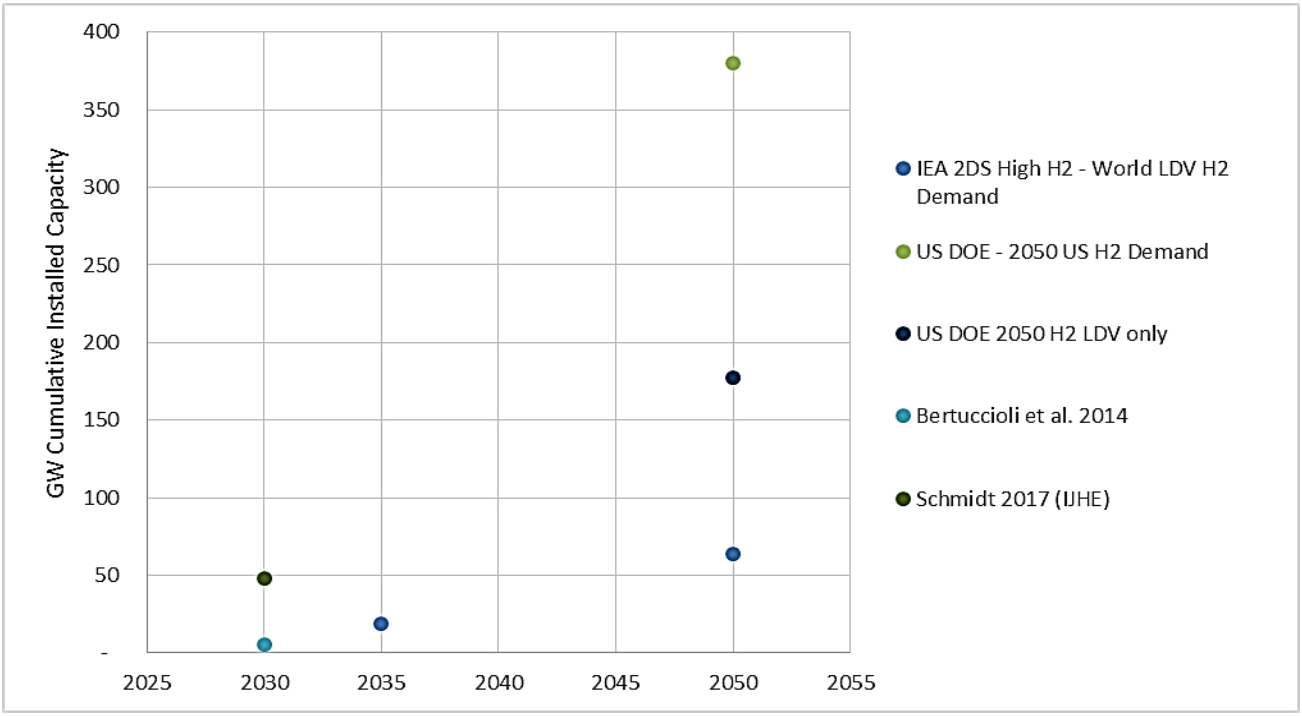

Figure 58. Future electrolyzer market size projections in 2030, 2035, and 2050 (based on assumed efficiency of 50kWh/kg and capacity factor of 90%)

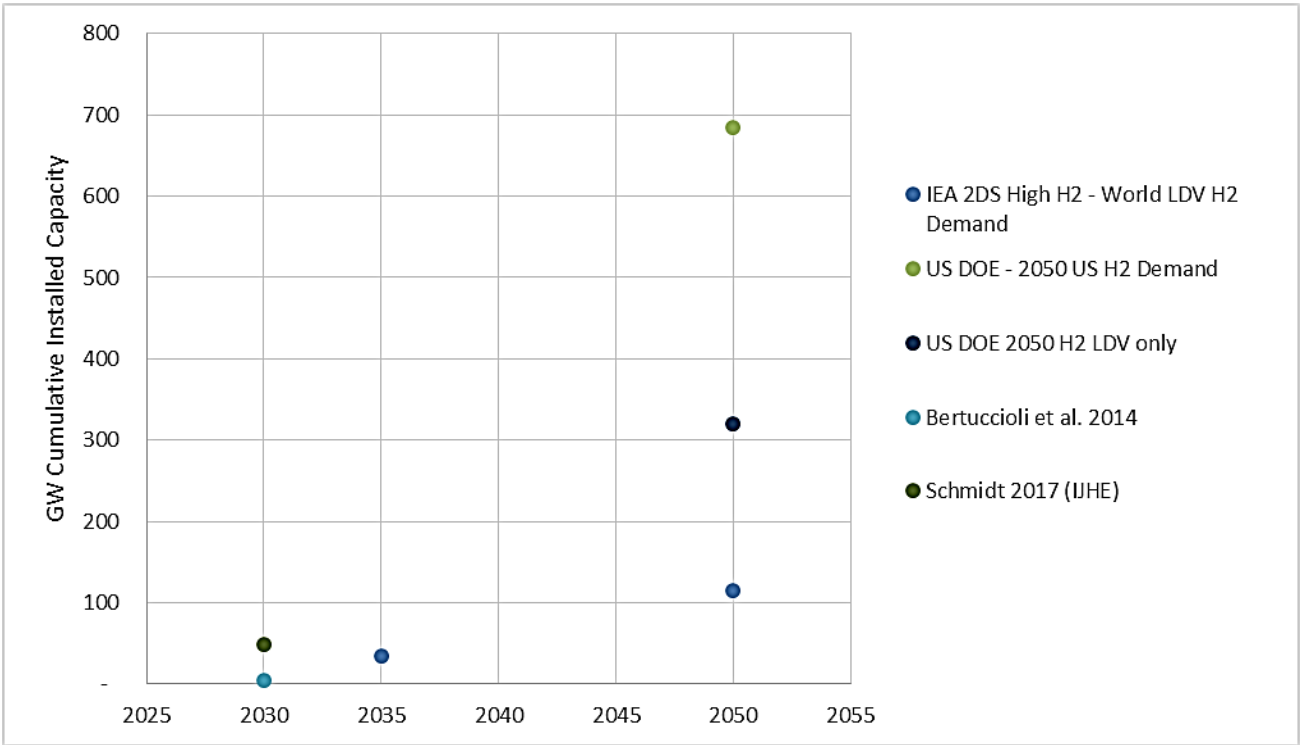

Figure 59. Future electrolyzer market size projections in 2030, 2035, and 2050 (based on assumed efficiency of 50kWh/kg and capacity factor of 50%)

Given the previous notes and plots using data from the literature, conservative and optimistic scenarios for electrolyzer production can be developed. Plots for the cumulative production limits of the three electrolyzer technologies for the conservative scenario and the optimistic scenario are found below in Figure 60 and Figure 61. Note that these electrolyzer production limits are the only limits applied to SNG production. Limits for the methanator equipment and the various carbon capture equipment are assumed not to be more stringent than these electrolyzer limits.

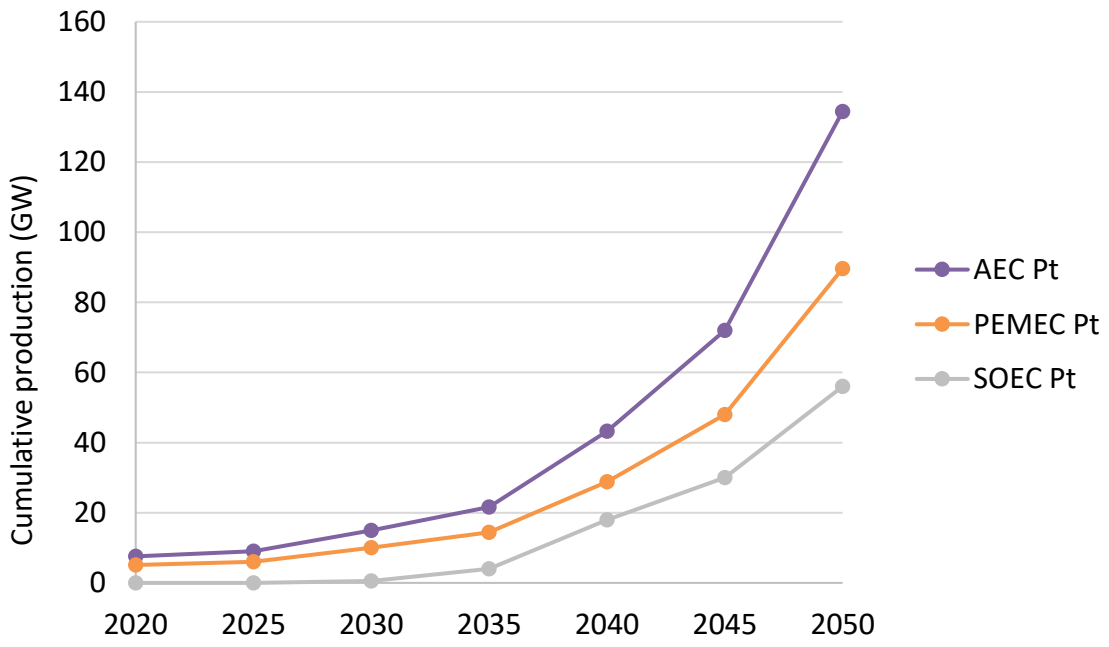

Figure 60. Conservative estimate on electrolyzer cumulative production limits

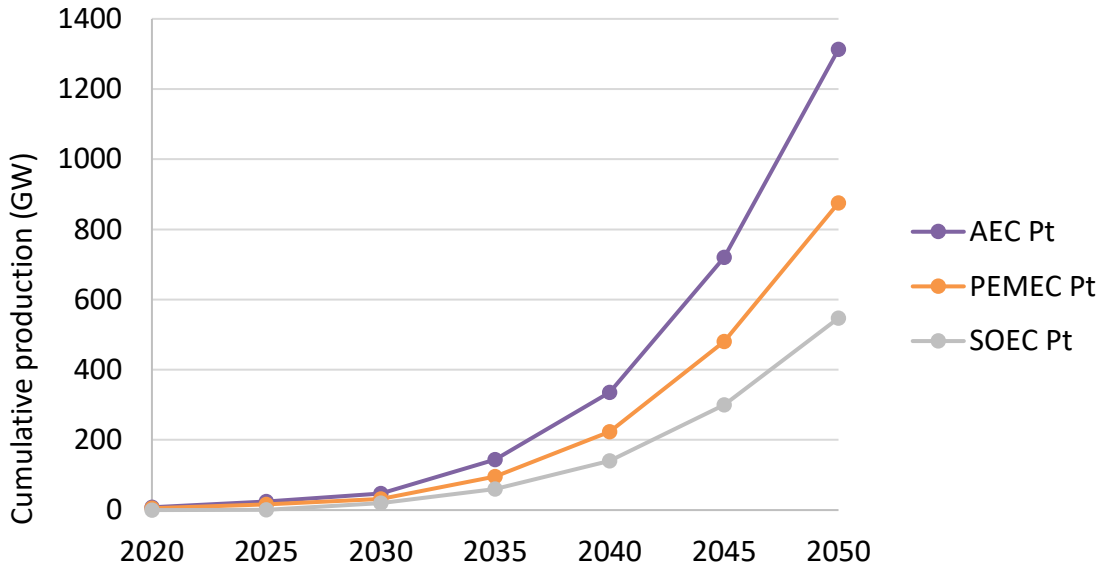

Figure 61. Optimistic estimate on electrolyzer cumulative production limits

The preceding conservative and optimistic technology growth limits are the cumulative installed capacities that dictate the cost evolution of electrolyzer technologies displayed in the tables and figures of Chapter 4.2. It was noted then that the growth in installations used to demonstrate Wright's Law were merely an example of a future scenario. In fact, those growth projections are practical limitations to the growth of the technologies. Recall that the present modeling work will in fact determine an optimal growth projection for each technology, and that is what will actually drive costs down.

6.3.2 Biomass Feedstock Fuel Production Equipment Cumulative Production Limits

The International Energy Agency projects a 1.7 times increase of bioenergy compared to current use by 2040, and a 4 times increase by 2050, which gives a reference to determine feasibility of biomass technology installed capacities [289], [290]. Gasification current installed technology is from the Global Syngas Technologies Council [291]. Similar to the electrolyzers, the upper limits are sourced from the U.S. Energy Information Administration (EIA) [288]. Plots

for the cumulative production limits of gasifiers, AD, gasifier-FT, hydrolysis, pyrolysis, and liquefaction are shown in Figure 62. Note that unlike the electrolyzers, which are more technically advanced and complicated than the biomass conversion processes as well as having less data in the literature, there are no conservative and optimistic projections; there is simply one projection.

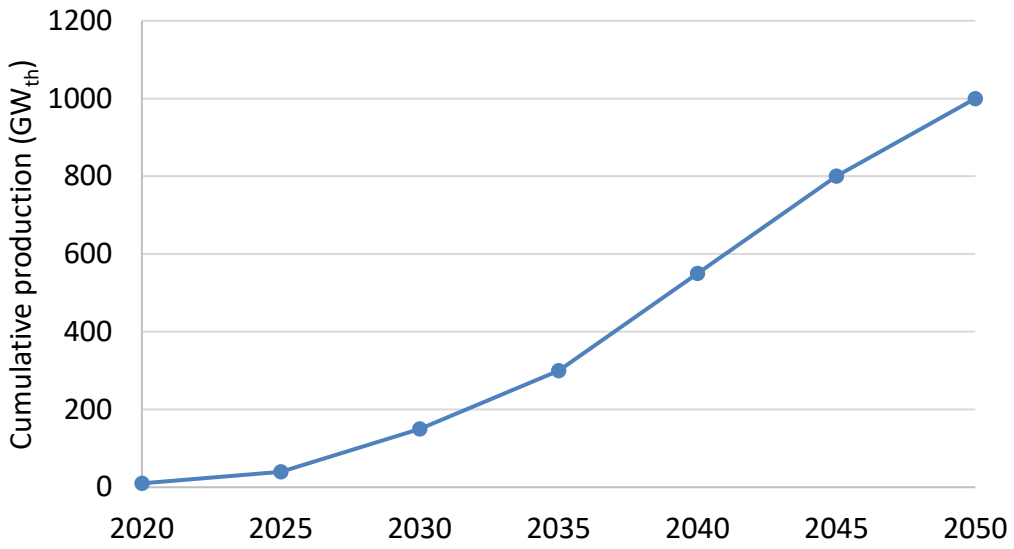

Figure 62. Biomass feedstock fuel production equipment cumulative production limits

As with the electrolyzer technologies, the preceding growth limits are what were displayed for the various biomass fuel production technologies in Chapter 4.2.

6.3.3 Future Vehicle Powertrain Availabilities

For LDVs, all of the powertrain configurations in this analysis are currently available except PFCEVs. However, at least one manufacturer has begun preparing for series production of a PFCEV, with the intention of selling it soon [160]. Therefore, this work assumes that PFCEVs will be available by 2020, for the first year of modeling.

For HDVs, regarding low-NOx engine technologies, low-NOx CNG engines are already available for purchase [273]. However, low-NOx diesel engines are not. The assumption is made that these engines will be available shortly, specifically in the year 2020. Note that this assumption does not have much impact on the results of this work as the GHG emissions constraints are the primary emissions constraints.

Zero-emission HDVs (BEVs, FCEVs, and PFCEVs) are all assumed to be available in 2025. A recent feasibility study has shown manufacturers expect both BEVs and FCEVs to come to the market after 2020, either in 2021 or shortly after [271]. Due to the current state of the art in 2019, the tendency for manufacturers to over-estimate their delivery timelines, as well as this work's timesteps of 5 years, the assumption is made to begin availability of these ZEVs as 2025. An additional implicit assumption is that PFCEVs will become available at nearly the same time, due to this powertrain's similarities to FCEVs with a larger battery and plug-in capability. A summary of the years that the various future HDV powertrains will be available is shown in Table 28.

Table 28. Future HDV powertrain availabilities

HDV powertrain	Year of availability
Low-NO_x diesel	2020
BEV	2025
FCEV	2025
PFCEV	2025

6.4 Fuel Feedstock Availability

The last set of constraints is for fuel feedstock availability. These take two forms: (1) for electricity, the electric grid can only feasibly grow a limited amount from year to year and (2) for biomass, there is only so much biomass available to be harvested.

6.4.1 Electricity

Electricity availability is constrained more by the infrastructure that distributes it than by the availability of its feedstocks (natural gas, solar, wind, nuclear, etc.). An in-depth assessment of the logistics of an electricity infrastructure upgrade is beyond the scope of this work, but a reasonable cap on growth is applied. Electricity for vehicle use is assumed to be up to about 20% of total electricity production by E3's work using their PATHWAYS model [189], [292]. Electricity limits for this present work are taken to be that 20% of the projected electricity capacity from E3's PATHWAYS work of the "straight line base" scenario [189], with an additional buffer of 20% on top of the total electricity production. To summarize, this present work assumes a quantity of electricity equal to 40% of the electricity production projected by E3 could be available for transportation fuel. These projections account for increased PEV adoption, and the additional 20% buffer applied is to account for a potentially high PEV adoption. However, it would be impractical to assume that every vehicle could become a PEV very rapidly due to the amount of time required to make the electric grid more robust. Similarly, electrolytic fuels that use electricity as a feedstock must be constrained as well. Therefore, the additional production limit prevents too drastic an increase in electricity throughput for either vehicle fuel or fuel feedstock. The electricity feedstock availability, along with biomass feedstock availability, is shown in Figure 63.

6.4.2 Biomass

Biomass feedstock limits are taken as previously shown in Figure 19 from the Billion Ton Report [31]. As a reminder, the availability is a function of both year as well as selling price.

A higher selling price of some biomass feedstocks leads to a higher quantity available. Some simplifications are made to aid in implementation, specifically in areas in which increasing selling price of biomass only slightly increases availability. In these cases, the slight increase in availability is neglected for the higher selling price. The maximum biomass feedstock availabilities used in the modeling, regardless of price, are shown in Figure 63, along with the electricity feedstock availability. Note that both forestry and tree biomass are interchangeable for the purpose of this work, so the combined availability is shown. Also, note that the biomass availabilities are displayed on the left y-axis and the electricity availability is displayed on the right y-axis, due to a difference in availability by nearly an order of magnitude.

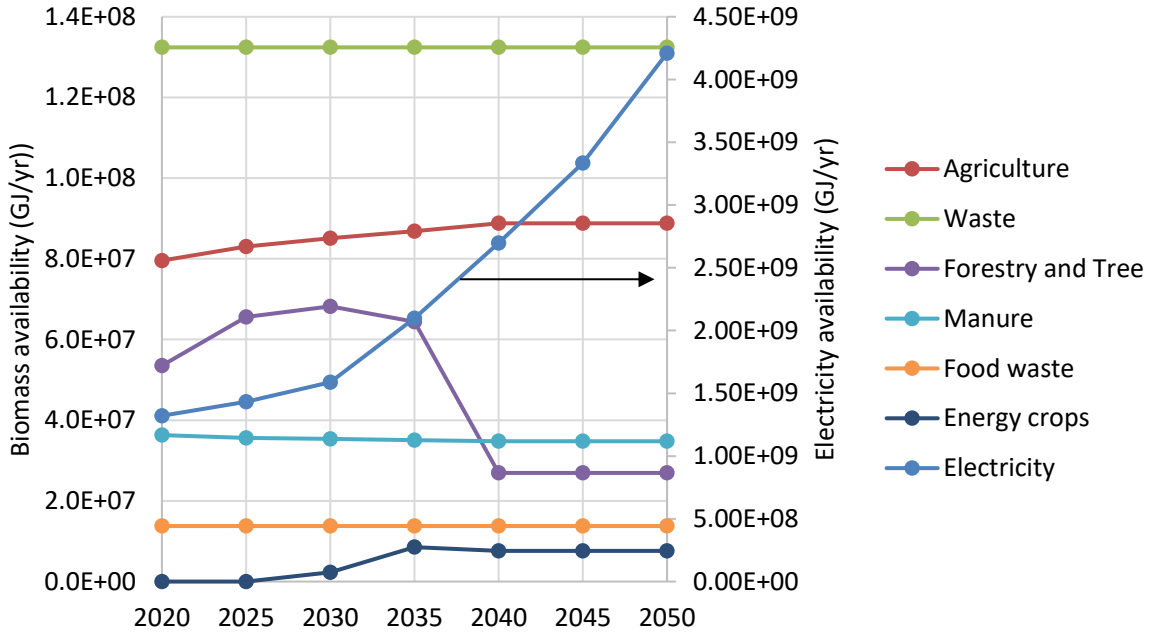

Figure 63. Fuel feedstock availability, data from [189] and [31]

7. ESTABLISHING THE OPTIMIZATION PROBLEM

The various components of the chain from fuel production to vehicles have been analyzed for efficiency, emissions, and cost; and Wright's Law has been identified as the methodology of projecting these costs into the future. With these data, it is now possible to calculate the total cost of each potential pathway. Additionally, the various constraints of the problem have been detailed. This chapter is devoted to describing how these costs and constraints are implemented into a formal optimization problem for the timeframe of 2020 (the near future) into 2050.

The modeling tool developed to solve the goal of this dissertation is christened Transportation Affecting Cost and Emissions (TRACE). The model, including projections and optimization, will hereafter be referred to as TRACE.

7.1 Optimization Method

Given the techno-economic data and constraints, it is evident that LP is an appropriate optimization tool for TRACE. One could argue that MILP is most appropriate as there can realistically only be an integer number of vehicles. However, given the scale of the problem being solved, approximating the number of vehicles chosen by this optimization as a continuous variable will not lead to any significant difference in results (2.9E10 new LDV miles traveled in 2020 with an average annual mileage of 11,346 miles per vehicle [140] leads to about 2.6 million LDVs in 2030; the same methodology for the HDV vocations leads to at least 166 vehicles being chosen, assumed to be a sufficiently large quantity that integer numbers are unnecessary for the results expected). Additionally, as there is no explicit spatial consideration in this work, individual fueling stations are not considered, but instead analyzed as a continuous quantity of

fuel being distributed and dispensed with costs varying continuously as well. Therefore, there is no need to incur the added computational burden of modeling this problem as a MILP problem.

IBM's CPLEX software integrates well with MATLAB, so it is the software of choice. Additionally, the MATLAB toolbox YALMIP is used to set up the constraints of the optimization problem [293].

The variables that describe this problem are the fuel pathways and the vehicle types. Fuel pathways are differentiated by feedstock (and, when appropriate, feedstock separated by distinct selling price) and fuel production technology. Vehicles are differentiated by LDVs and each of the HDV vocations for all appropriate vehicle powertrain configurations. This leads to a total of 151 variables, 109 of which are for fuel production and 42 are for vehicles.

7.2 Cost Function

The cost function of TRACE is determined by the techno-economic data gathered and projection methods described in Chapters 4 and 5. Each fuel pathway and corresponding vehicle powertrain configuration will have an associated cost per amount of energy of fuel and correspondingly number of vehicles.

The cost function is generally split into two categories: (1) fuel feedstock, production, distribution, and dispensing; and (2) vehicles. The reason for this splitting is some fuels can be used in multiple vehicles. Separating into the two categories allows the modeling to independently select fuel production pathway and vehicle type without having to code each and every potential fuel and vehicle pathway. Note that a modeling constraint, to be introduced shortly, links the fuel variables to the vehicle variables.

One exception to the above is for PEVs. For PEVs, the electricity feedstock cost is calculated separately and both electricity distribution and dispensing costs are lumped with the PEV cost (recall that electricity production costs are incorporated into the feedstock cost). This is because electricity distribution and dispensing costs are dependent upon the level of charging power required by the PEV as noted in Chapter 4.4.1. For example, light-duty PHEVs and PFCEVs only require level 1 charging. Therefore, distribution costs are assumed negligible for these vehicles and dispensing costs are much lower than scenarios that require level 2 or level 3 dispensing. Due to these infrastructure cost differences, the distribution and dispensing costs are grouped with the vehicle cost so the appropriate numbers are used.

The TRACE cost function is presented in Equation 13. This cost function is minimized for each timestep (i.e. 2020 to 2050 in five year increments). After each timestep, costs and efficiencies are updated as noted in the last section of this chapter.

Equation 13. TRACE cost function

$$\min\left(\sum_{i,j,k,m,t}\left(\frac{feedstock_{i,t}+\frac{\left(\frac{(production_{j,t}*CRF)+FOM_j}{CF_i*8760\frac{h}{yr}}+VOM_j\right)}{0.0036\frac{GJ}{kWh}}}{\eta_{production,j,t}*\eta_{distribution,k}*\eta_{dispensing,m}}+\frac{distribution_k}{\eta_{dispensing,m}}+dispensing_m\right)*x_{n,t}+\sum_{p,q,t}\left(\frac{vehicle_{p,t}*CRF}{aaVMT_q}\right)*y_{p,t}\right)$$

The sets, variables, and parameters used in Equation 13 are described in Table 29.

Table 29. Description of optimization problem sets, variables, and parameters for TRACE cost function

Sets	**Description**	**Units**
$i \in I$	Set of fuel feedstocks at each selling price	-
$j \in J$	Set of fuel production equipment technologies	-
$k \in K$	Set of fuel distribution methods	-
$m \in M$	Set of fuel dispensing methods	-
$n \in N$	Set of appropriate combinations for the fuel feedstocks, production technologies, distribution methods, and dispensing methods for fuel pathways	-
$p \in P$	Set of vehicle types including specific class, HDV vocation, and powertrain configuration	-
$q \in Q$	Set of vehicle class and HDV vocations	-
$t \in T$	Set of timesteps modeled	-
Variables	**Description**	**Units**
$x_{n,t}$	Fuel decision variable	GJ/yr
$y_{p,t}$	Vehicle decision variable	mi/yr
Parameters	**Description**	**Units**
$feedstock_{i,t}$	Cost of fuel feedstock i at timestep t	$/GJ
$production_{j,t}$	Cost of fuel production equipment j at timestep t	$/kW
CRF	Economic term to convert capital cost into annual payments	-
FOM_j	Cost of FOM for fuel production equipment j	$/kW-yr
VOM_j	Cost of VOM for fuel production equipment j	$/kWh
CF_i	Fraction of nameplate capacity a fuel production facility uses on average	-
$distribution_k$	Cost of fuel distribution method k	$/GJ
$dispensing_m$	Cost of fuel dispensing method m	$/GJ
$\eta_{production,j,t}$	Efficiency of fuel production equipment j at timestep t	-
$\eta_{distribution,k}$	Efficiency of fuel distribution method k	-
$\eta_{dispensing,m}$	Efficiency of fuel dispensing method m	-
$vehicle_{p,t}$	Cost of vehicle type p at timestep t	$
$aaVMT_q$	Average annual vehicle miles traveled by vehicle class and vocation q	Mi/yr

Note that for PEVs, as mentioned previously, the fuel distribution and dispensing costs of the electricity are grouped with the vehicle costs instead of with the fuel feedstock and production to accommodate different distribution and dispensing costs for the different levels of electric chargers appropriate for the different PEVs. These distribution and dispensing costs are

divided by the PEV's CD efficiency to convert from cost on a per mile energy basis to a per mile basis for consistency with the vehicle cost.

Both electrolytic fuels and biomass fuels can have different capacity factors, which could affect the cost of the associated fuel. For electrolytic fuels is a high capacity factor of 0.8, which depicts a scenario in which P2G is run nearly continually to maximize the usage and fuel output. This is most appropriate for use with the distribution electricity grid with a mix of both renewable and non-renewable resources, which fits the data from E3 detailed in Chapter 4.1.1. Using the high capacity factor decreases capital cost of fuel production equipment compared to fuel output. For biomass feedstocks, a 0.8 capacity factor is also used, assuming a relatively high biomass throughput to capitalize on the biofuel production plants purchased but also allowing for downtime of repairs and other necessary upkeep. Later scenarios detailed in Chapter 8 will determine the effect of capacity factor on cost, which is most relevant for electrolytic fuels due to the decreased cost of electricity that could accompany a low-capacity factor P2G plant. Biomass cost is not as dependent on capacity factor as electricity cost is.

7.3 Constraints

The emissions regulations, VMT requirements, realistic technology growth rates, and feedstock availability from Chapter 6 compose the major constraints of TRACE. These and the rest of the constraints included are given in Equation 14 through Equation 22.

The first constraint, Equation 14, ensures that both fuel production and vehicle adoption are positive and finite values to ensure they make physical sense.

Equation 14. Constraint: Positive and finite values for fuel production and vehicle adoption

$$0 \leq x_{n,t}, y_{p,t} \leq 1e15$$

Next, Equation 15 ensures VMT for LDVs and each HDV vocation are met.

Equation 15. Constraint: VMT requirement

$$\sum_{p,t} y_{p,t} = VMT_{p,t}$$

Equation 16 constrains fuel production to respect the amount of feedstock that is available at each timestep.

Equation 16. Constraint: Feedstock capacity

$$\sum_{i,j,k,m,n,t} \frac{x_{n,t}}{\eta_{production,j,t} * \eta_{distribution,k} * \eta_{dispensing,m}}$$

$$\leq feedstockCapacity_{i,t} \;\; for\ each\ x_{n,t} that\ uses\ feedstock\ i$$

Equation 17 constrains fuel production equipment adoption to limits established from the literature in Chapter 6.3.

Equation 17. Constraint: Fuel production equipment technology capacity

$$\sum_{i,j,k,m,n,t}^{n} \frac{x_{n,t}}{CF_i * \eta_{production,j,t} * \eta_{distribution,k} * \eta_{dispensing,m}}$$

$$\leq \; productionCapacity_{j,t}\ for\ each\ x_{n,t} that\ uses\ production\ technology\ j$$

Equation 18 links fuel production to VMT to ensure there is no excess fuel production that is not used in a vehicle, or any vehicle that is produced that does not have fuel to power it.

Equation 18. Constraint: Fuel and vehicle pairing

$$\sum_{n,t} x_{n,t} = \frac{y_{p,t}}{\eta_{vehicle,p,t}} \; for\ every\ corresponsing\ fuel\ that\ can\ be\ used\ in\ each\ vehicle\ type$$

Equation 19 acts as the market release of heavy-duty BEVs, FCEVs, and PFCEVs in 2025.

Equation 19. Constraint: HDV future powertrain availability

$$y_{p=HDV\ BEV,t=2020} = 0$$

$$y_{p=HDV\ FCEV,t=2020} = 0$$

$$y_{p=HDV\ PFCEV,t=2020} = 0$$

Equation 20 limits the amount of VMT that can be met by BEVs for LDVs and heavy-duty linehaul and drayage vocations to account for range limitations as detailed in Chapter 6.2.

Equation 20. Constraint: BEV range limitation

$$y_{p=LDV\ BEV,t} \leq 0.61 * y_{LDV,t}$$

$$y_{p=HDV\ linehaul\ BEV,t} \leq 0.6 * y_{HDV\ linehaul,t}$$

$$y_{p=HDV\ drayage\ BEV,t} \leq 0.25 * y_{HDV\ drayage,t}$$

Equation 21 sets limits on GHG emissions according to the legislation and Executive Order of Chapter 6.1.

Equation 21. Constraint: GHG emissions limits

$$\sum_{j,k,m,n,t} \frac{x_{n,t}}{\eta_{production,j,t} * \eta_{distribution,k} * \eta_{dispensing,m}} * EF_{n,t} + \sum_{p,t}^{n} \frac{y_{p,t}}{\eta_{vehicle,p,t}} * EF_{p,t}$$

$$+ legacyGHG_t \leq limitsGHG_t$$

Lastly, the use of CRFs to turn capital costs into annual payments requires that TRACE continues to use fuel production equipment if it is adopted. Otherwise, it is conceivable that TRACE might select a fuel production technology for one timestep but stop using it in the next timestep. This is akin to signing up for a three year car lease, making one month's payment for using it, and then returning the car and neglecting the rest of the lease contract. This would not be acceptable, so Equation 22 is implemented to ensure the large capital investments of fuel production plants are used for their lifetime. The lifetime of the equipment used is expected to be long enough to last the timeframe of this problem (at most 30 years if adopted in 2020), which for some technologies is aided by regular upkeep costs as part of the FOM and VOM costs [66], [120], [244], [294].

Equation 22. Constraint: Continued fuel production plant use

$$x_{i,t} \geq x_{i,t-1} \; for\ each\ individual\ production\ technology\ type$$

Any additional parameters included in Equation 14 through Equation 22 not described in Table 29 are described in Table 30.

Table 30. Description of additional optimization parameters for TRACE constraints

Parameters	Description	Units
$VMT_{p,t}$	VMT requirement for vehicle type p at timestep t	Mi/yr
$feedstockCapacity_{i,t}$	Capacity of feedstock i at timestep t	GJ/yr
$productionCapacity_{j,t}$	Capacity of production technology j at timestep t	GJ/yr
$\eta_{vehicle,p,t}$	Vehicle efficiency of vehicle type p at timestep t	mi/GJ
$EF_{n,t}$	GHG emission factor for fuel production pathway n at timestep t	
$EF_{p,t}$	GHG emission factor for vehicle type p at timestep t	
$legacyGHG_t$	GHG tailpipe emissions from on-road vehicles made prior to 2020 at timestep t	
$limitsGHG_t$	GHG emission limits in California from legislation and Executive Order at timestep t, adjusted for the transportation sector and only the vehicle types modeled in TRACE assuming equal reduction economy-wide	

7.4 Cost and Efficiency Updates

After each timestep of optimization in TRACE, fuel production technology and vehicle component costs are updated based on Wright's Law (Equation 6). The cumulative installed capacity of every piece of technology is increased by the quantity of each that TRACE determines is the lowest cost option of meeting the constraints. Recall that vehicle costs are split into major powertrain components and the glider that remains to account for different learning rates of the various equipment within the vehicle.

Additionally, efficiencies of each vehicle technology are increased after each timestep. The efficiency projections for each fuel production technology are detailed in Chapter 4.2. The efficiency improvements of each vehicle technology are those detailed in Chapter 5.1, namely 1.15 MPGGE improvement every five years for LDVs [268] and 1.0 MPPGE improvement every five years for HDVs [269]. Note that these efficiency improvements are an approximation for those detailed in Chapter 4.

8. OPTIMAL FUEL AND VEHICLE DEPLOYMENT

This chapter analyzes the Reference Case, which is included to have a comparison for TRACE results, as well as the TRACE results. Default parameters are used at first for a baseline result of what future transportation sector could look like when adopting clean fuels and meeting all constraints outlined in Chapter 7.3. Additionally, some additional constraints are imposed and several sensitivity analyses are conducted to exercise TRACE in interesting ways and gather insight into factors that affect transportation technology evolution.

8.1 Reference Case

The Reference Case which serves as a comparison for TRACE optimization results uses conventional fossil gasoline, diesel, and natural gas as fuels and ICVs for all vehicle types. For this Reference Case, all LDVs use gasoline as fuel, 47% of refuse HDVs use natural gas as found in EMFAC 2020 projections [141], and the rest of the refuse HDVs as well as all other vocations of HDVs use diesel.

The Reference Case handles vehicle efficiency and cost the same as detailed for TRACE. All ICVs have the same improved efficiencies over time as described in Chapter 5.1 and Chapter 7.4. The Reference Case uses the same starting cost of ICVs as detailed in Chapter 5.2 and applies Wright's Law on each vehicle component based on cumulative production for vehicle cost reductions. Emissions for the gasoline, diesel, and natural gas used in ICVs are from the GREET WTW Calculator [295]. This tool lists the WTW emissions for the fossil fuels of interest. These data are gathered on a per-energy basis so the modeled ICV efficiency can be incorporated.

Price of the fossil fuels is from U.S. Energy Information Administration Annual Energy Outlook 2019 [296], as shown in Figure 64. Note that the price for gasoline and diesel are very close to each other, while that of natural gas is much lower and shown on a secondary axis with values shown on the right of the figure. While cost and price are not the same, these fuel prices will be used as proxies for the cost of fossil fuel feedstock, production, distribution, and dispensing added together.

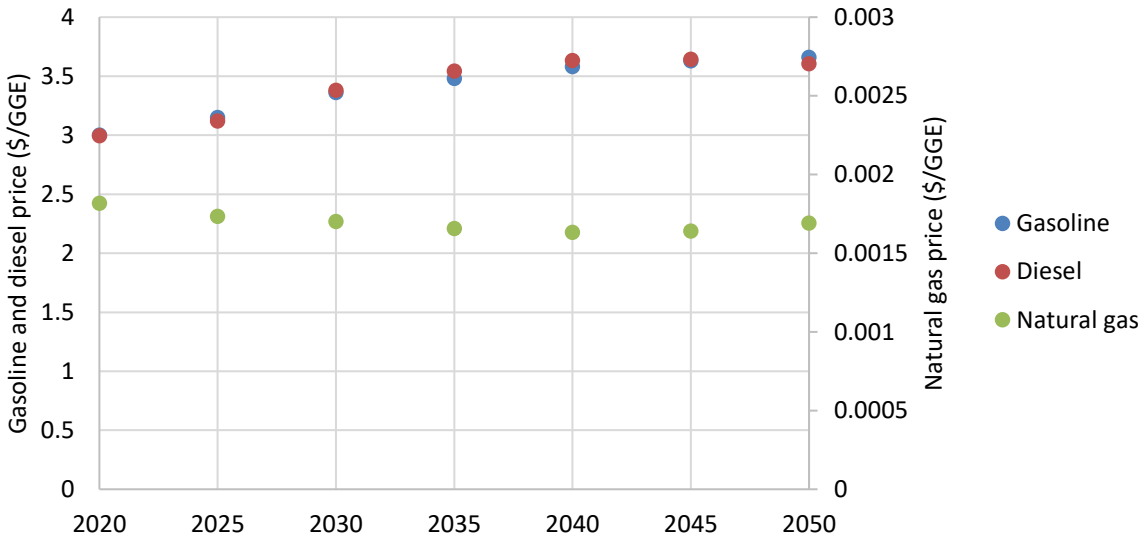

Figure 64. Fossil fuel price projections, data from [296]

To ensure a fair comparison with the TRACE cases, the cost of fuel for the legacy vehicles is not included and neither is the cost of the legacy vehicles themselves.

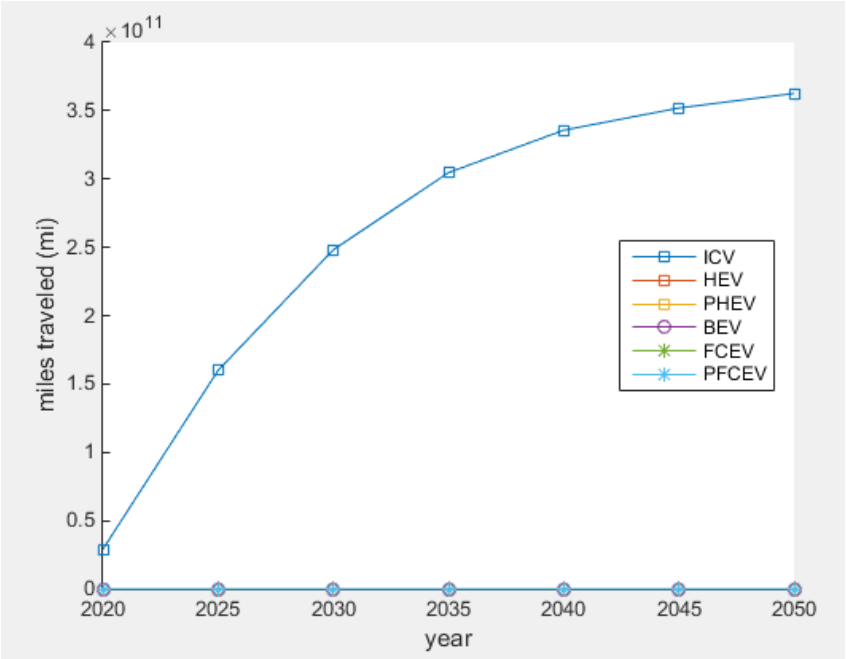

Figure 65. Reference Case LDV miles traveled

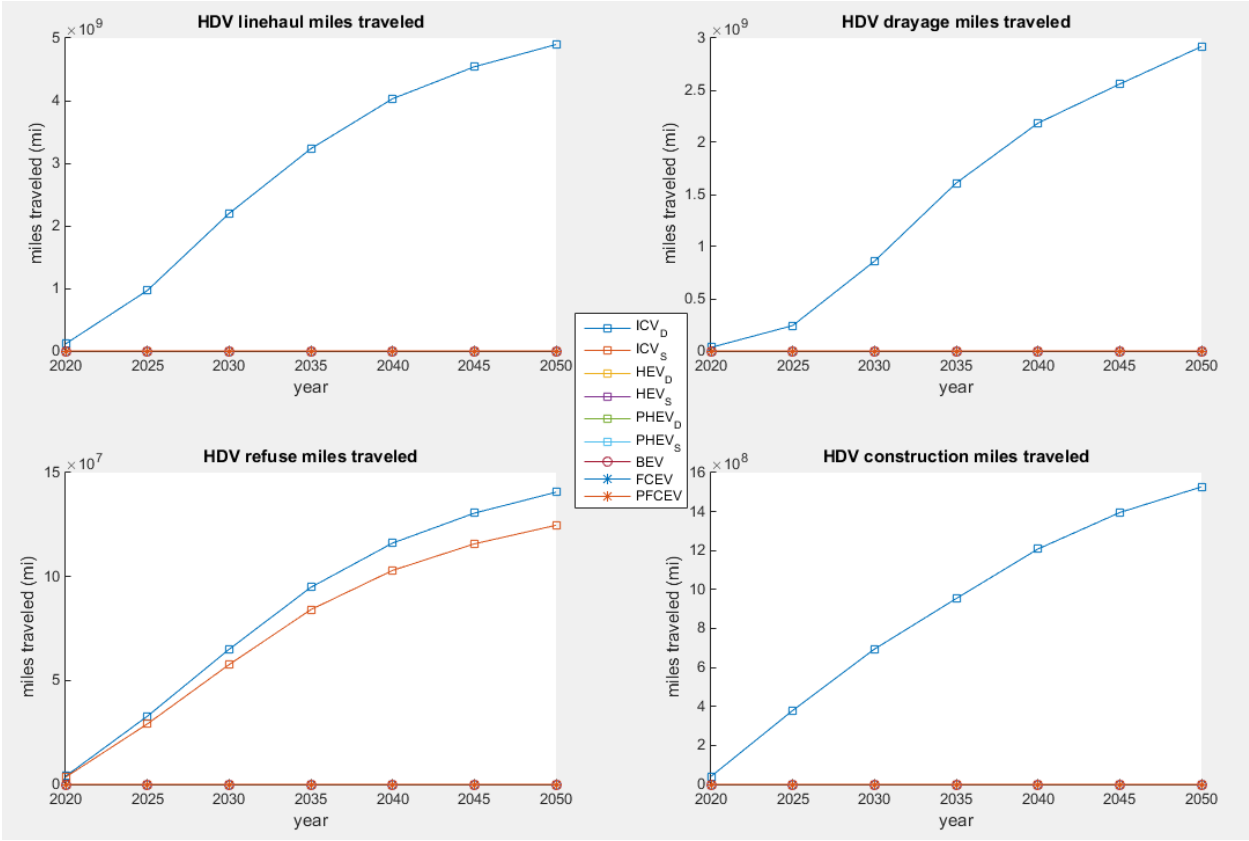

Figure 66. Reference Case HDV miles traveled by vocation

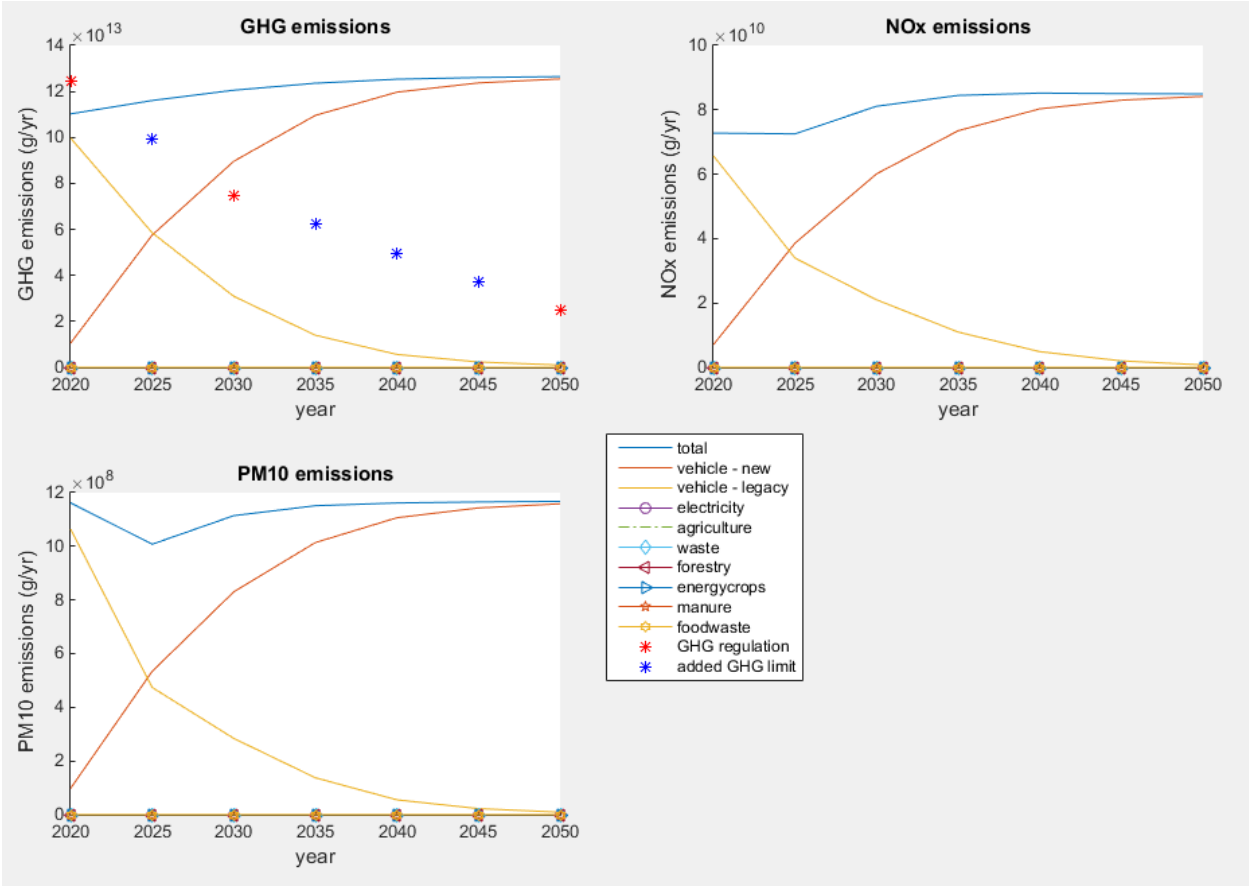

Figure 67. Reference Case emissions

Note that the GHG emissions legislation and Executive Order are not met, except for the constraint at 2020. Therefore, this Reference Case would not be acceptable in California.

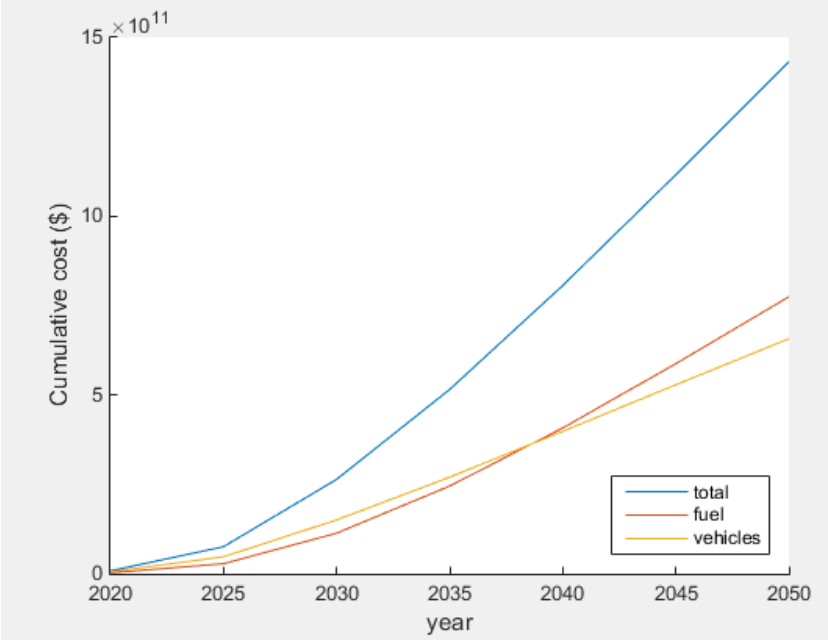

Figure 68. Reference Case cumulative cost

8.2 TRACE Non-ZEV Constrained Case

TRACE results with the default techno-economic data and constraints of Chapters 4 through 6 without ZEV requirements are presented below.

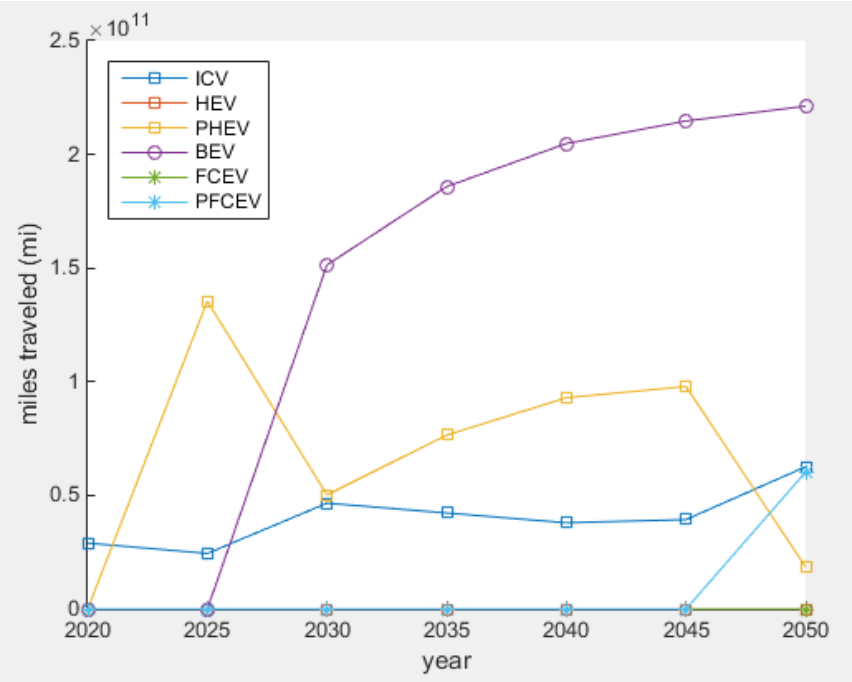

Figure 69. TRACE Non-ZEV Constrained Case LDV miles traveled

LDVs have a continual baseline of ICVs. PHEVs are adopted significantly beginning in 2025, and BEVs begin to be the major LDV choice in 2030. PFCEVs are adopted in significant quantity in 2050.

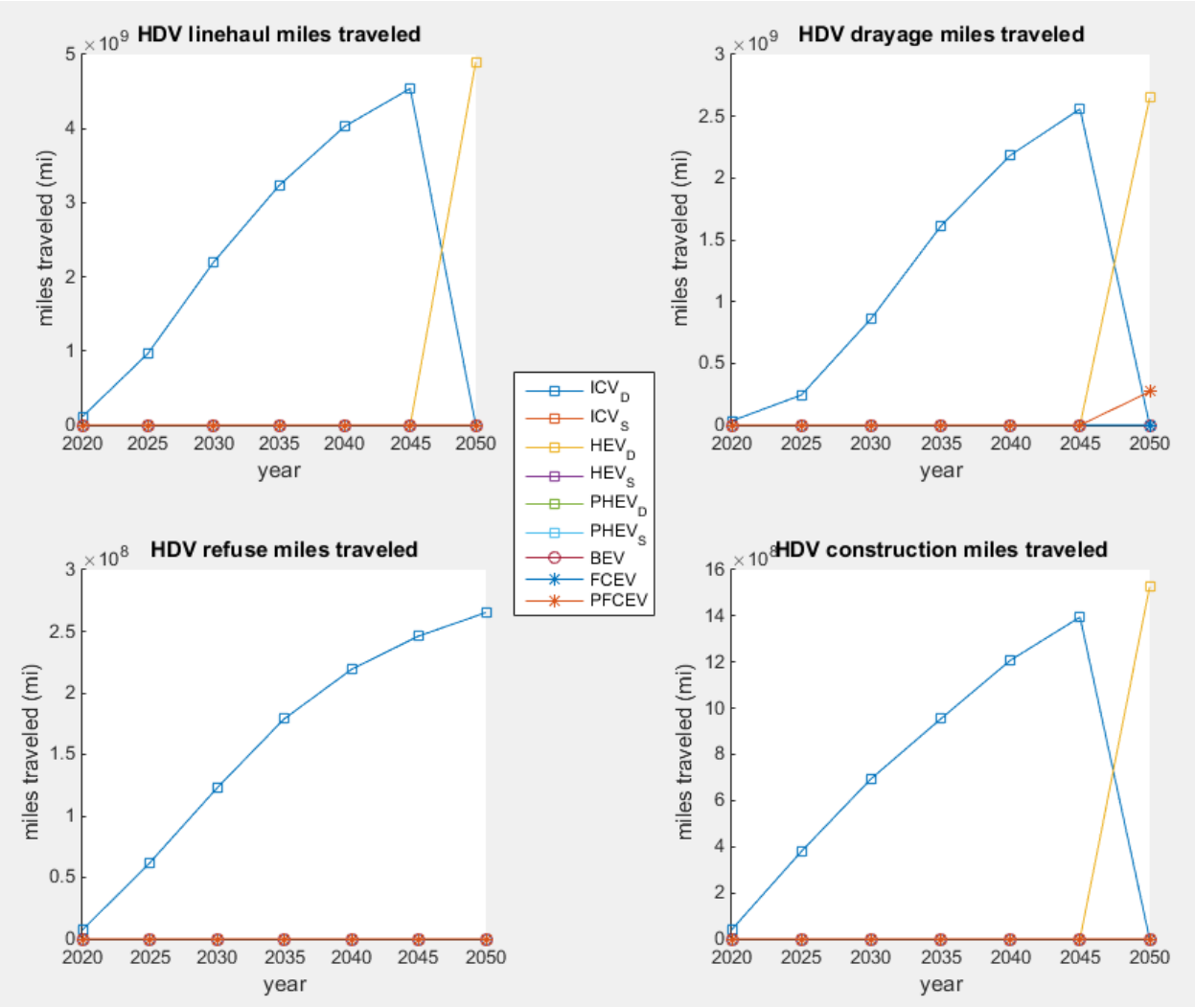

Figure 70. TRACE Non-ZEV Constrained Case HDV miles traveled by vocation

HDVs of all vocations are composed solely of diesel-fueled ICVs up to and including in 2045. In 2050, diesel-fueled HEVs are the dominant or sole powertrain option for all vocations except refuse. PFCEVs are also adopted for drayage trucks in somewhat significant quantities in 2050.

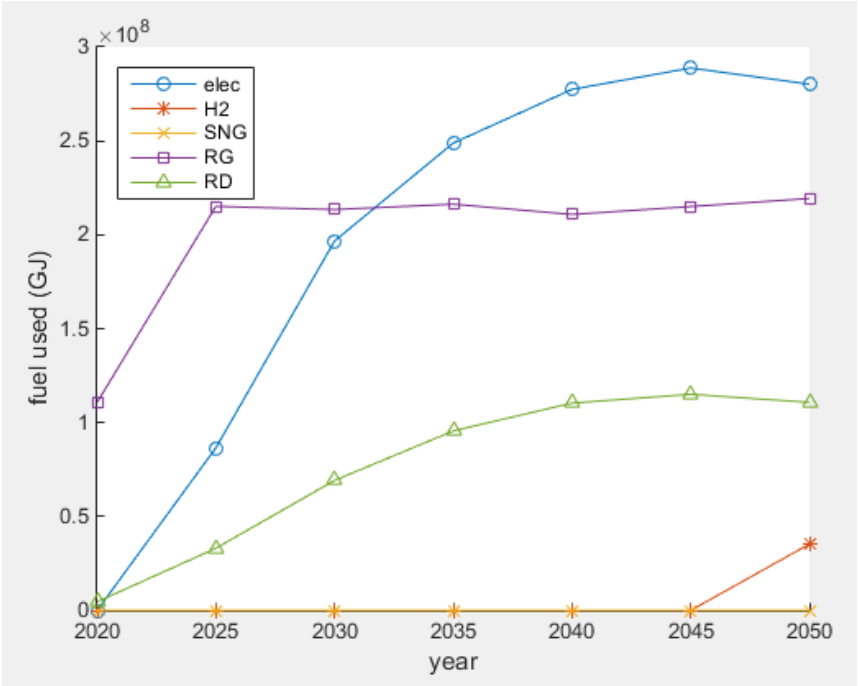

Figure 71. TRACE Non-ZEV Constrained Case fuels used

Fuel production follows the vehicle powertrains adopted for LDVs and HDVs. Renewable gasoline is produced to fuel the light-duty ICVs and PHEVs. Electricity is produced to fuel light-duty PHEVs and BEVs. Renewable diesel is produced to fuel heavy-duty ICVs. Hydrogen is produced to fuel the light- and heavy-duty PFCEVs in 2050.

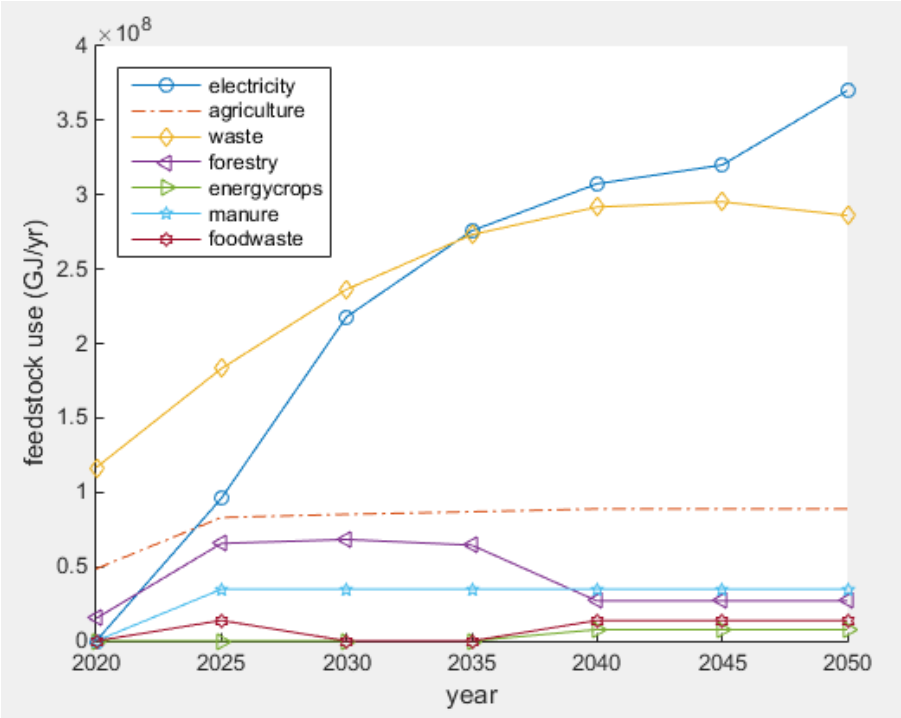

Figure 72. TRACE Non-ZEV Constrained Case feedstocks used

While waste begins as the most used fuel feedstock until 2030, electricity then becomes the most used fuel feedstock as LDVs are primarily BEVs in later years and LDVs have significantly higher VMT than HDVs. All biomass feedstock categories are used in various quantities throughout the years of simulation.

Even though manure has a very negative GHG emission factor, it is not used much in these results. This is because it is very expensive compared to waste, which is the most-used biomass feedstock. Manure is about twice as expensive as the lowest cost waste on an energy basis and 22% higher cost at waste's highest cost (recall that many of the biomass feedstocks have increasing cost as utilization increases). Therefore, TRACE finds another more cost-effective fuel and vehicle pathway using waste to meet GHG emissions constraints.

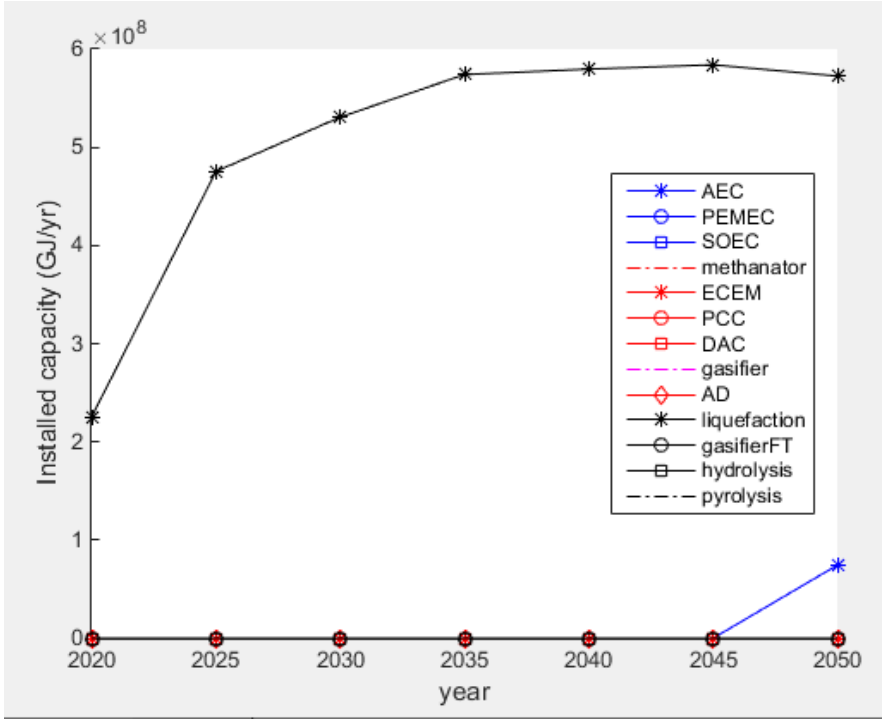

Figure 73. TRACE Non-ZEV Constrained Case fuel production equipment used

Liquefaction is the only fuel production equipment selected by TRACE up to 2045, and then in 2050 some AECs are used to produce hydrogen. Recall that while electricity needs to be produced to support the vehicle technologies as chosen by TRACE (particularly light-duty PHEVs and BEVs), the production of electricity is beyond the scope of this work and therefore electricity is considered only a feedstock. Liquefaction produces all of the renewable gasoline and diesel required by the LDVs and HDVs.

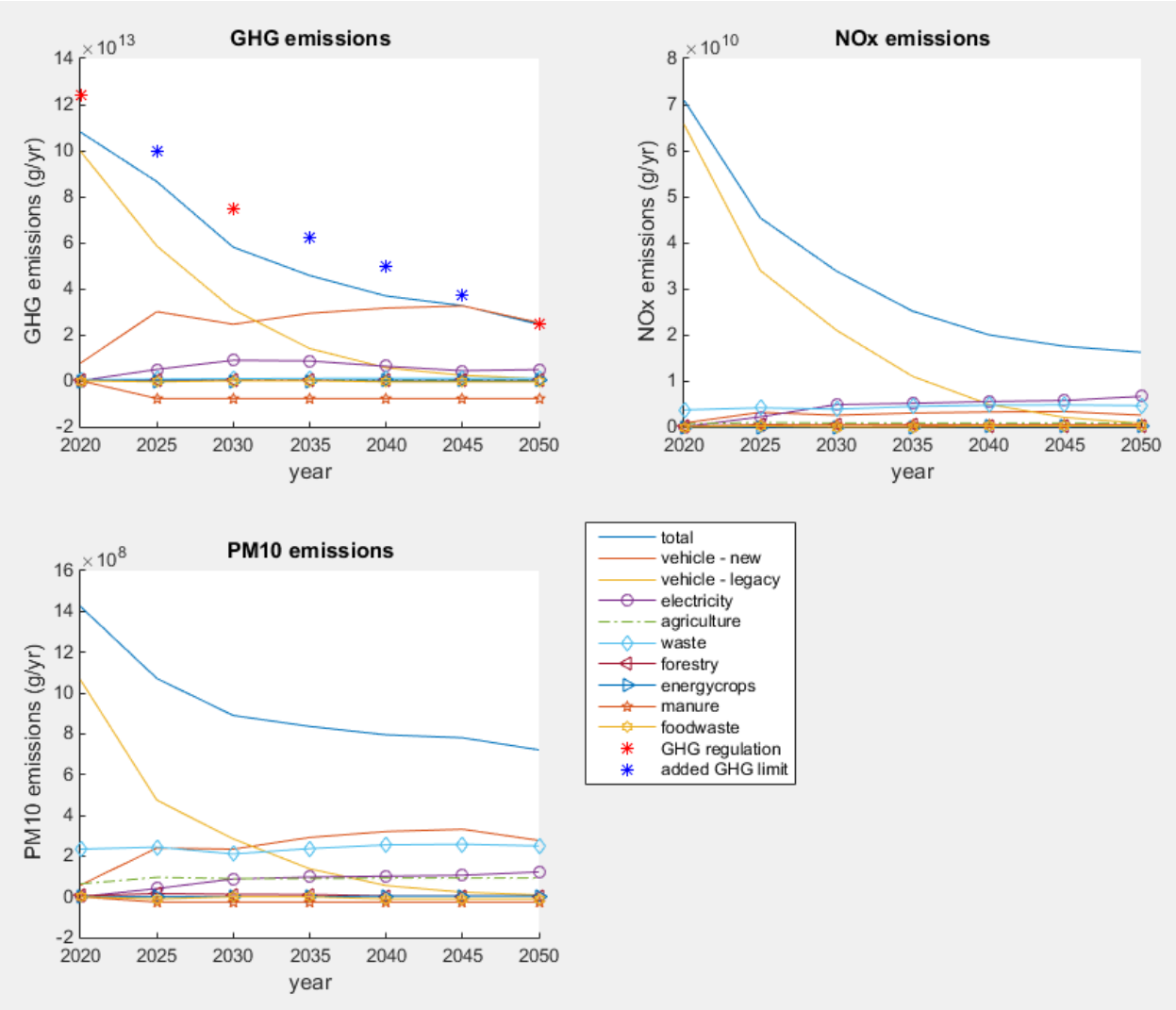

Figure 74. TRACE Non-ZEV Constrained Case emissions

GHG emissions goals are met, as they should be due to the constraints added. The year 2050 is modeled to just meet the goal, while the other years have some further GHG emissions reductions beyond the goals.

NO_x emissions are not modeled to have any constraint by default, but the technologies adopted significantly reduce NO_x emissions, by 80% in 2050 compared to 2020.

PM_{10} emissions are also not modeled to have any constraints by default, but the technologies adopted reduce PM10 emissions by 54% in 2050 compared to 2020.

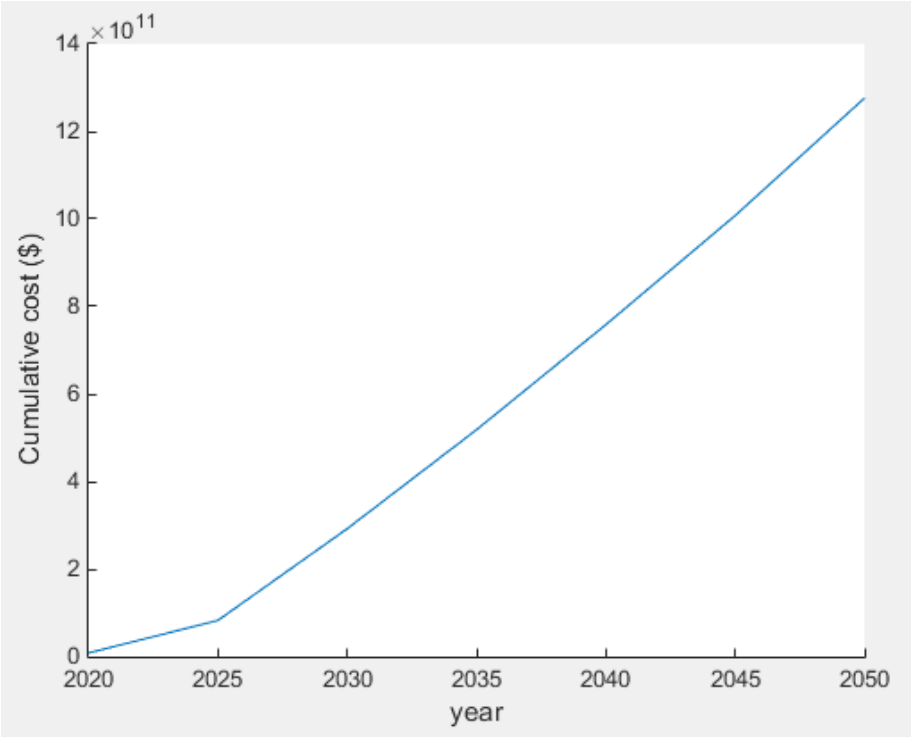

Figure 75. TRACE Non-ZEV Constrained Case cumulative cost

The total cumulative cost of this TRACE result out to 2050 is approximately $1.28 trillion.

To ensure the cost calculations are as desired and to get insight into why TRACE is making the illustrated choices, it is wise to pick some of the pathways and calculate those costs by hand. The LDV sector and linehaul HDVs are focused on here, and a selection of key fuels and feedstocks are included. See the selected costs on a per mile basis in Table 31 for LDVs and Table 32 for linehaul HDVs.

Table 31. LDV cost per mile of selected vehicles and fuel pathways in 2020

Vehicle fuel pathway	Feedstock cost ($/mi)	Production cost ($/mi)	Distribution cost ($/mi)	Dispensing cost ($/mi)	Vehicle cost ($/mi)	Total cost ($/mi)
BEV – CA electricity	0.013	0.000	0.002	0.017	0.455	0.487
FCEV – AEC, CA electricity	0.038	0.023	0.075	0.000	0.638	0.773
FCEV – gasifier, $30/dry ton agriculture	0.008	0.033	0.075	0.000	0.638	0.755
ICV – liquefaction, $30/dry ton MSW	0.005	0.077	0.006	0.000	0.189	0.277
PHEV – CA electricity and liquefaction, $30/dry ton MSW	0.010	0.030	0.001	0.000	0.290	0.331

Table 32. Linehaul HDV cost per mile of selected vehicles and fuel pathways in 2020

Vehicle fuel pathway	Feedstock cost ($/mi)	Production cost ($/mi)	Distribution cost ($/mi)	Dispensing cost ($/mi)	Vehicle cost ($/mi)	Total cost ($/mi)
BEV – CA electricity	0.143	0.000	0.026	0.902	0.443	1.514
FCEV – AEC, CA electricity	0.386	0.232	0.768	0.000	0.476	1.862
FCEV – gasifier, $30/dry ton agriculture	0.084	0.340	0.768	0.000	0.476	1.668
ICV – liquefaction, $30/dry ton MSW	0.035	0.530	0.040	0.000	0.176	0.780
PHEV – CA electricity and liquefaction, $30/dry ton MSW	0.033	0.510	0.038	0.000	0.214	0.795

Given the goal of TRACE is to minimize cost while meting environmental constraints, it is apparent that TRACE is selecting the cheapest technology (ICVs) to the extent possible before moving to a more expensive but less GHG-polluting option (PHEVs and BEVs). The extent to

which cost is sacrificed to achieve lower GHG emissions depends on the GHG emission constraint, which gets stricter as the years progress. Therefore, as time goes on, TRACE selects more BEVs which have lower GHG emissions than ICVs and PHEVs while maintaining a lower cost per mile than FCEVs at the default input values.

In 2025, GHG emissions constraints force adoption of PHEVs, which are more expensive than ICVs but have lower emissions. Then, in 2030, emissions constraints tighten and therefore BEVs are adopted, which have lower overall GHG emissions as legislation forces cleaner electricity as time progresses.

8.3 Comparison of Reference Case and TRACE Non-ZEV Constrained Case

Note that the results for the Reference Case and TRACE Non-ZEV Constrained Case are similar in cumulative cost. At first, the Reference Case is cheaper than the TRACE Non-ZEV Constrained Case. However, by 2035, the TRACE Non-ZEV Constrained Case begins to have lower cumulative cost than the Reference Case. By 2050, the Reference Case is 19% more expensive than the TRACE Non-ZEV Constrained Case results. See Table 33 and Figure 76 for the comparison of cumulative costs of the Reference Case and the TRACE Non-ZEV Constrained Case.

Table 33. Comparison of cumulative cost for Reference Case and TRACE Non-ZEV Constrained Case

	2020	**2025**	**2030**	**2035**	**2040**	**2045**	**2050**
Reference	8.16E+09	7.57E+10	2.64E+11	5.16E+11	8.06E+11	1.12E+12	1.43E+12
TRACE Non-ZEV Constrained	8.31E+09	8.27E+10	2.92E+11	5.18E+11	7.58E+11	1.01E+12	1.28E+12

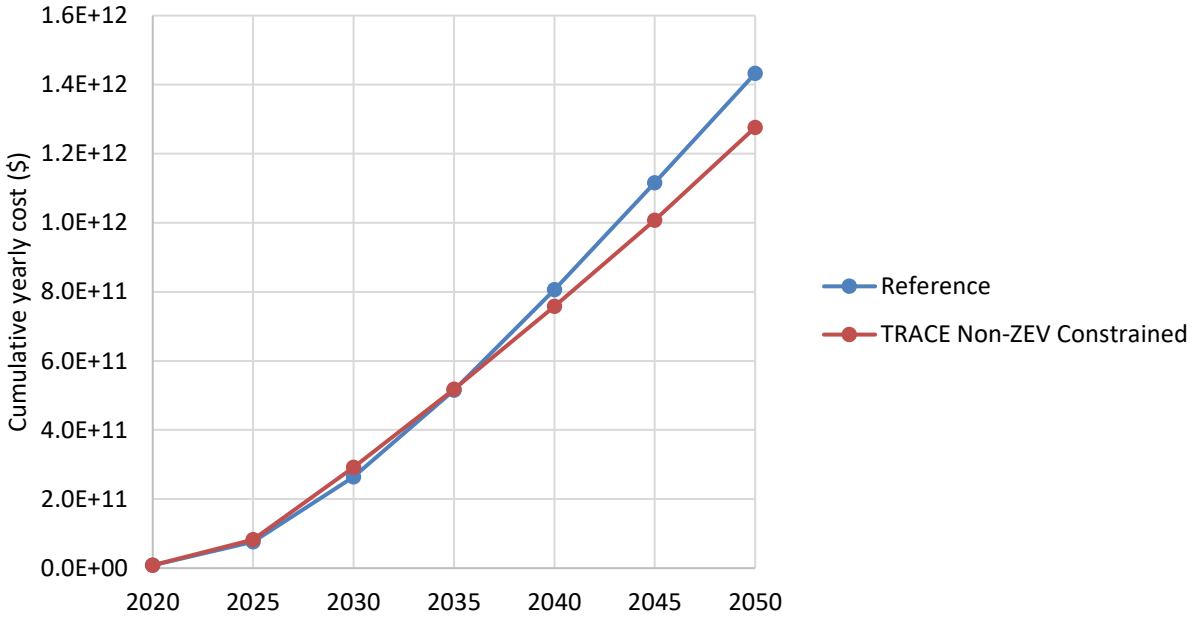

Figure 76. Comparison of cumulative cost for Reference Case and TRACE Non-ZEV Constrained Case

While it may seem surprising that it is cheaper to adopt clean and renewable fuels compared to fossil fuels, there is precedent for results similar to these. Offer et al. show that by 2030, both BEVs and PFCEVs have lower combined fuel and vehicle cost than ICVs, in the context of LDVs [163]. The University of California, Davis Institute of Transportation Studies has released a report that shows a sensitivity analysis that in some cases projects alternative HDVs (namely FCEVs, catenary vehicles, and vehicles with modest batteries and on-road charging) have lower cost per mile than conventional diesel ICVs [270]. The International Council on Clean Transportation notes that when excluding infrastructure costs, heavy-duty FCEVs and other alternative HDVs (the catenary and on-road charging configurations) have lower cost per mile than conventional diesel ICVs [297]. Therefore, if infrastructure costs for these alternative vehicles are low enough, it is conceivable that overall cost could be lower than ICVs operating on fossil diesel fuel.

Consider the fact that LDVs are fueled majorly by BEVs in the latter half of the TRACE Non-ZEV Constrained Case. LDVs have much higher VMT than any of the HDV vocations, so fuel and vehicle costs form a major portion of total cost. While BEVs are more expensive than ICVs currently, fueling a BEV is significantly cheaper than fueling an ICV with gasoline. From Figure 18 and Figure 64, both the electricity and fossil fuel costs are projected to increase modestly, so the current trend of cheap BEV fuel is modeled to continue in TRACE.

Regarding emissions for the TRACE Non-ZEV Constrained Case and the Reference Case, GHG emissions are reduced 80.6%, NO_x emissions are reduced by 83.2%, and PM_{10} emissions are reduced by 44.0% in the year 2050. Comparisons of each of these emissions between the Reference Case and the TRACE Non-ZEV Constrained Case results are displayed in Figure 77 through Figure 79.

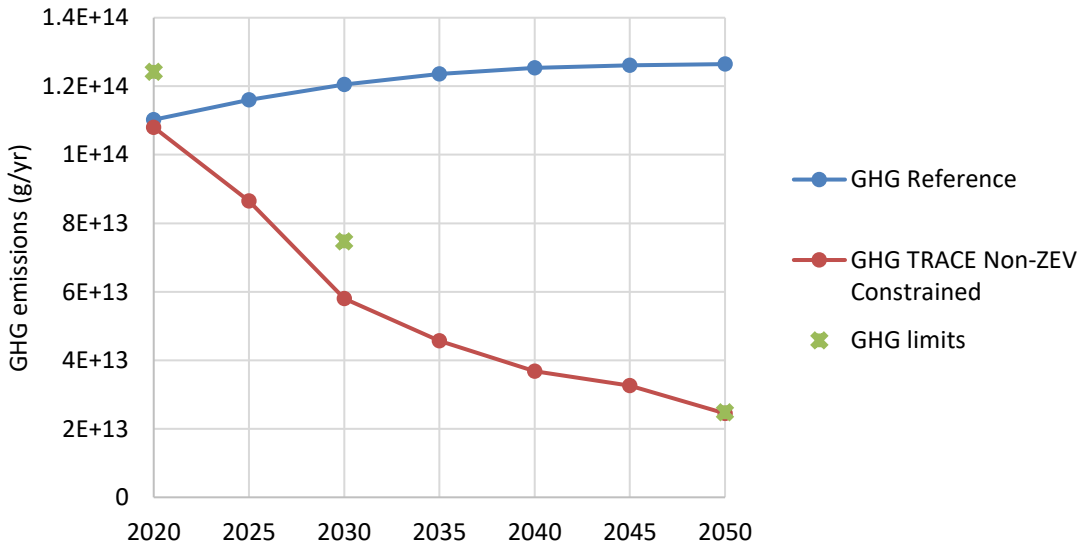

Figure 77. GHG emissions comparison between Reference Case and TRACE Non-ZEV Constrained Case

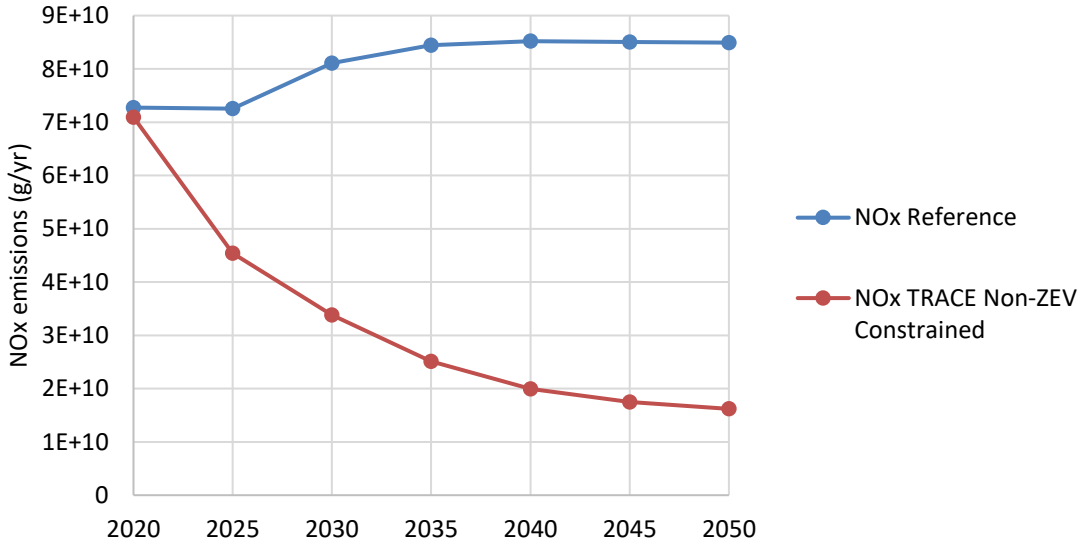

Figure 78. NO_x emissions comparison between Reference Case and TRACE Non-ZEV Constrained Case

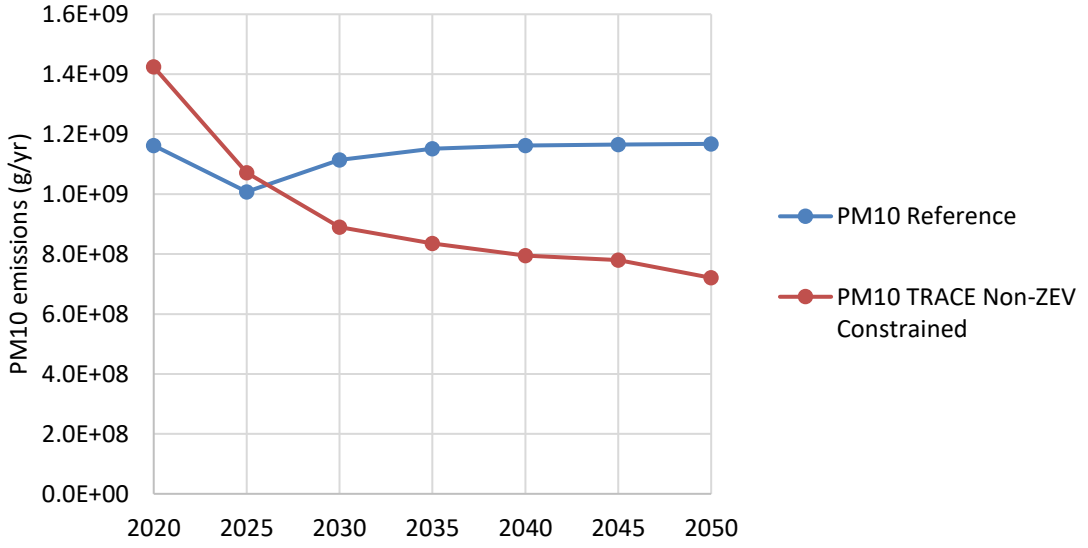

Figure 79. PM_{10} emissions comparison between Reference Case and TRACE Non-ZEV Constrained Case

8.4 Additional Constraints

The following are some additional constraints included to exercise TRACE and gather more insight beyond the default constraints included.

8.4.1 Effect of ZEV Constraints

While California has the goal in the form of Executive Order S-3-05 to reduce GHG emissions 80% below 1990 levels, it should be the ultimate goal of bringing GHG emissions down to zero. One step of achieving that goal is to require ZEVs.

Requiring all LDVs to be ZEVs increases costs in 2020 by 90%, and total cumulative cost is increased by 55% in 2050. This case projects 61% of LDVs to be BEVs and 39% to be PFCEVs. All HDVs are diesel ICVs. The result is 33.8% lower GHG emissions than required by Executive Order S-3-05 in 2050.

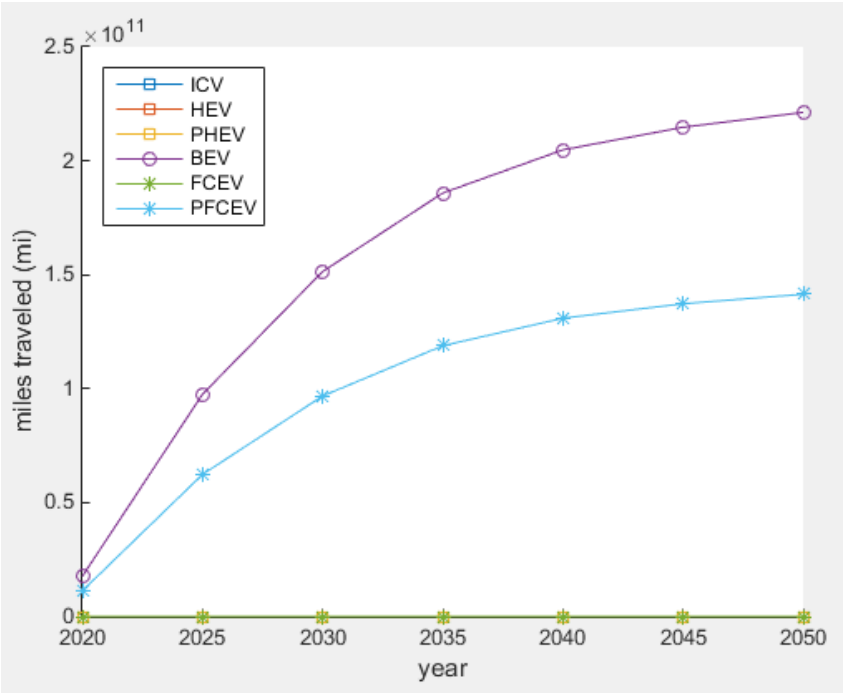

Figure 80. Light-duty ZEV constraint LDV miles traveled

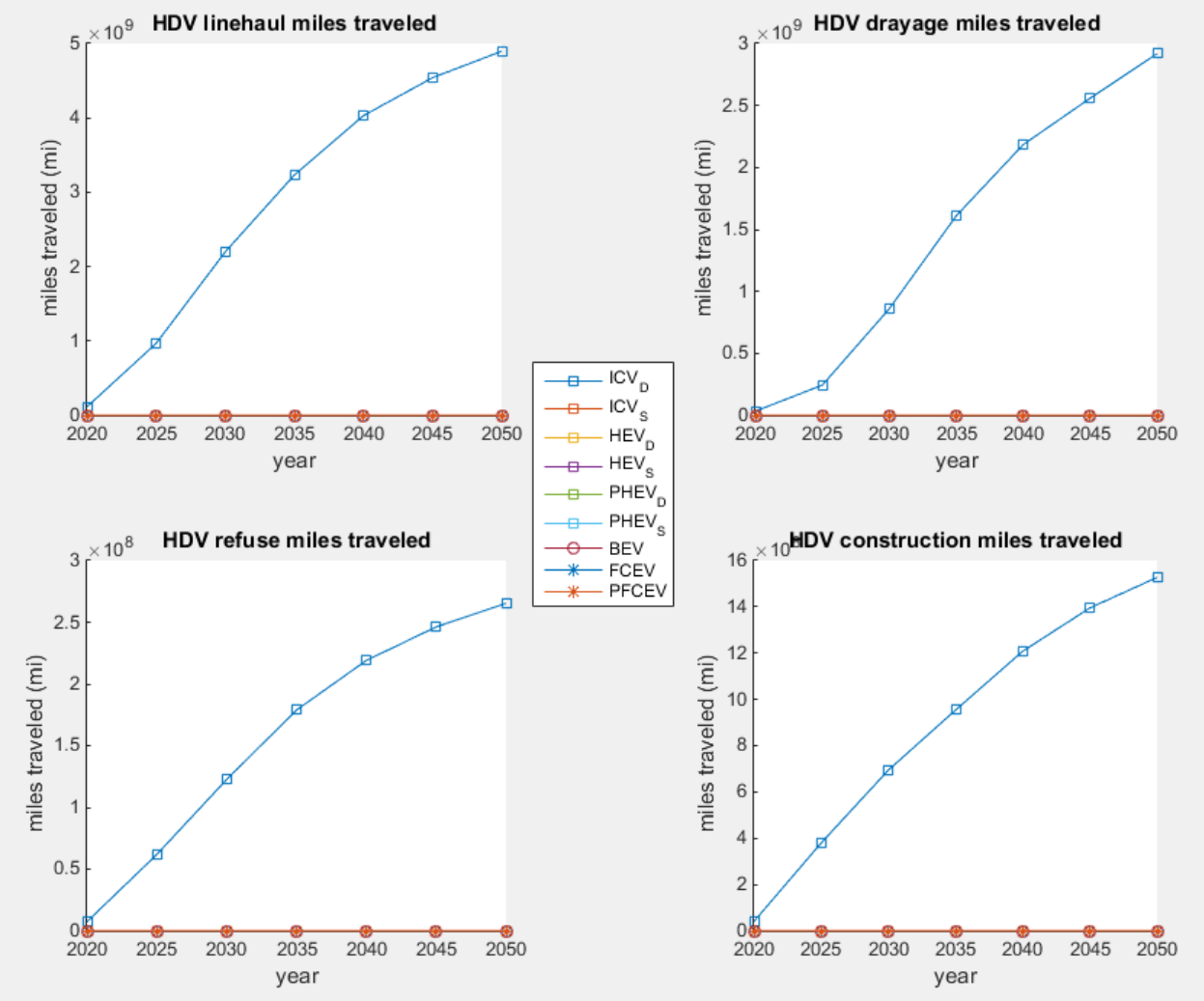

Figure 81. Light-duty ZEV constraint HDV miles traveled

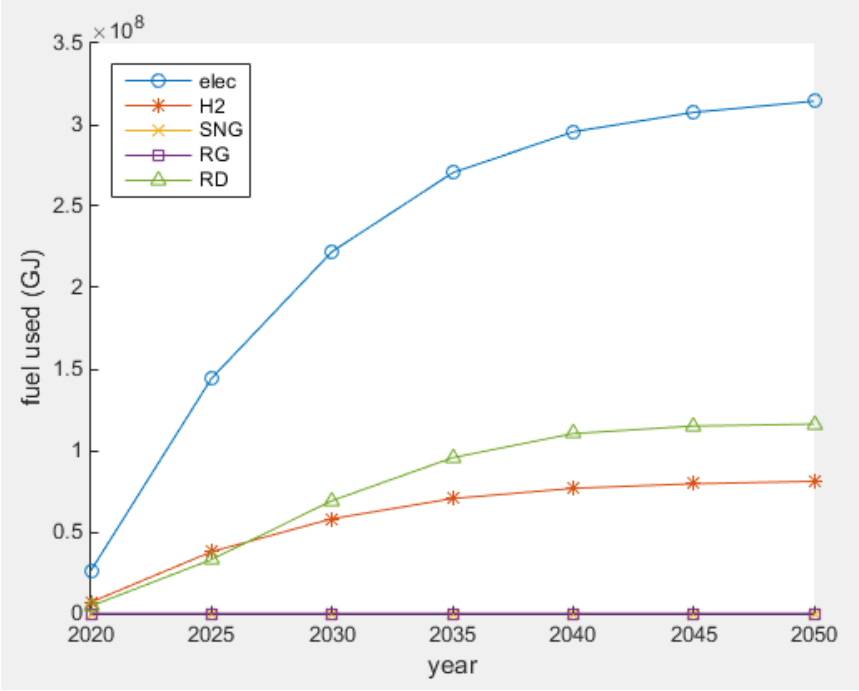

Figure 82. Light-duty ZEV constraint fuels used

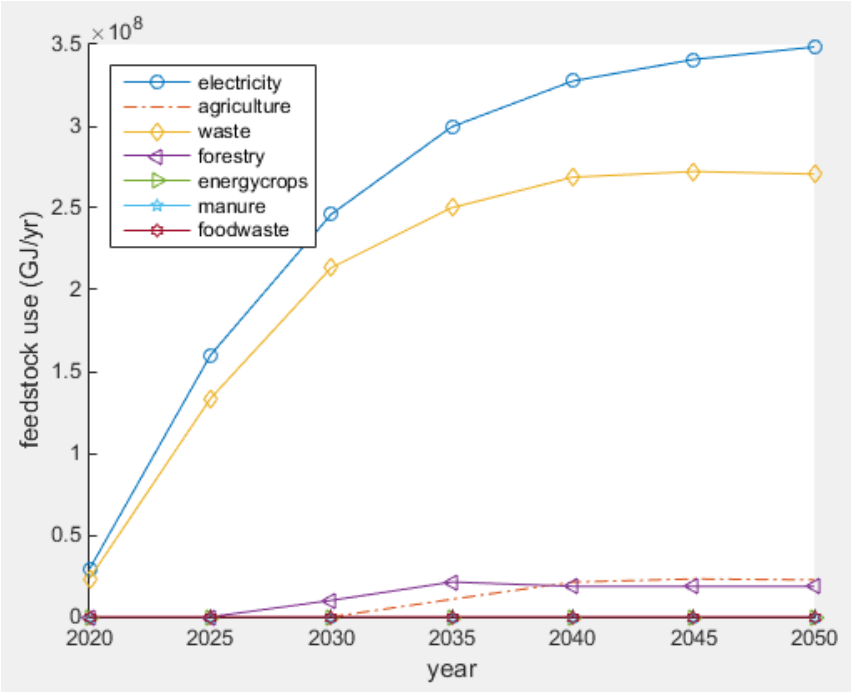

Figure 83. Light-duty ZEV constraint feedstocks used

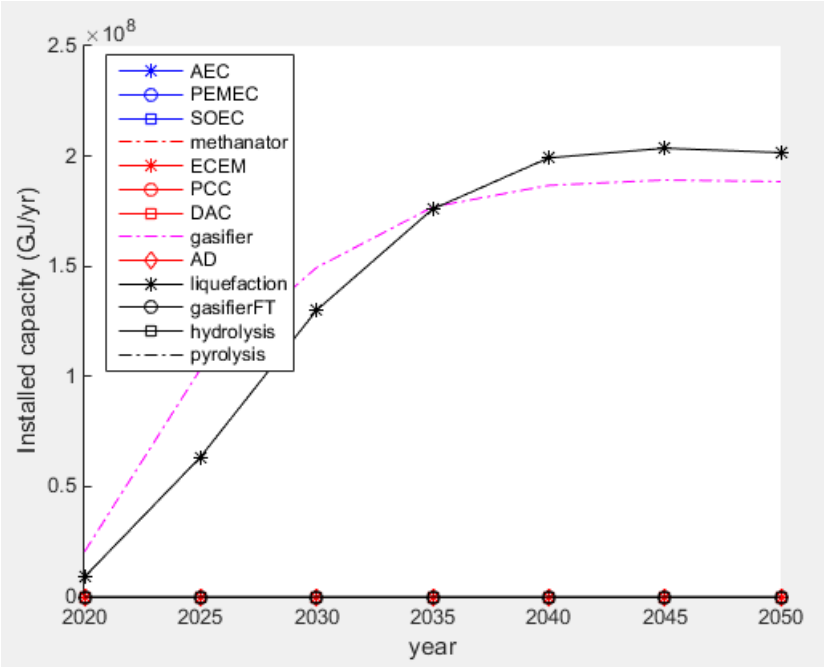

Figure 84. Light-duty ZEV constraint fuel production equipment used

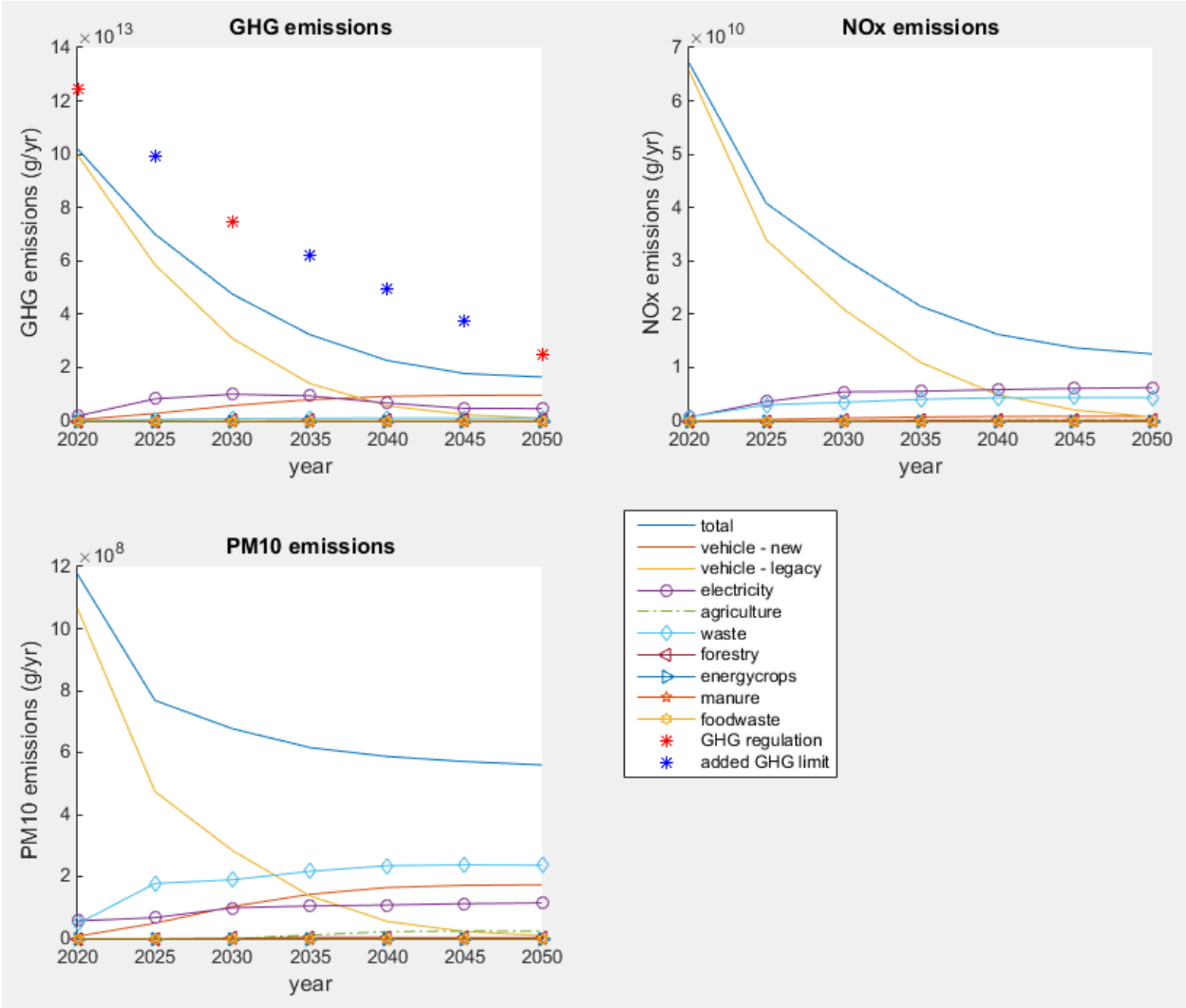

Figure 85. Light-duty ZEV constraint emissions

Requiring all vehicles to be ZEVs (which requires the removal of the constraint that no heavy-duty ZEVs are available until 2025) increases costs 91% compared to the default results, and total cumulative cost is increased by 59% in 2050. This case projects 61% of LDVs to be BEVs and 39% to be PFCEVs, as before in the light-duty ZEV constraint case. All HDVs are projected to be PFCEVs. Note the significant decrease in GHG emissions this case leads to, drastically undercutting the GHG emissions constraints, with 72.4% lower levels than Executive Order S-3-05 requires in 2050, as well as significant further PM_{10} and NO_x emissions reductions.

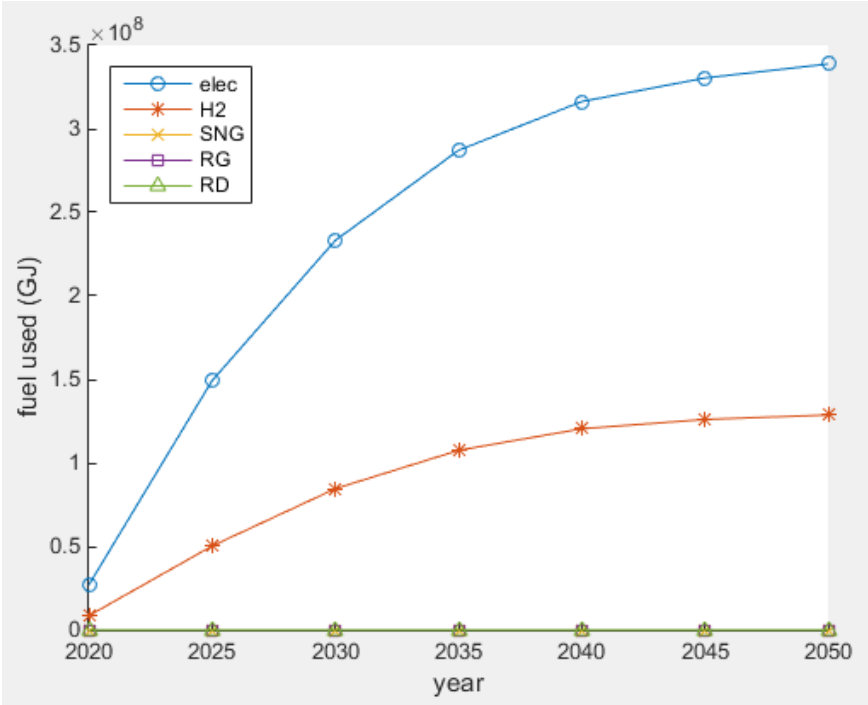

Figure 86. All ZEV constraint fuels used

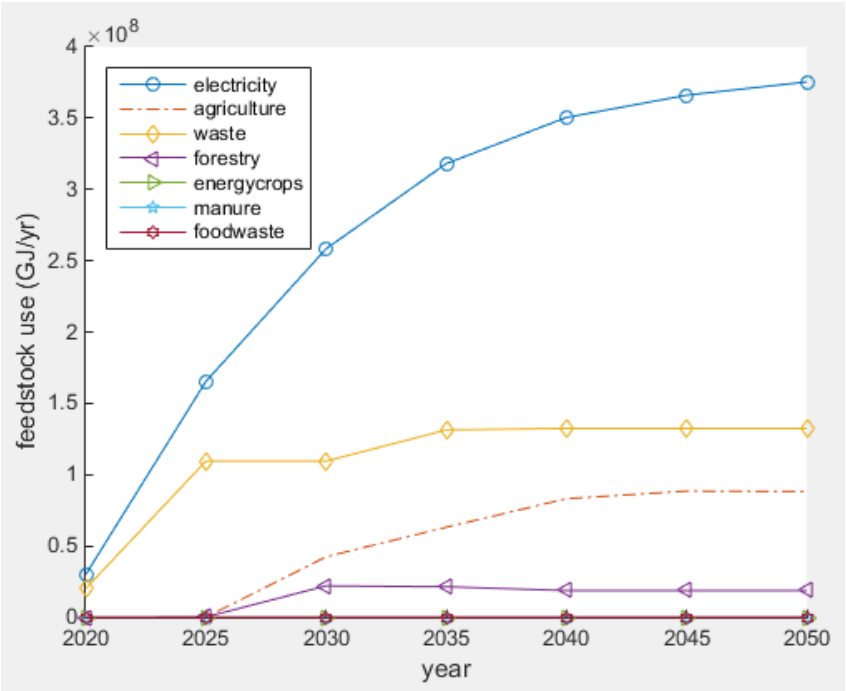

Figure 87. All ZEV constraint fuel feedstocks used

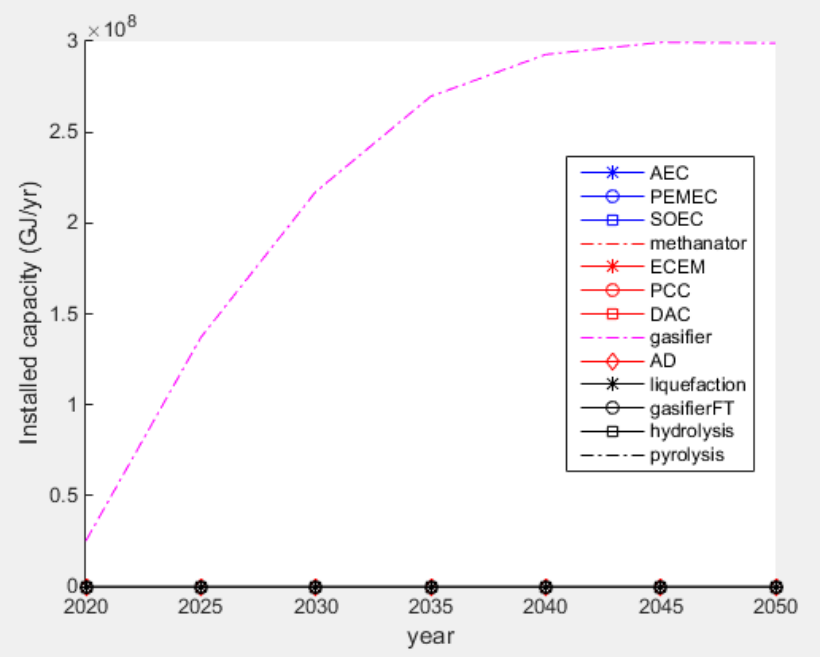

Figure 88. All ZEV constraint fuel production equipment use

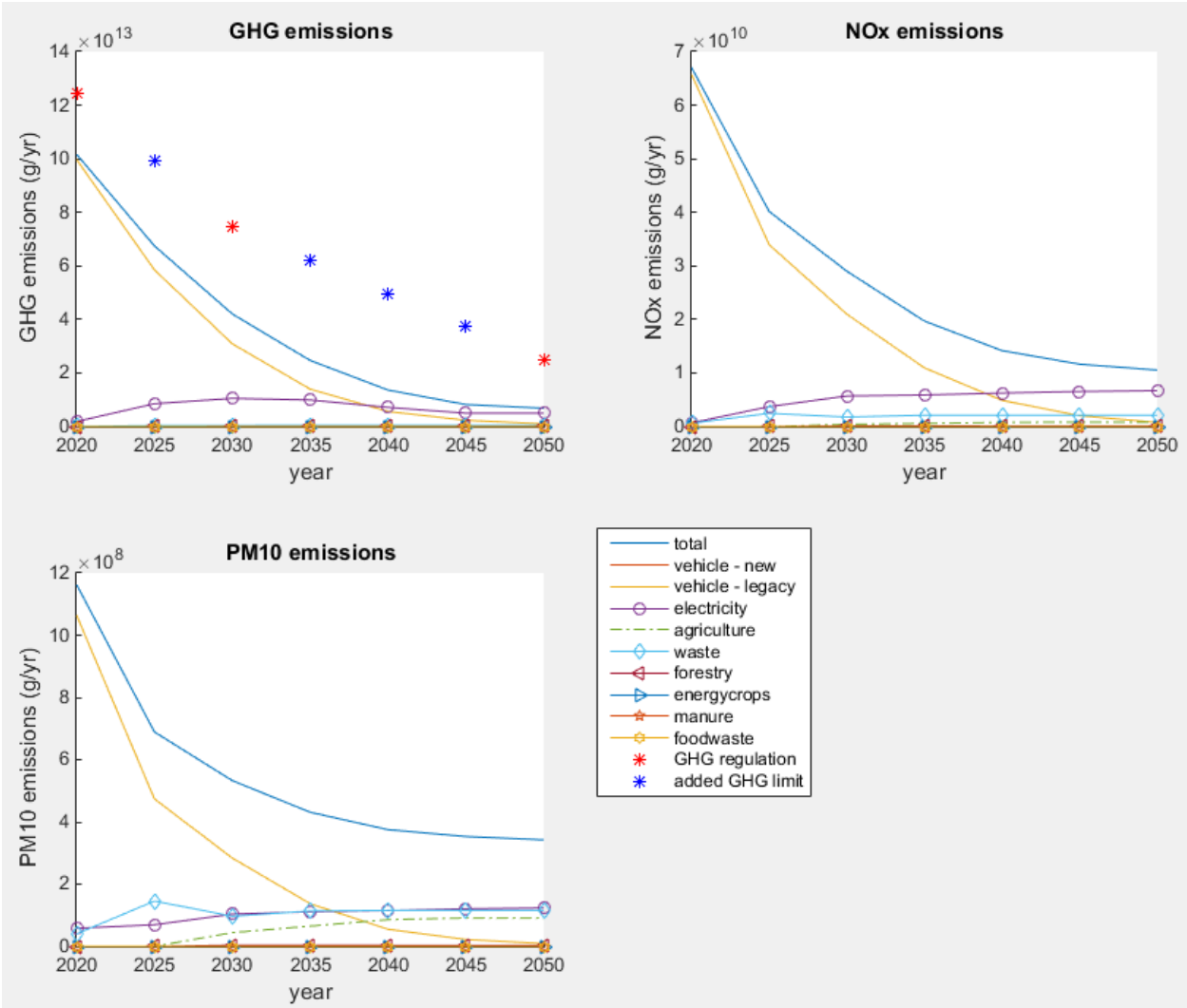

Figure 89. All ZEV constraint emissions

8.4.2 Effect of Drayage CAP Emissions Constraints

There are goals to reduce nitrogen oxide (NO_x) tailpipe emissions by 80% and diesel particulate matter (PM) tailpipe emissions by 45% by 2031 in the South Coast Air Basin (SoCAB) [298]. For the year 2035, 81% of drayage NO_x emissions and 82% of drayage PM_{10} emissions (these are the PM emissions 10 micrometers in diameter or smaller) in California are projected to be from ports in the SoCAB (Port of Los Angeles and Port of Long Beach) according to the California Air Resources Board Standard Emission Tool [299]. Therefore, due

to the high emissions impact of SoCAB drayage trucks on California drayage in general, the additional constraints of 80% NO_x tailpipe reductions and 45% PM_{10} tailpipe emissions by 2030, the modeled year closest to 2031 of the goal, are applied to all drayage trucks.

To get the baseline for these emissions for 2020, the default NO_x and PM_{10} emissions from EMFAC are determined to be 6,590 metric tons per year of NO_x and 40.7 metric tons per year of PM_{10}. NO_x emissions are assumed to decrease linearly to the 80% reduction goal in 2030, then are held constant afterward. PM_{10} emissions are assumed to decrease linearly to the 45% reduction goal in 2030, then are held constant afterward.

These constraints force the adoption of PFCEVs in 2030, first as secondary to diesel ICVs, but by 2035 PFCEVs become the main drayage HDV powertrain choice with the hydrogen produced by biomass gasifiers. LDVs are unaffected by these additional drayage CAP constraints. This case leads to a 0.48% increase in total cumulative cost in 2050.

Note that total emissions of both NO_x and PM_{10} are not affected as much as GHG emission reductions in other scenarios (1.81% reduction for NO_x and 4.51% reduction for PM_{10} in 2050) due to the relatively low portion of VMT from drayage HDVs compared to LDVs. However, recall that CAP emissions are a local issue, and reductions in areas with high CAP emissions and high population would be greatly served by reductions such as these.

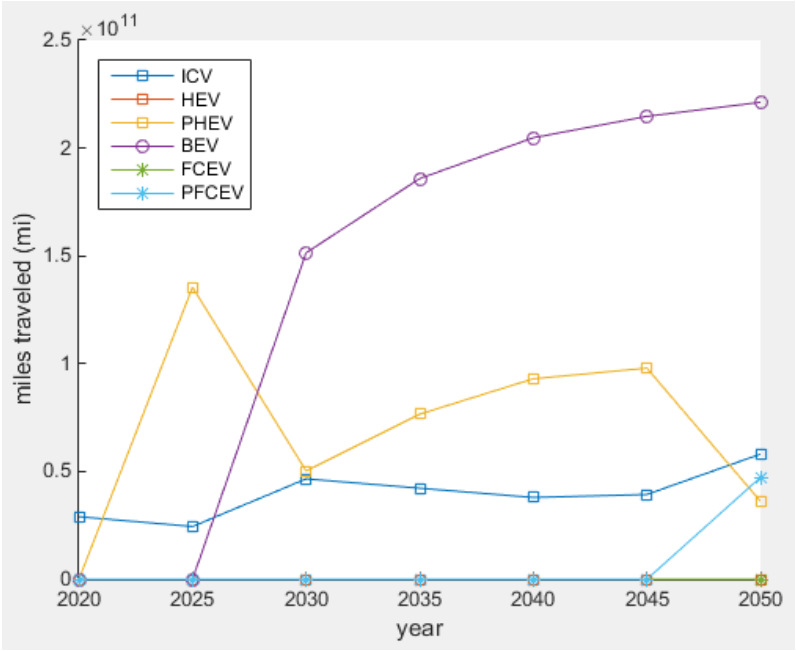

Figure 90. Drayage CAP emissions constraints LDV miles traveled

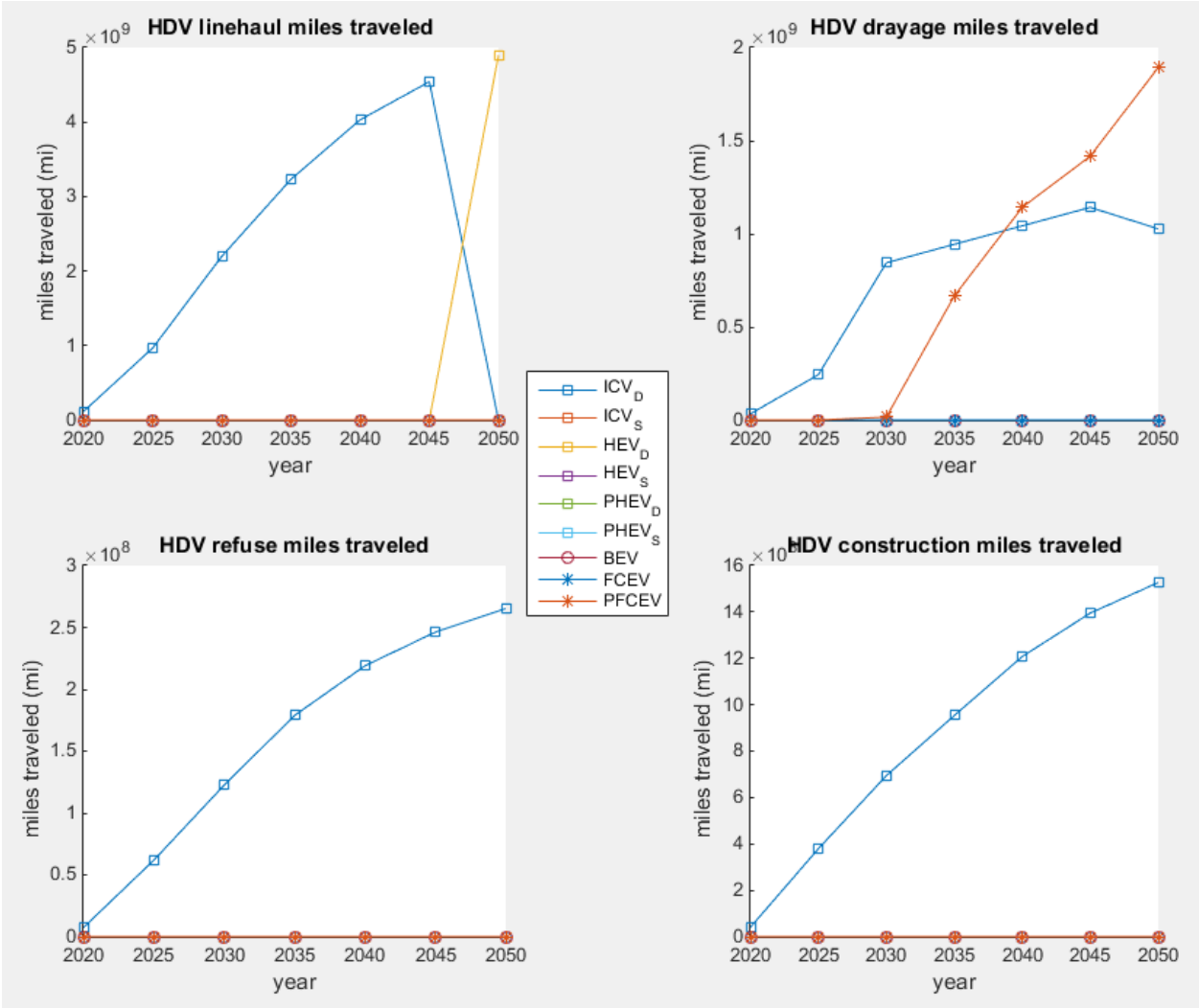

Figure 91. Drayage CAP emissions constraints HDV miles traveled

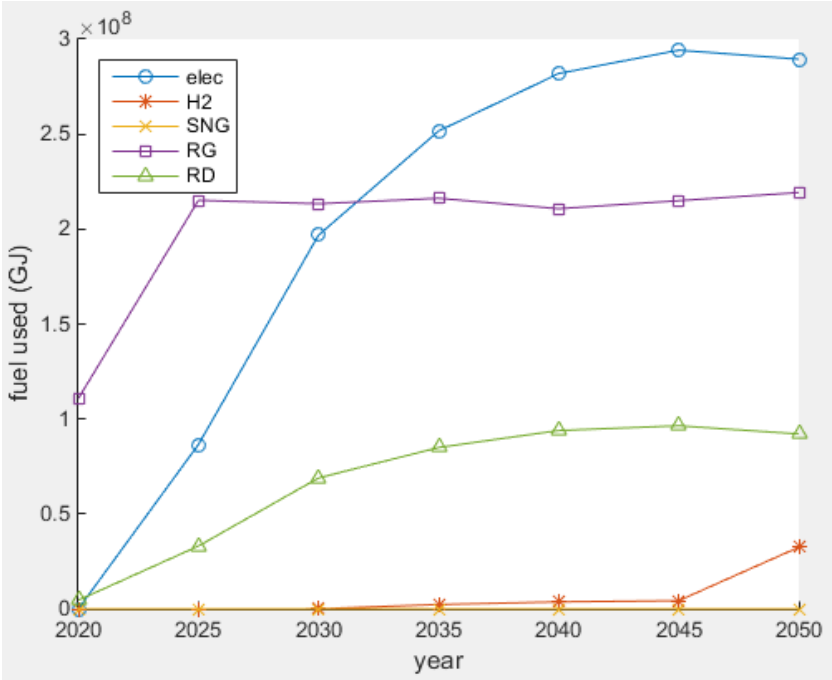

Figure 92. Drayage CAP emissions constraints fuels used

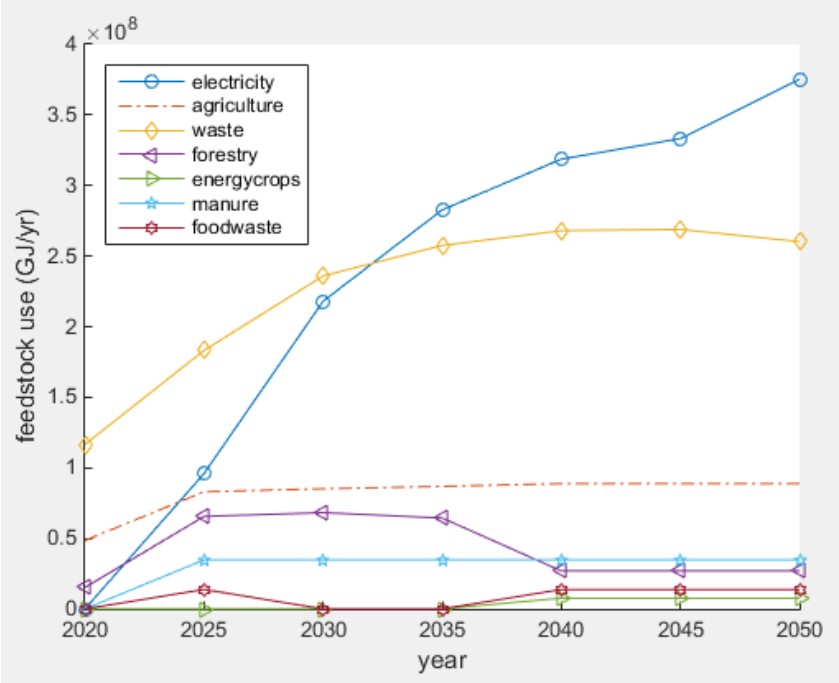

Figure 93. Drayage CAP emissions constraints feedstocks used

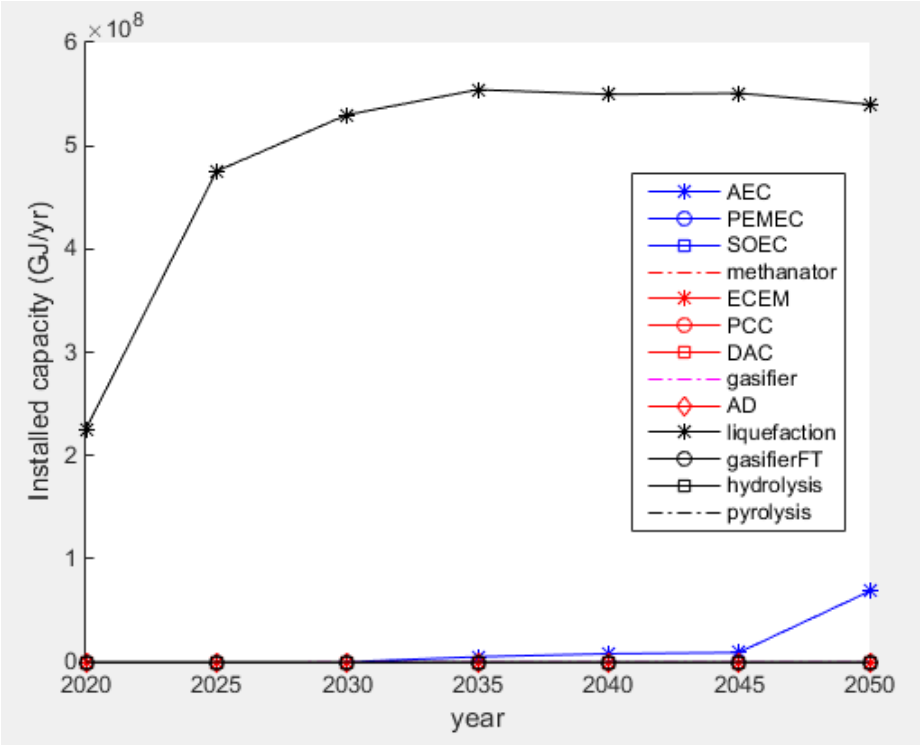

Figure 94. Drayage CAP emissions constraints fuel production equipment used

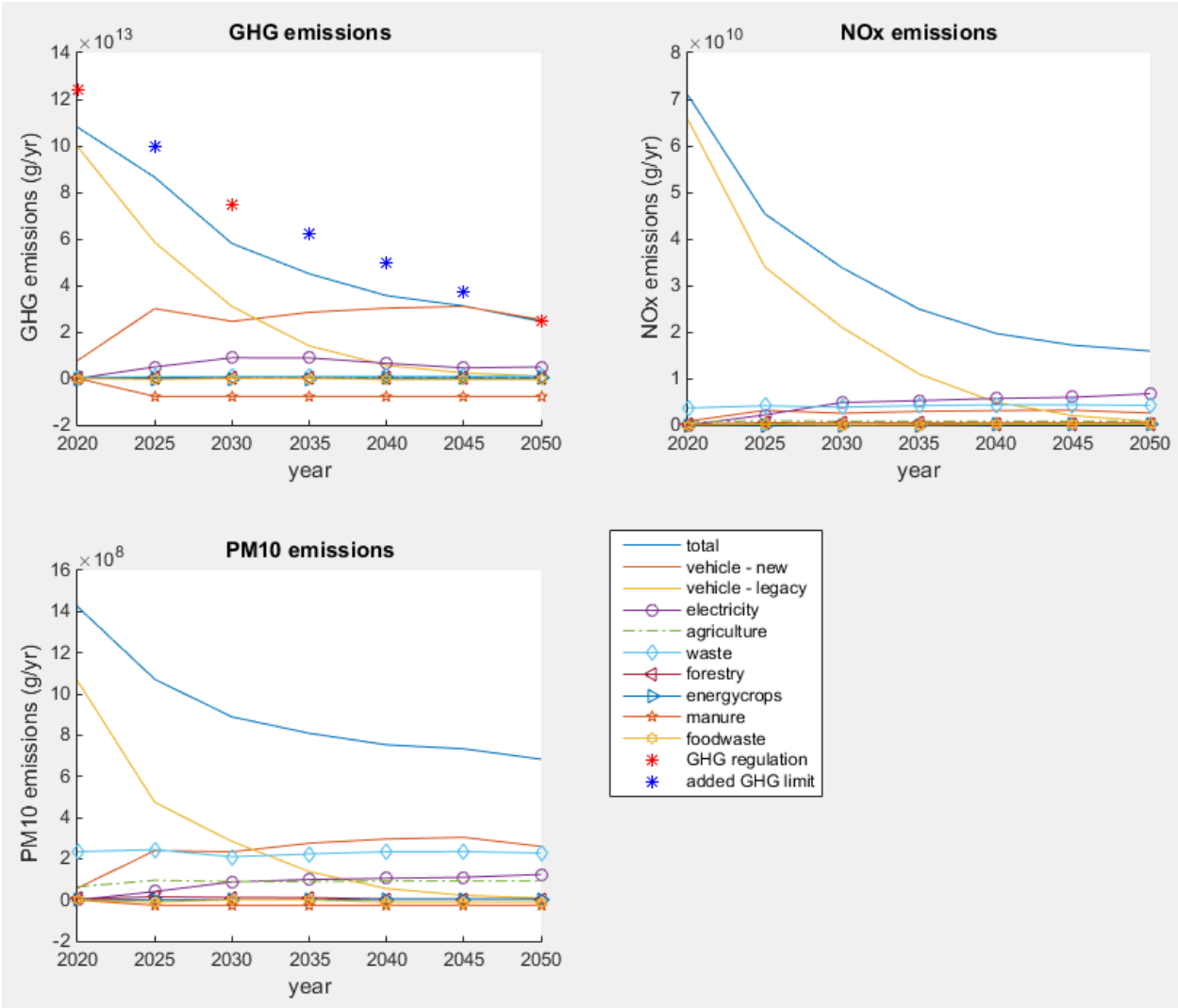

Figure 95. Drayage CAP emissions constraints emissions

8.5 Sensitivity Analyses

The following are several sensitivity analyses conducted to give insight into the relative importance of the various techno-economic data included in TRACE. Some key parameters are selected and analyzed below.

8.5.1 Effect of Continued Production Plant Constraint

The use of CRFs to convert the capital cost of fuel production plants requires the constraint that when a production technology is adopted, it will continue to be used and paid for until the end of its lifetime (or the end of this analysis in 2050, after which is beyond the scope of this work). However, it would be interesting to see the effect of removing that constraint, effectively making the fuel production market infinitely flexible to respond to change in cost of fuel and vehicle pathways. Doing so causes a drastic decrease in liquefaction production plant use in 2050.

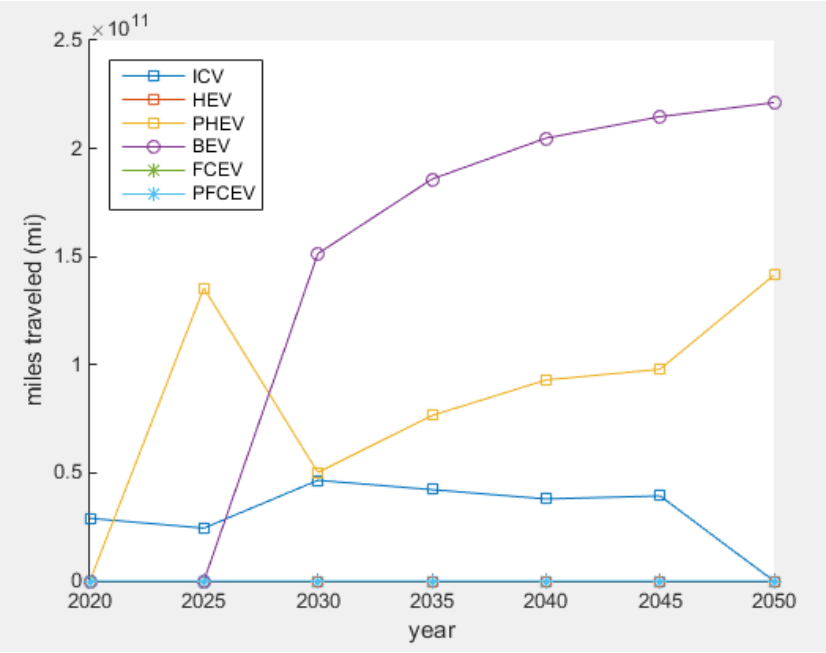

Figure 96. No continued production plant constraint LDV miles traveled

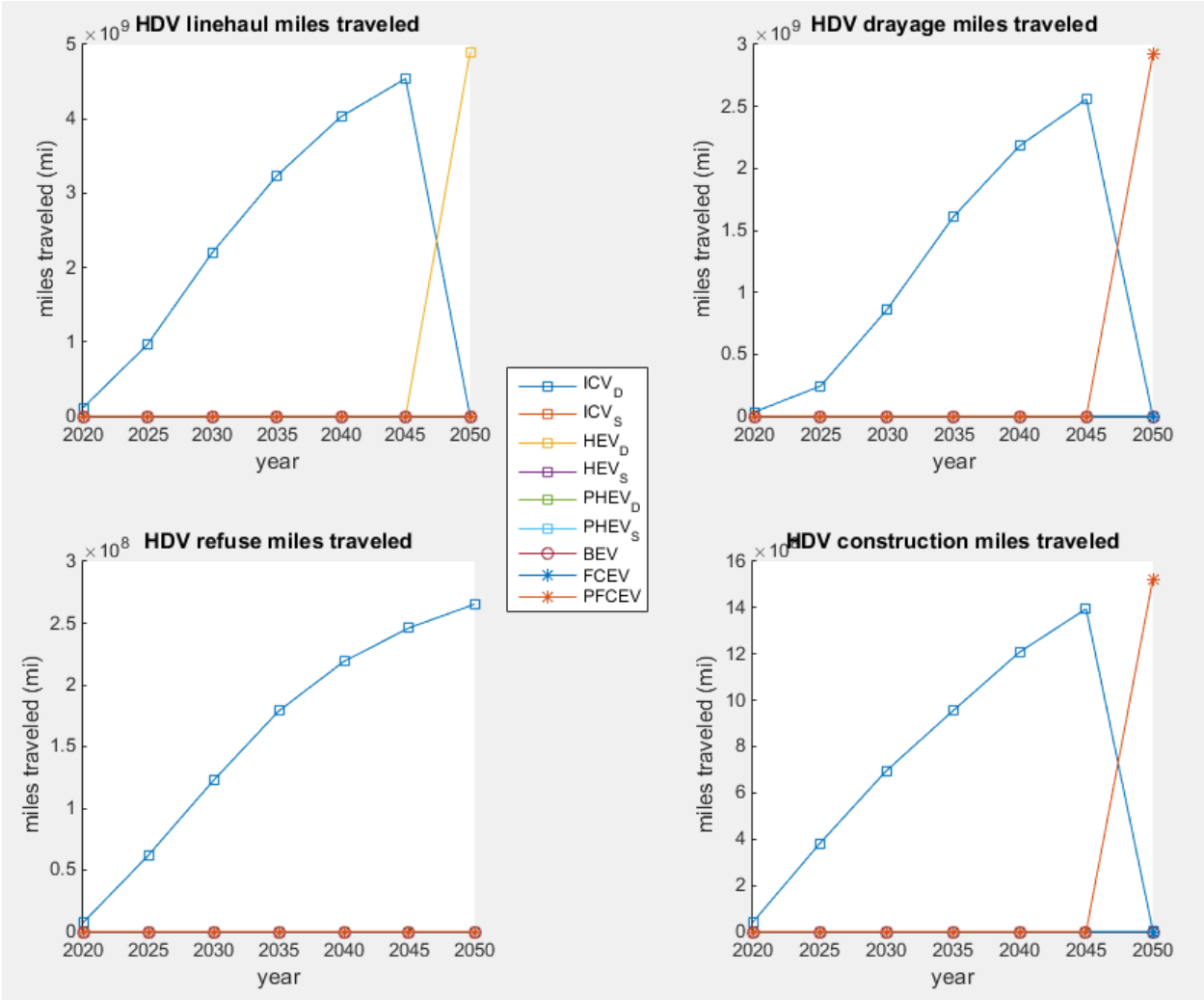

Figure 97. No continued production plant constraint HDV miles traveled by vocation

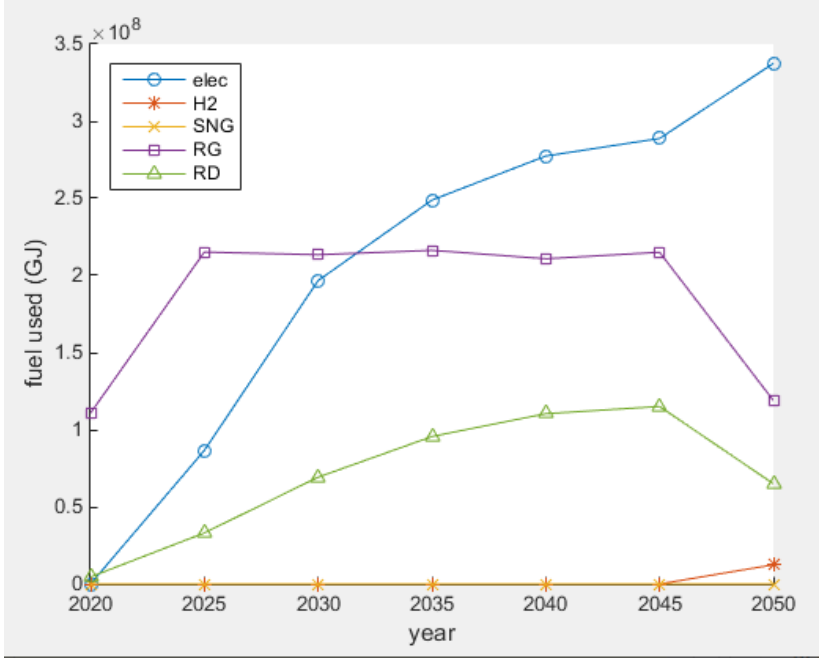

Figure 98. No continued production plant constraint fuels used

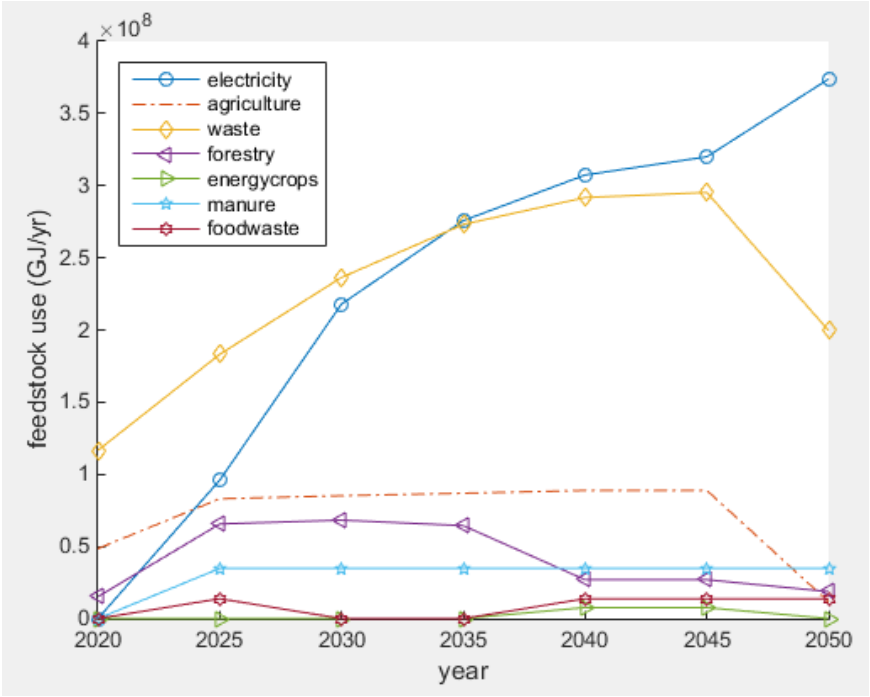

Figure 99. No continued production plant constraint feedstocks used

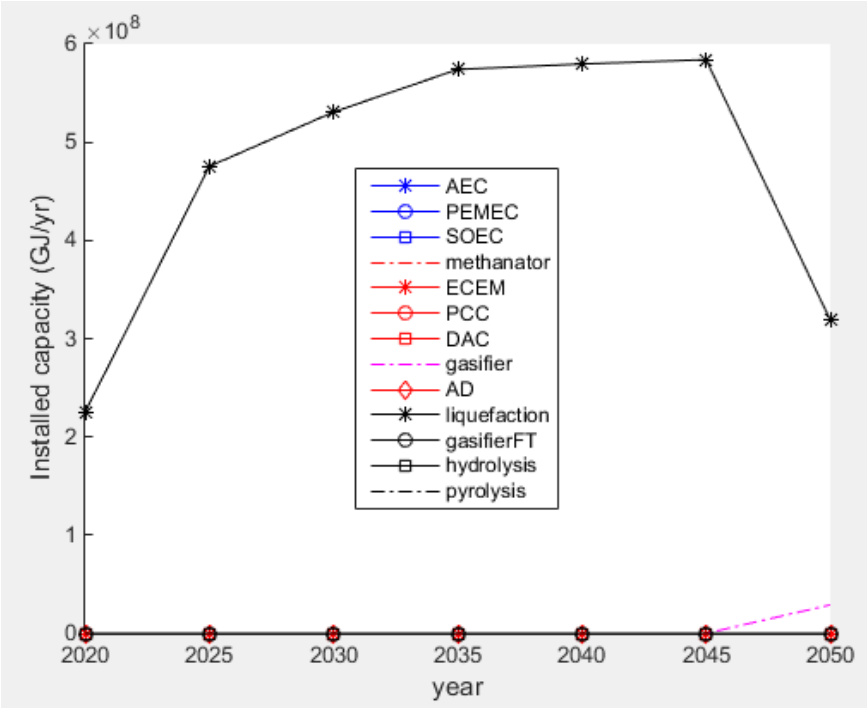

Figure 100. No continued production plant constraint fuel production equipment used

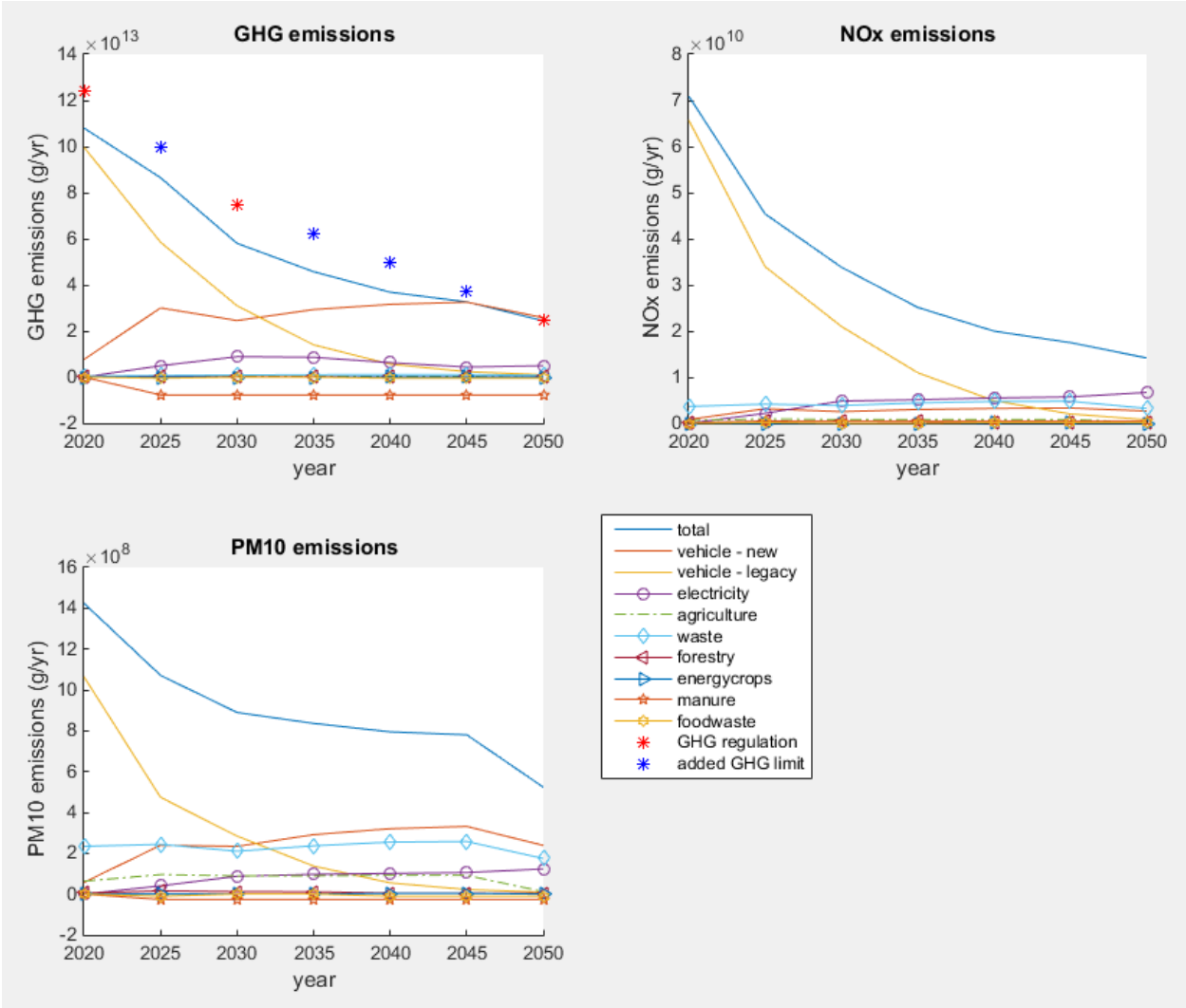

Figure 101. No continued production plant constraint emissions

8.5.2 Effect of Electricity Distribution Cost

Recall that level 1 charging is modeled with no electricity distribution cost. Only level 2 and level 3 electric charging is modeled to have an associated electricity distribution cost. Reducing electric distribution costs by 50% decreases the total cumulative cost by 0.41%, because very little level 2 electric charging is used (for some drayage PFCEVs in 2050) and level

1 charging does not have an associated distribution cost. This does not affect technology adoption.

An increase of electric distribution costs by 50% has no impact on technology adoption but increases total cumulative cost by 0.41%%. An increase of electric distribution costs by a factor of five also has no impact on vehicle adoption but increases total cumulative cost by 3.2%.

8.5.3 Effect of Electricity Dispensing Cost

Another major component that mainly affects LDVs in the TRACE Non-ZEV Constrained Case results is the electricity dispensing cost. If each of the electric charging levels has its costs cut in half, the total cumulative cost is decreased by 2.6% and technology adoptions are not changed.

If each of the electric charging levels has its cost doubled, the effect is an increased total cumulative cost of 5.1%, but there is no change in vehicle technology adoption.

Given the results of this section as well as the previous on electricity distribution cost, it is clear that TRACE results are more sensitive to electricity dispensing cost than electricity distribution cost.

8.5.4 Effect of Electrolyzer Technology Cost

No matter how low electrolyzer capital costs go, there is no significant change in vehicle technology adoption. Furthermore, zeroing out the FOM and VOM for the electrolyzer technologies still does not bring hydrogen into the results with all other inputs held constant.

This is not surprising as the vehicle cost per mile of FCEVs is higher than the total cost of BEVs for LDVs (note Table 31), so even making the feedstock, production, distribution, and

dispensing costs all zero for hydrogen pathways would not be enough to stimulate an adoption of fuel cell-powered vehicles beyond that required to make up for range and fueling time constraints of BEVs.

8.5.5 Effect of Gasifier Cost

Similar to the electrolyzer costs, zeroing out gasifier capital, FOM, and VOM costs still is not enough to get hydrogen adopted and results are the same as default. The same reason as above regarding high FCEV cost is relevant here.

8.5.6 Effect of Fuel Cell Cost

Reducing fuel cell cost to $0 does not encourage the adoption of either FCEVs or PFCEVs beyond what is adopted in the Non-ZEV Constrained Case.

8.5.7 Effect of Liquefaction Cost

Reducing the starting liquefaction cost 10% lowers the total cumulative cost by 0.55% and does not change technology adoption. Increasing the starting liquefaction cost by 10% increases the total cumulative cost by 0.54% and also does not change technology adoption.

Doubling liquefaction capital costs leads to a total cumulative cost reduction of 2.9% due to technologies adopted. This causes LDVs to be primarily PHEVs and BEVs beginning in 2025, while HDV vocations assume several alternative powertrain options except for refuse trucks. PHEVs to be adopted in 2020 instead of ICVs. The amount of liquefaction adopted is significantly decreased and electricity use is correspondingly increased.

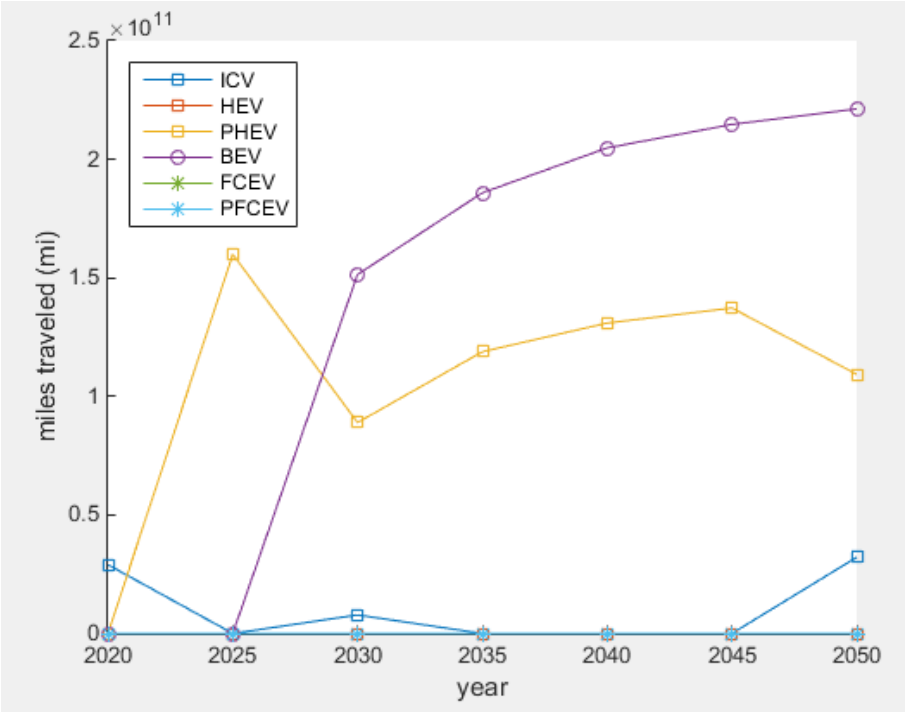

Figure 102. Doubled liquefaction cost LDV miles traveled

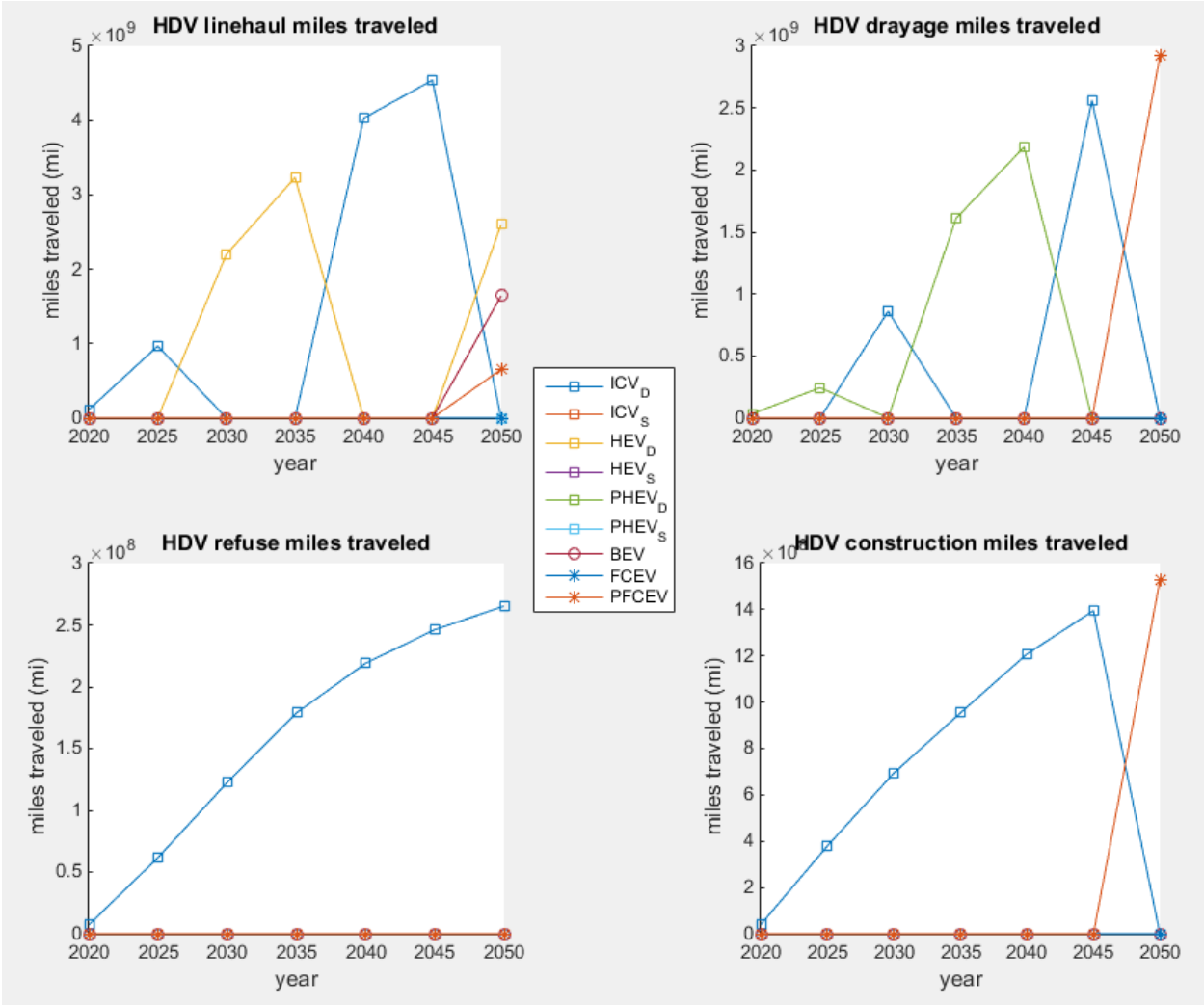

Figure 103. Doubled liquefaction cost HDV miles traveled by vocation

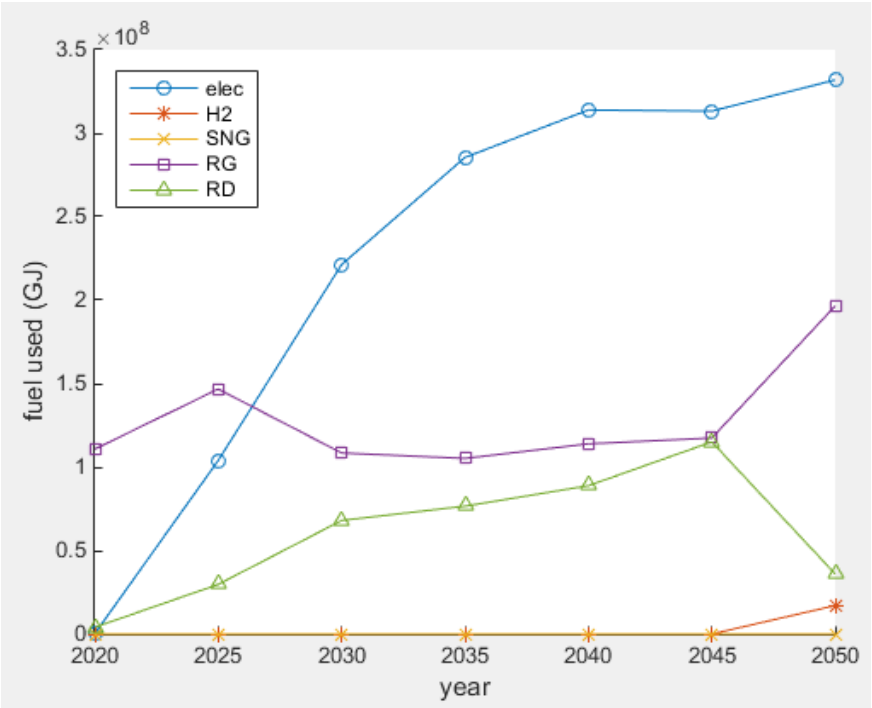

Figure 104. Doubled liquefaction cost fuels used

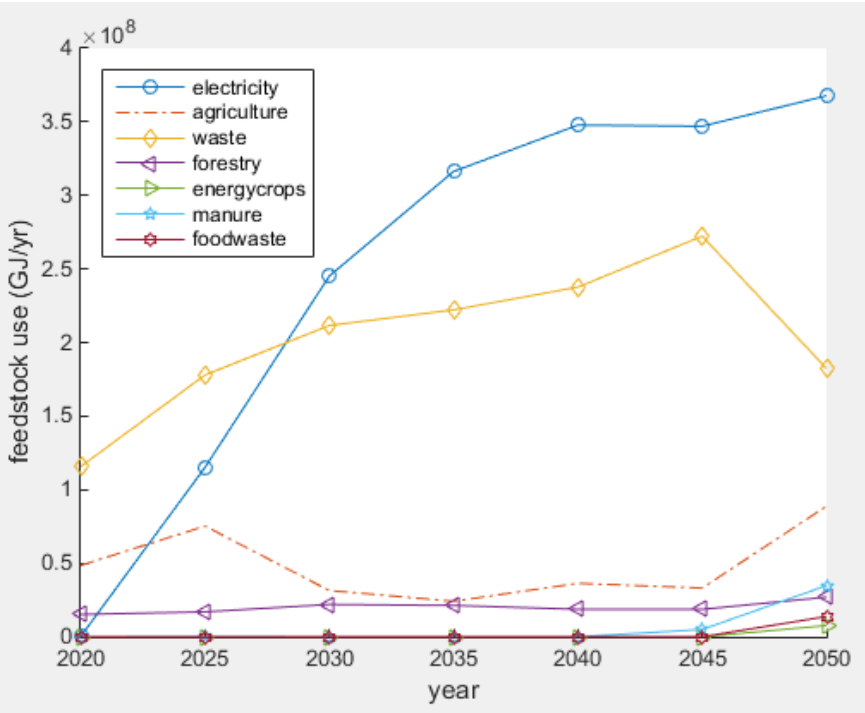

Figure 105. Doubled liquefaction cost feedstocks used

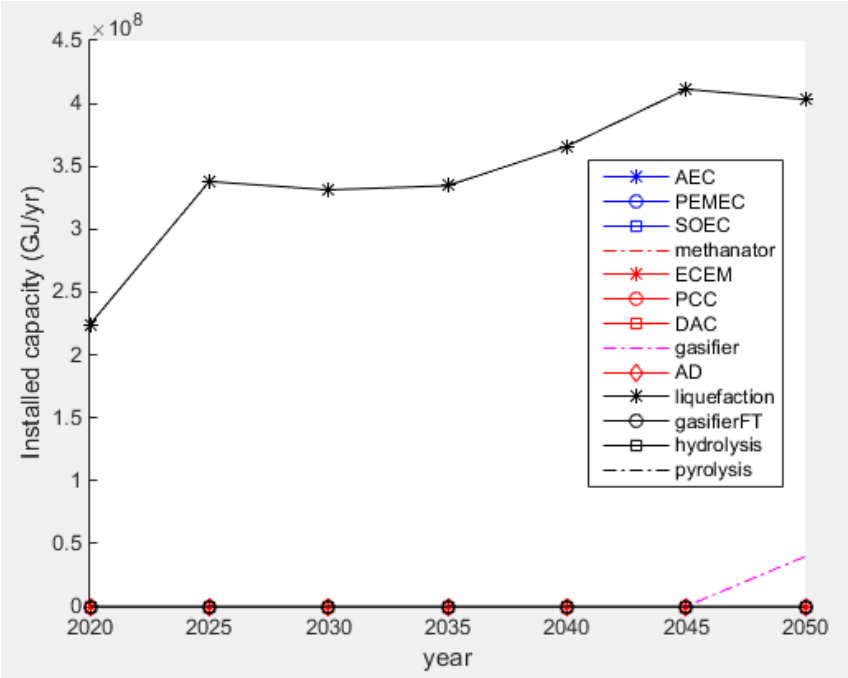

Figure 106. Doubled liquefaction cost fuel production equipment used

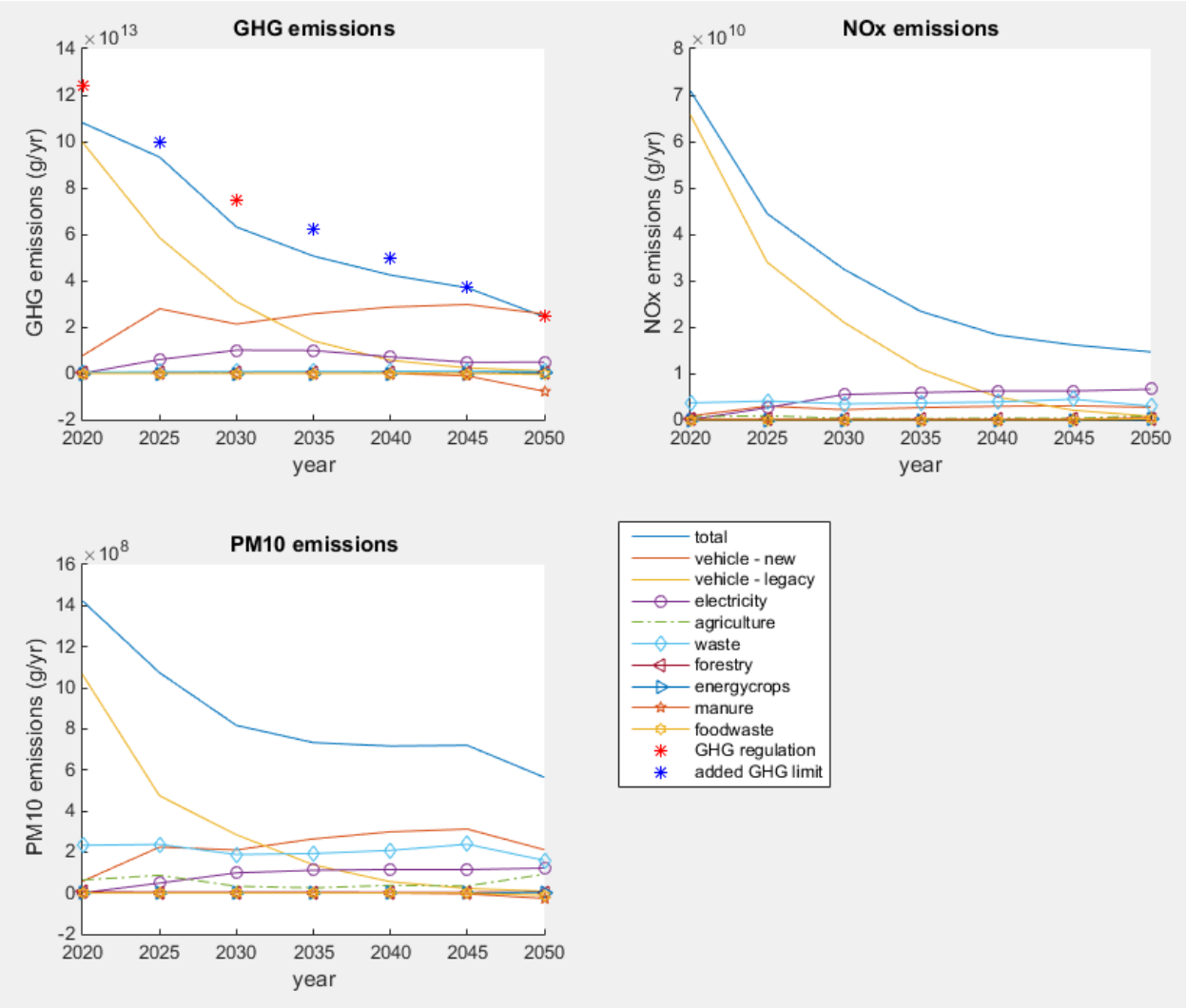

Figure 107. Doubled liquefaction cost emissions

8.5.8 Effect of Electricity Feedstock Constraints

The electricity feedstock constraint can be tightened to include 57% lower electricity use for vehicles than the original constraint and still produce a feasible solution with TRACE. At this point, all of the biomass feedstocks are used at their full potential. This change in constraint leads to a similar vehicle adoption for LDVs and HDVs, with a total increase in cumulative cost by 0.23%.

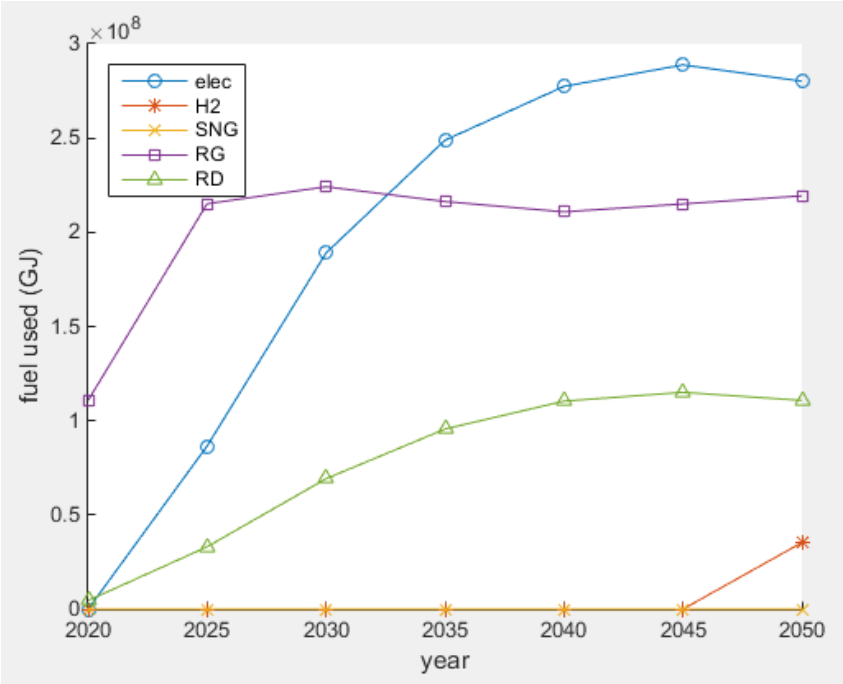

Figure 108. Reduction of electricity feedstock availability by 57% fuels used

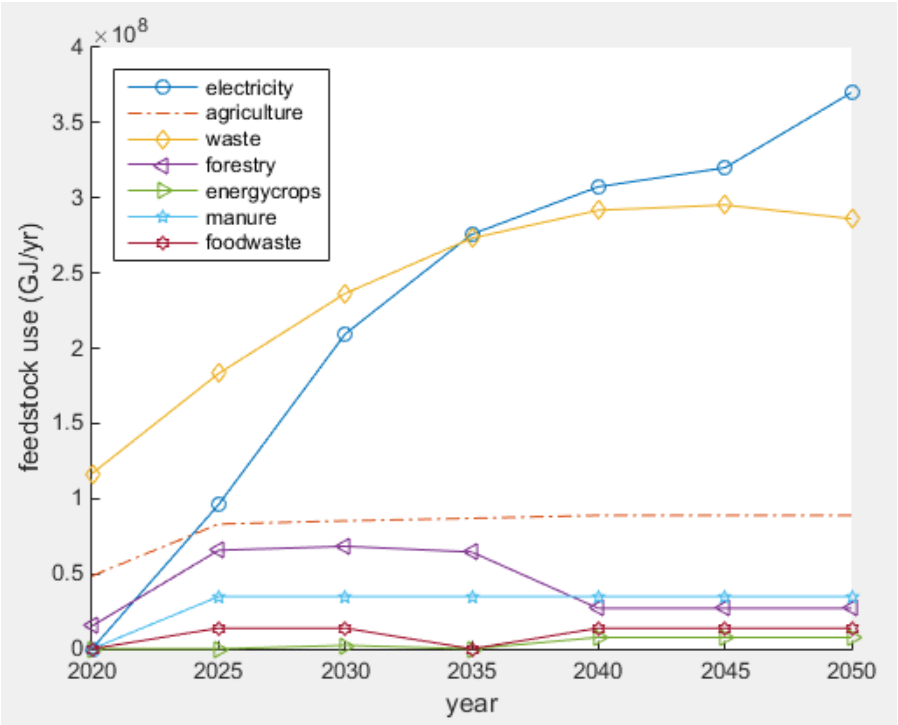

Figure 109. Reduction of electricity feedstock availability by 57% feedstocks used

8.5.9 Effect of CF and Electricity Cost on P2G Technology

Electricity costs from E3 are somewhat low [300], ranging from 3.7 cents per kWh in 2020 to 4.2 cents per kWh in 2050 with some fluctuation in the middle [189]. Consider a case with a 50% increase in the electricity cost for BEVs, which is more conservative, and negligible cost for electricity going into P2G plants, a scenario that could exist given the already existing curtailed energy from solar and wind power in California [301][302]. However, if a P2G plant is using otherwise-curtailed electricity, the capacity factor would be low; assume a capacity factor of 0.2 instead of the default 0.8. With these changes in electricity cost and P2G plant capacity factor, the technology adoption stays the same as for the default electricity costs. Total cumulative cost increases 2.5% due to the heavy light-duty BEV use and the 50% increase of fuel cost for those vehicles.

8.5.10 Effect of Battery Learning Rate

Decreasing the battery learning rate to zero, meaning there is no decrease in battery cost with increasing cumulative production amount, has a number of impacts on technology adoption. For LDVs, PHEVs are used into later years of modeling and PFCEVs are adopted as the primary powertrain type in 2045 and 2050. Linehaul HDVs have significant diesel HEV adoption in 2030 and some significant PFCEV adoption in 2035 and 2040, respectively. Drayage HDVs have significant PFCEV adoption in 2030 and beyond, except in 2040. Refuse HDVs continue to use diesel ICVs. For construction HDVs, there is some significant PFCEV and FCEV adoption in 2030 and 2040, respectively. Total cumulative cost is increased 22%, showing battery cost is a major contributor to total cost of these TRACE results.

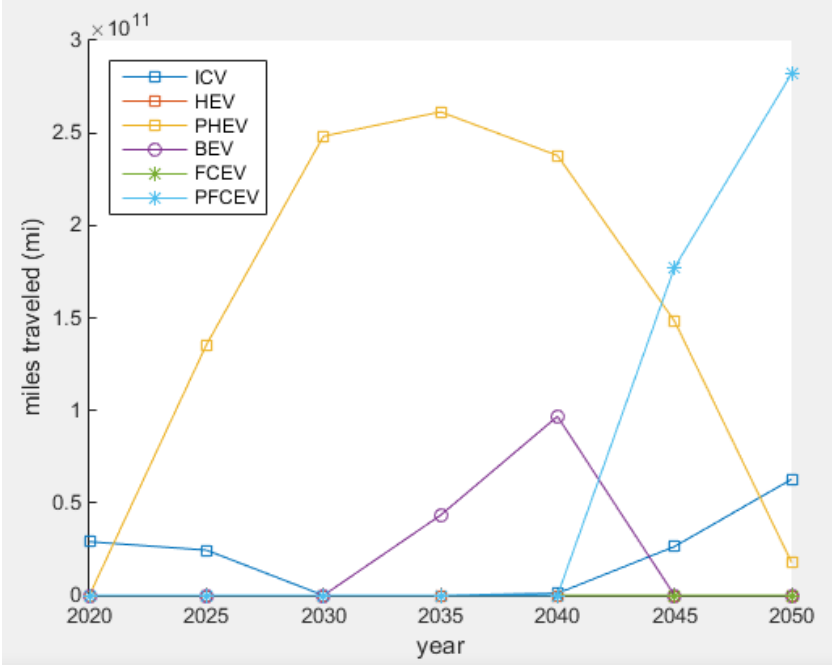

Figure 110. Zero battery LR LDV miles traveled

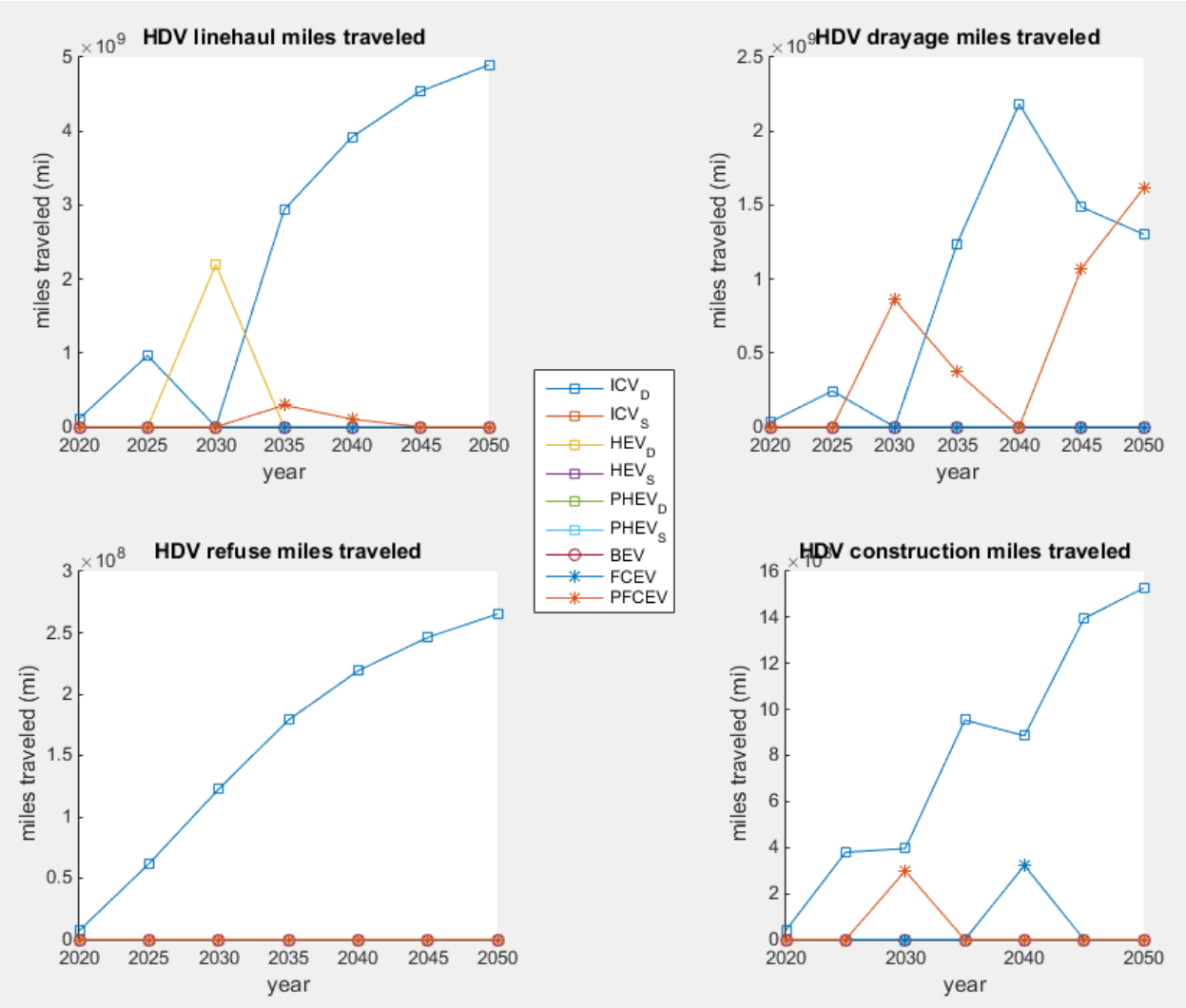

Figure 111. Zero battery LR HDV miles traveled by vocation

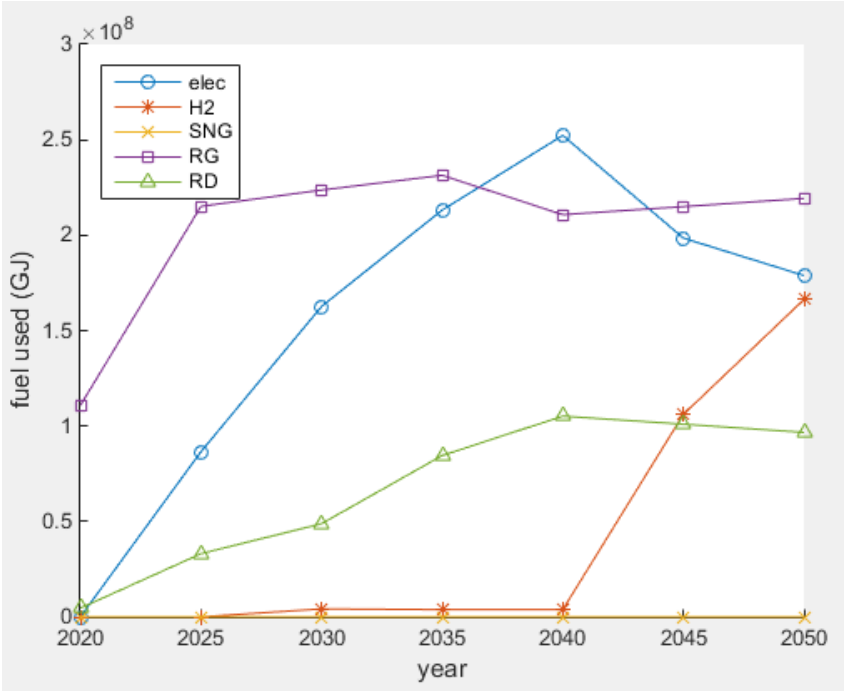

Figure 112. Zero battery LR fuels used

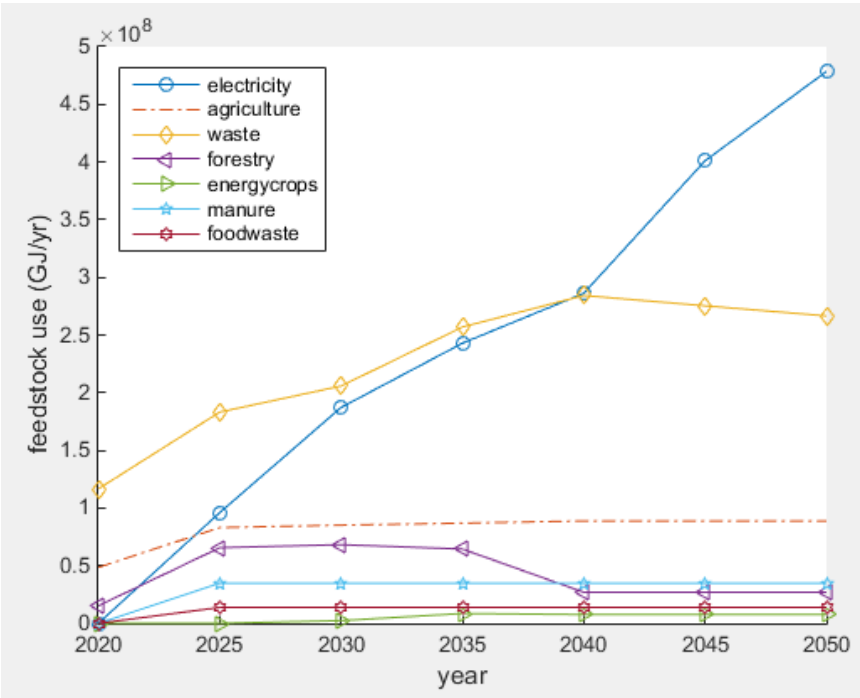

Figure 113. Zero battery LR feedstocks used

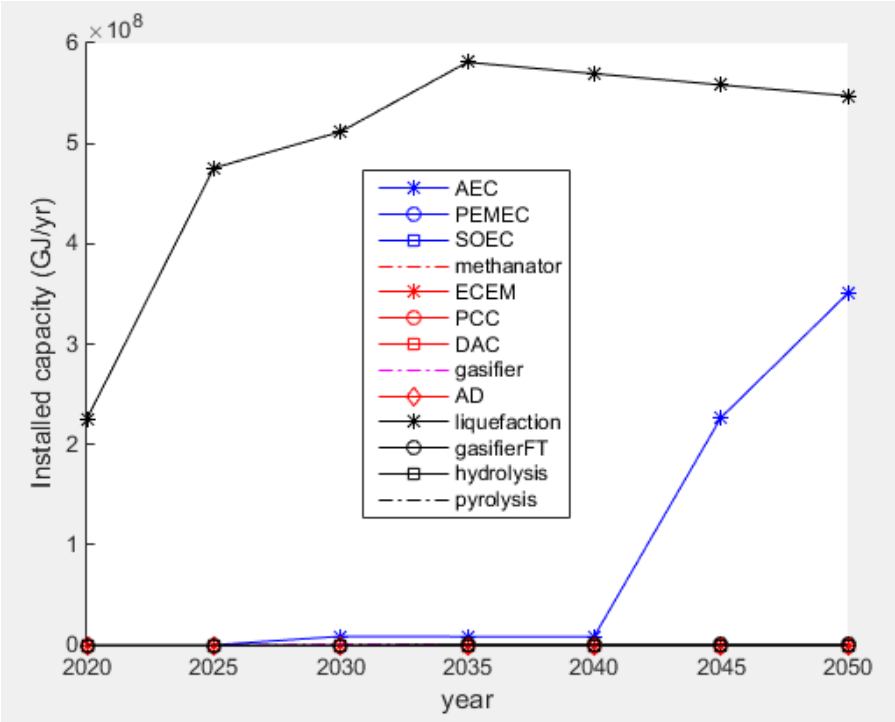

Figure 114. Zero battery LR fuel production equipment used

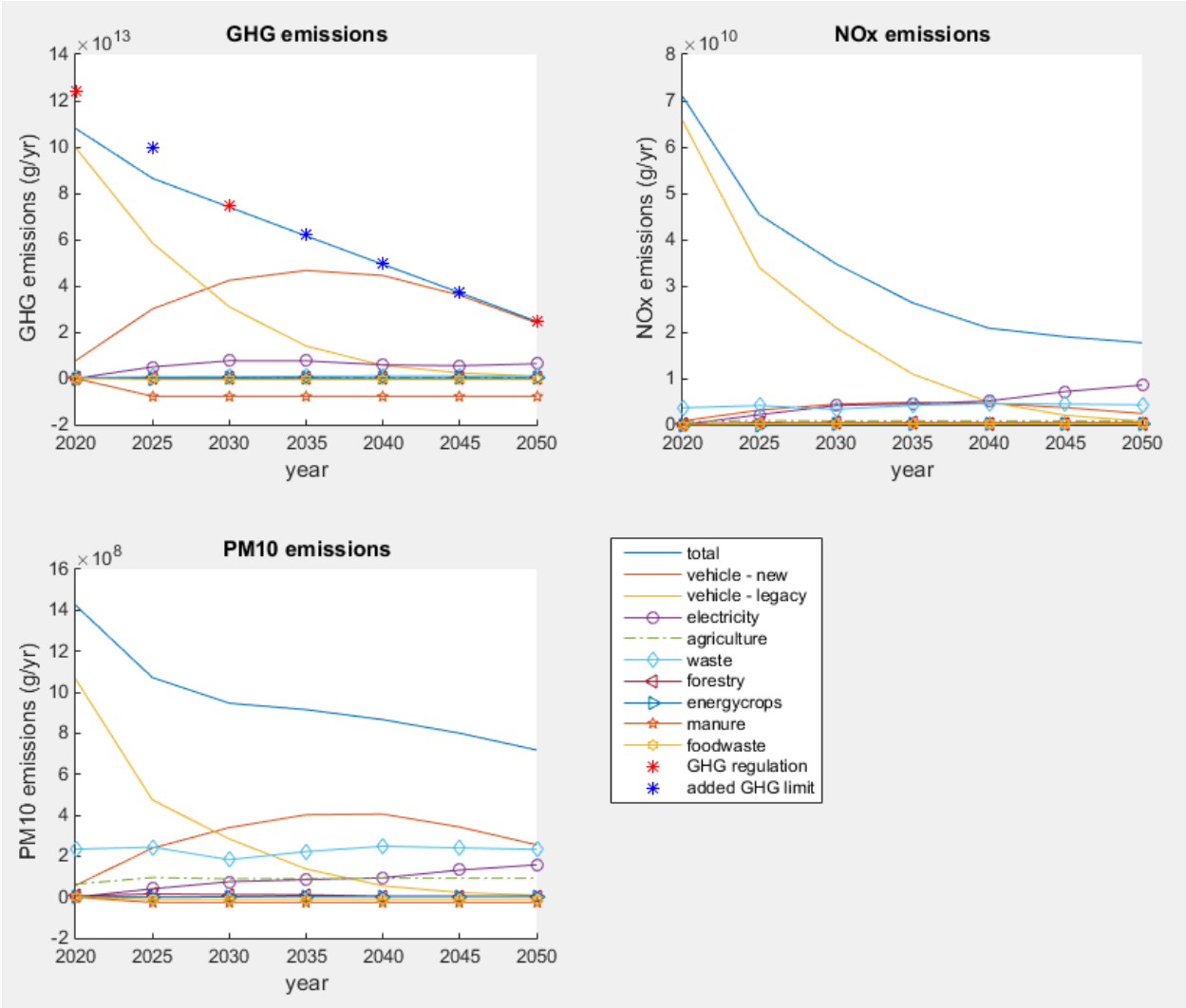

Figure 115. Zero battery LR emissions

8.5.11 Effect of VMT Changes

As previously mentioned, VMT projections are from EMFAC [141]. As with all projections, it would be unwise to assume that these projections are entirely accurate. This is especially true as drastically increasing alternative fuel and vehicle use (as projected by TRACE using default values) would affect cost of transportation, particularly in early years of adoption. TRACE is perfectly inelastic to demand, meaning changes in cost do not affect demand (i.e. VMT). Therefore, it is important to include a sensitivity analysis for VMT. Additionally, the

literature shows a range of VMT changes due to autonomous vehicles, with some projections up to 100% increase of VMT [303]–[312]. While the changes in efficiency and cost of autonomous vehicles compared to human-driven vehicles is beyond the scope of this work (and therefore no changes are made to the efficiency or cost in the following cases), the potential change in VMT is modeled so a general idea of the effect of varying VMT demand can be analyzed. Note that only the VMT of the new vehicles using the alternative fuels is affected here, as the legacy vehicles are assumed to use fossil fuels with consistent fuel price so VMT for those vehicles is assumed constant.

Decreasing VMT has the potential to drastically change adopted technologies, depending on the magnitude of increase in VMT. Decreasing VMT 10% for all years decreases cumulative cost by 9.9%, but does not affect the rollout of fuel and vehicle technologies. Decreasing VMT 50% for all years decreases cumulative cost by 48% and does affect the rollout of fuel and vehicle technologies. Due to significantly lower VMT, meeting emissions reductions goals does not require as many alternative vehicle types. The result is more reliance on ICVs for both LDVs and HDVs while still meeting the GHG emissions goals.

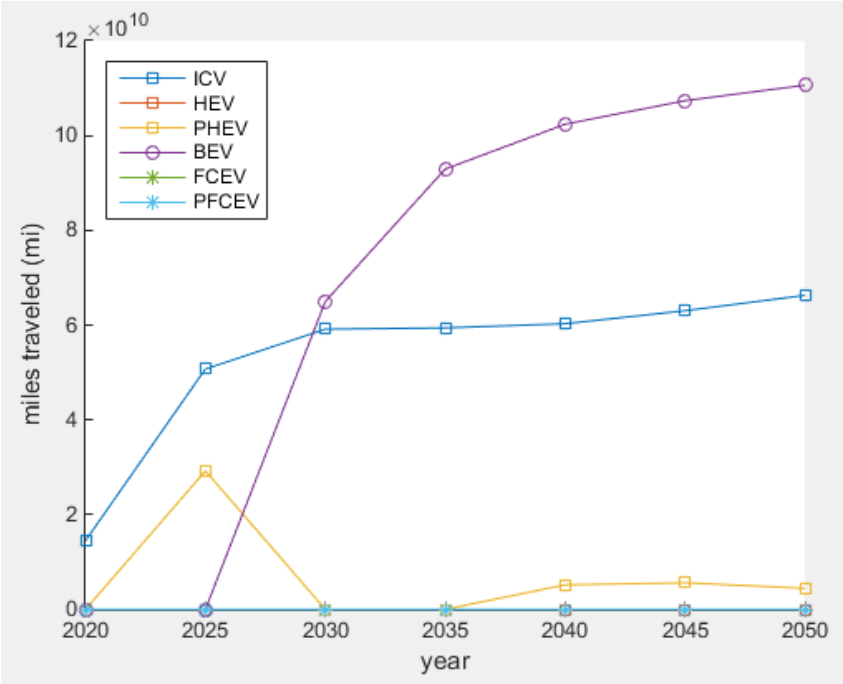

Figure 116. Decrease in all VMT by 50% LDV miles traveled

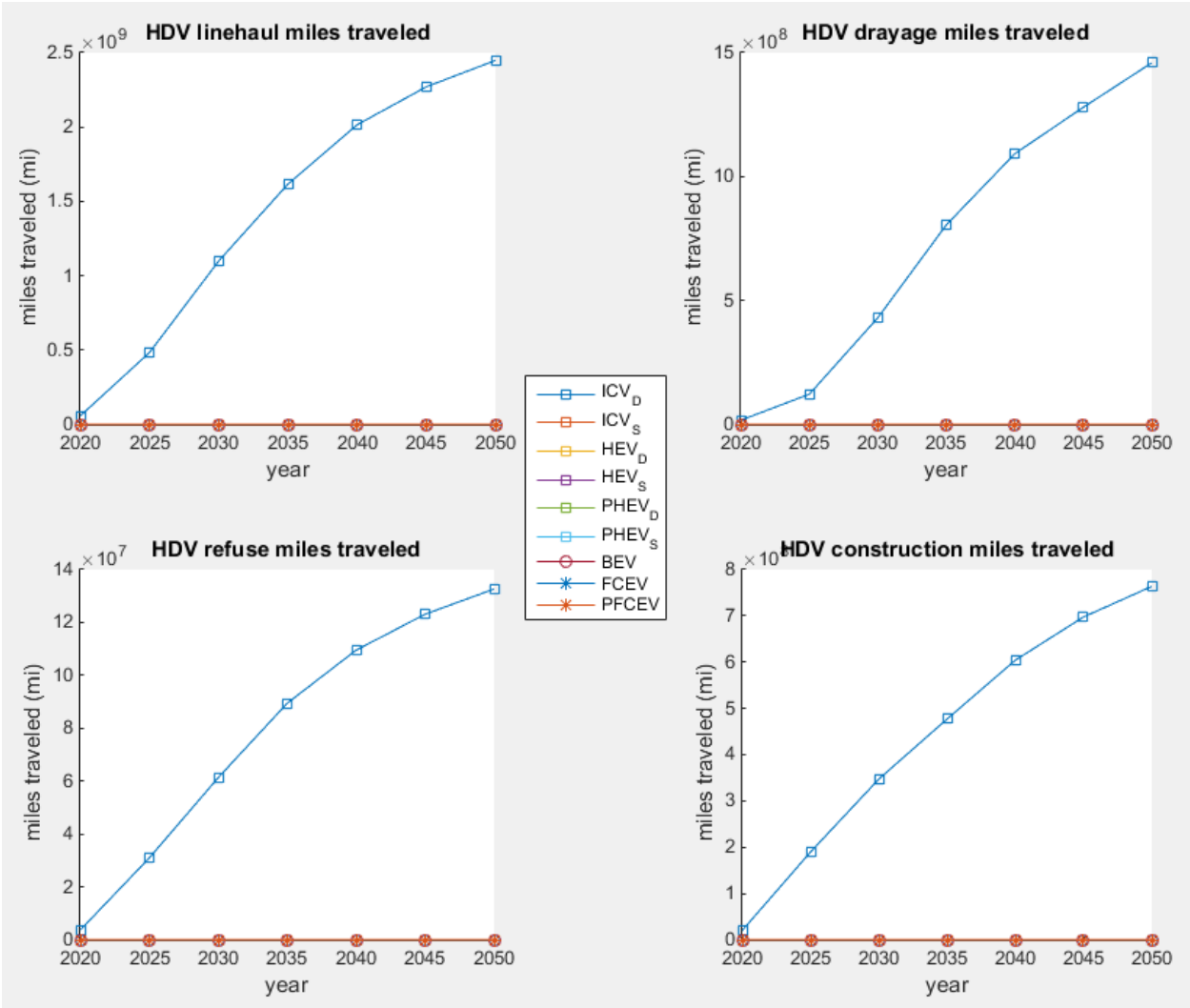

Figure 117. Decrease in all VMT by 50% HDV miles traveled

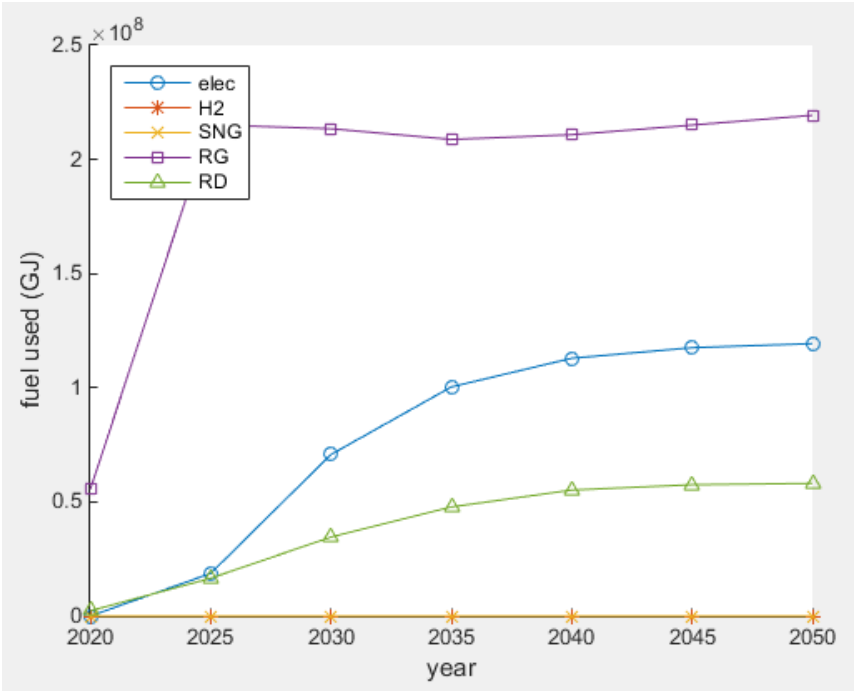

Figure 118. Decrease in all VMT by 50% fuels used

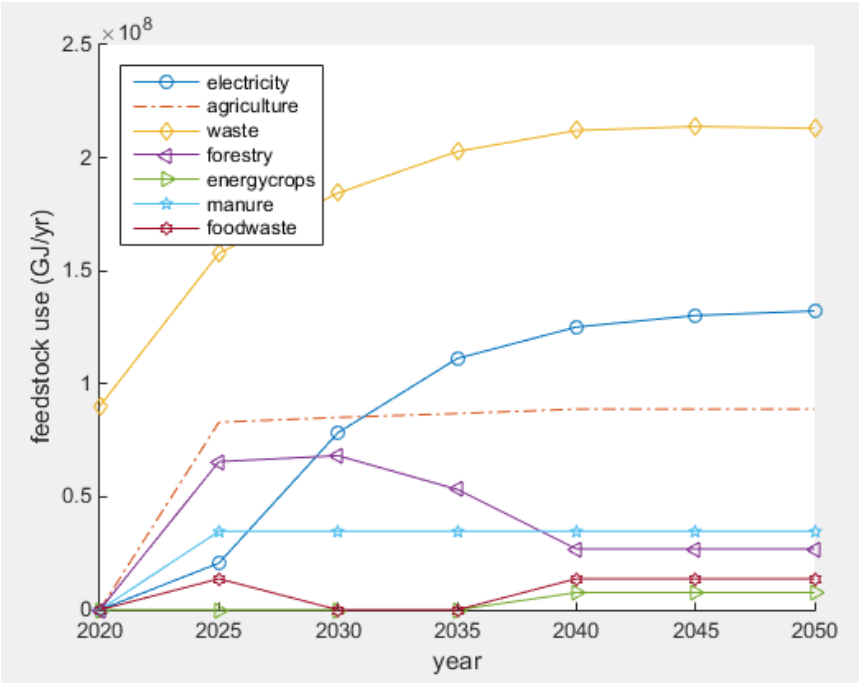

Figure 119. Decrease in all VMT by 50% feedstocks used

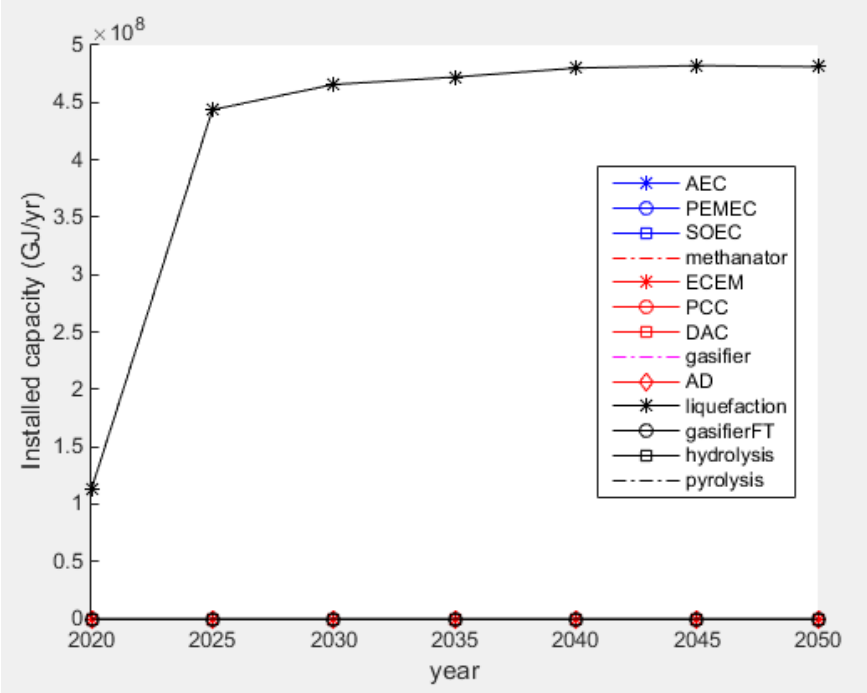

Figure 120. Decrease in all VMT by 50% fuel production equipment used

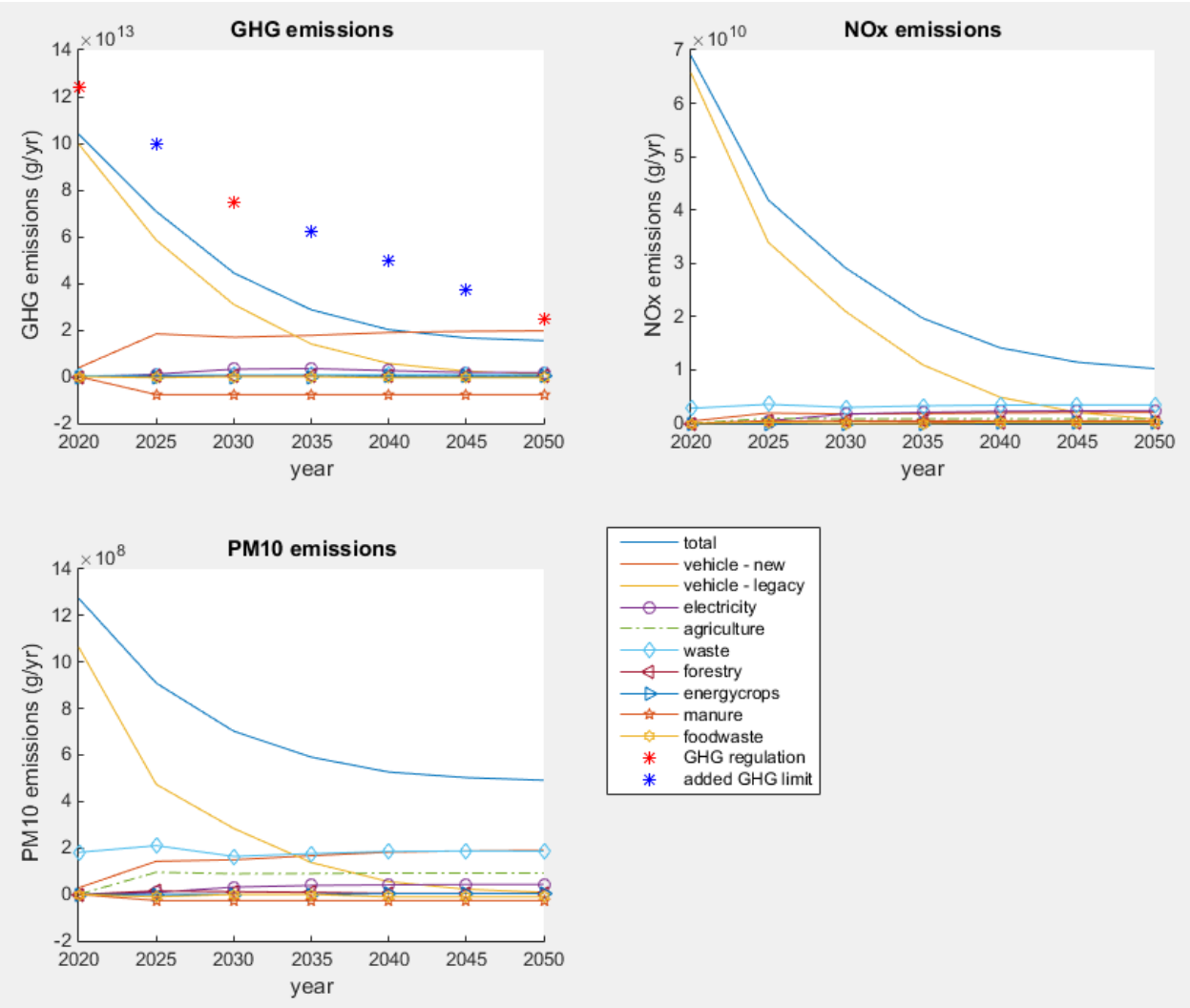

Figure 121. Decrease in all VMT by 50% fuel production equipment used

Increasing VMT also has the potential to drastically change adopted technologies, depending on the magnitude of increase in VMT. Increasing VMT 10% for all years does not affect technology adoption, but cumulative cost is increased by 10%. Increasing VMT 50% for all years has a number of changes in technology adoptions as an increase in VMT makes meeting emissions goals more stringent. For LDVs, ICVs are reduced while PHEVs and PFCEVs are increased in later years. For linehaul HDVs, there is a majority of diesel-fueled HEVs for all years with some diesel-fueled ICVs in 2035 and some BEVs in 2050. For drayage HDVs,

PFCEVs become the major vehicle type beginning in 2040. For refuse and construction HDVs, most continue to be diesel ICVs except for construction PFCEVs in 2045 and diesel-fueled ICVs for both refuse and construction in 2050. The total cumulative cost for this 50% increase in VMT is 40% above the default value.

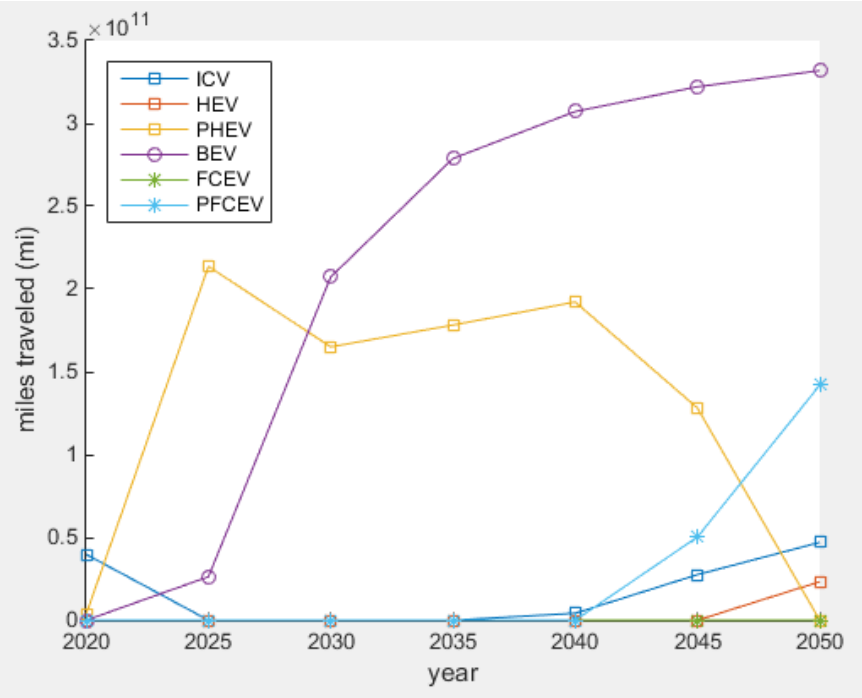

Figure 122. Increase in all VMT by 50% LDV miles traveled

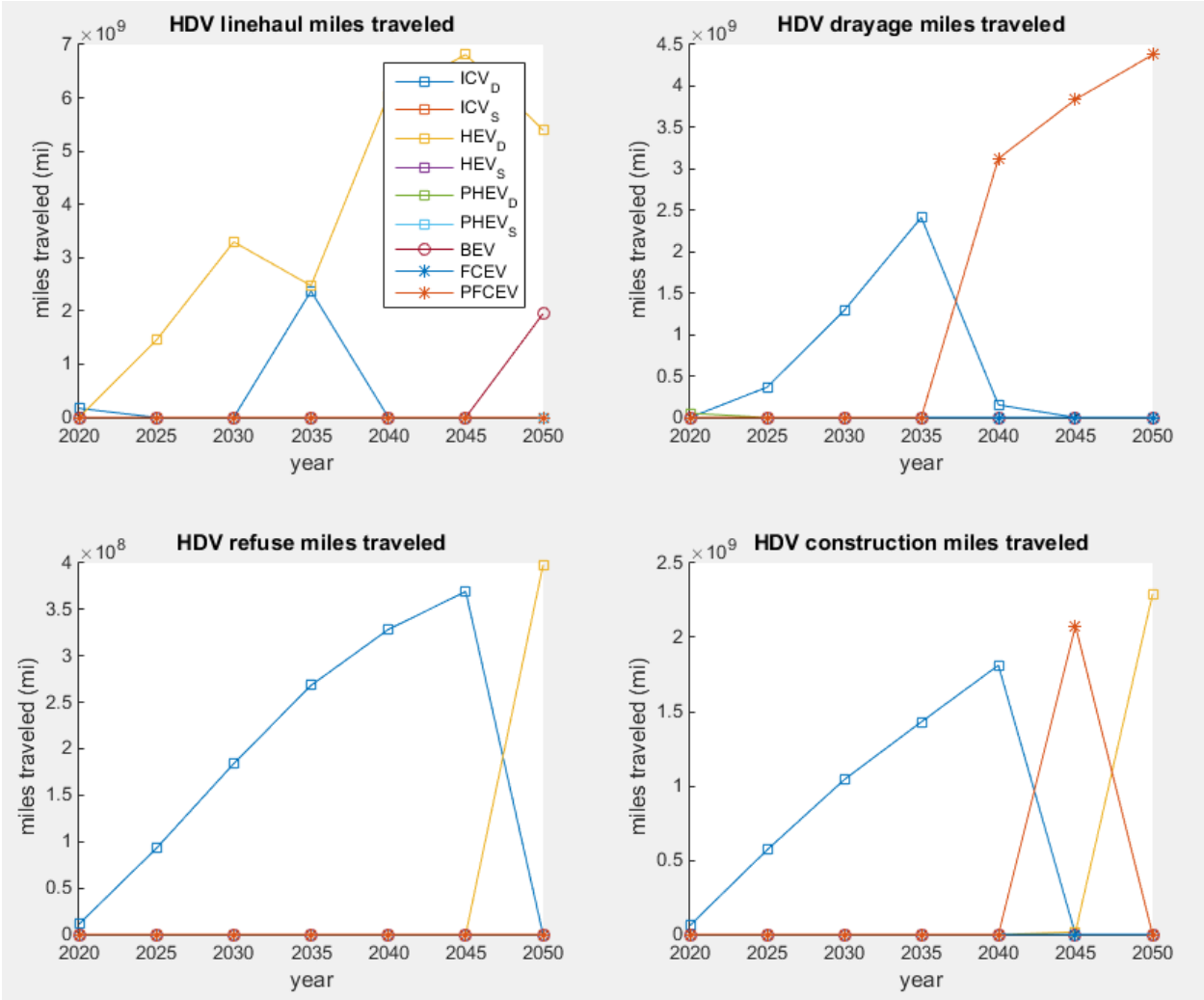

Figure 123. Increase in all VMT by 50% HDV miles traveled

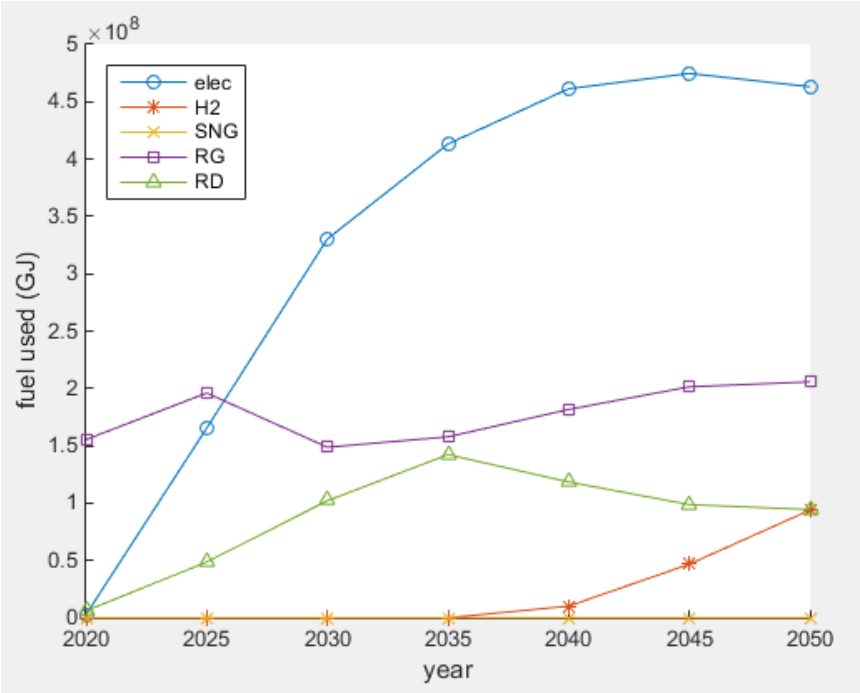

Figure 124. Increase in all VMT by 50% fuels used

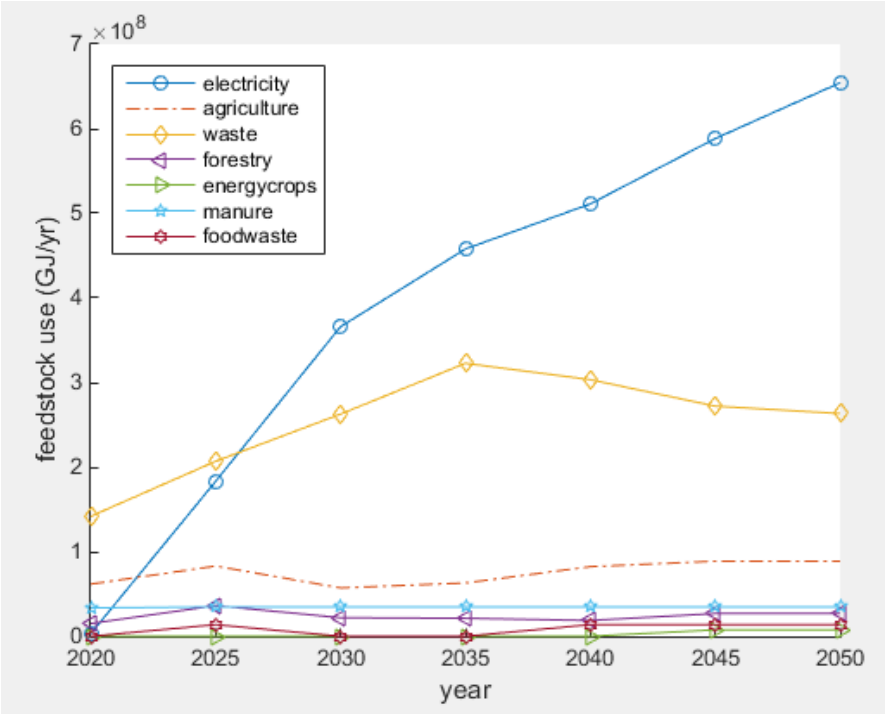

Figure 125. Increase in all VMT by 50% feedstocks used

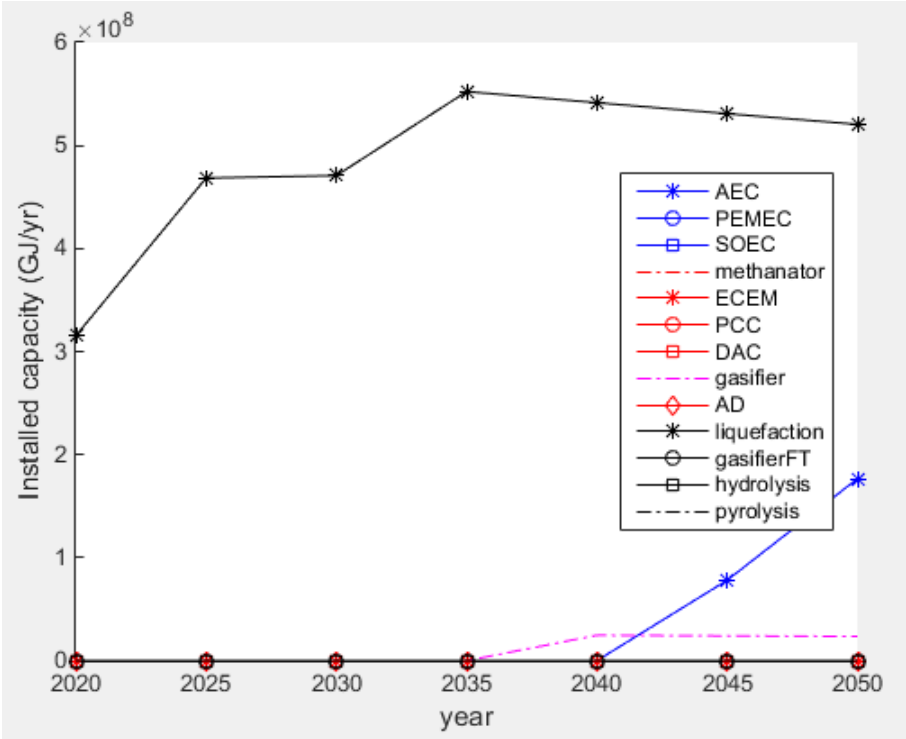

Figure 126. Increase in all VMT by 50% fuel production equipment used

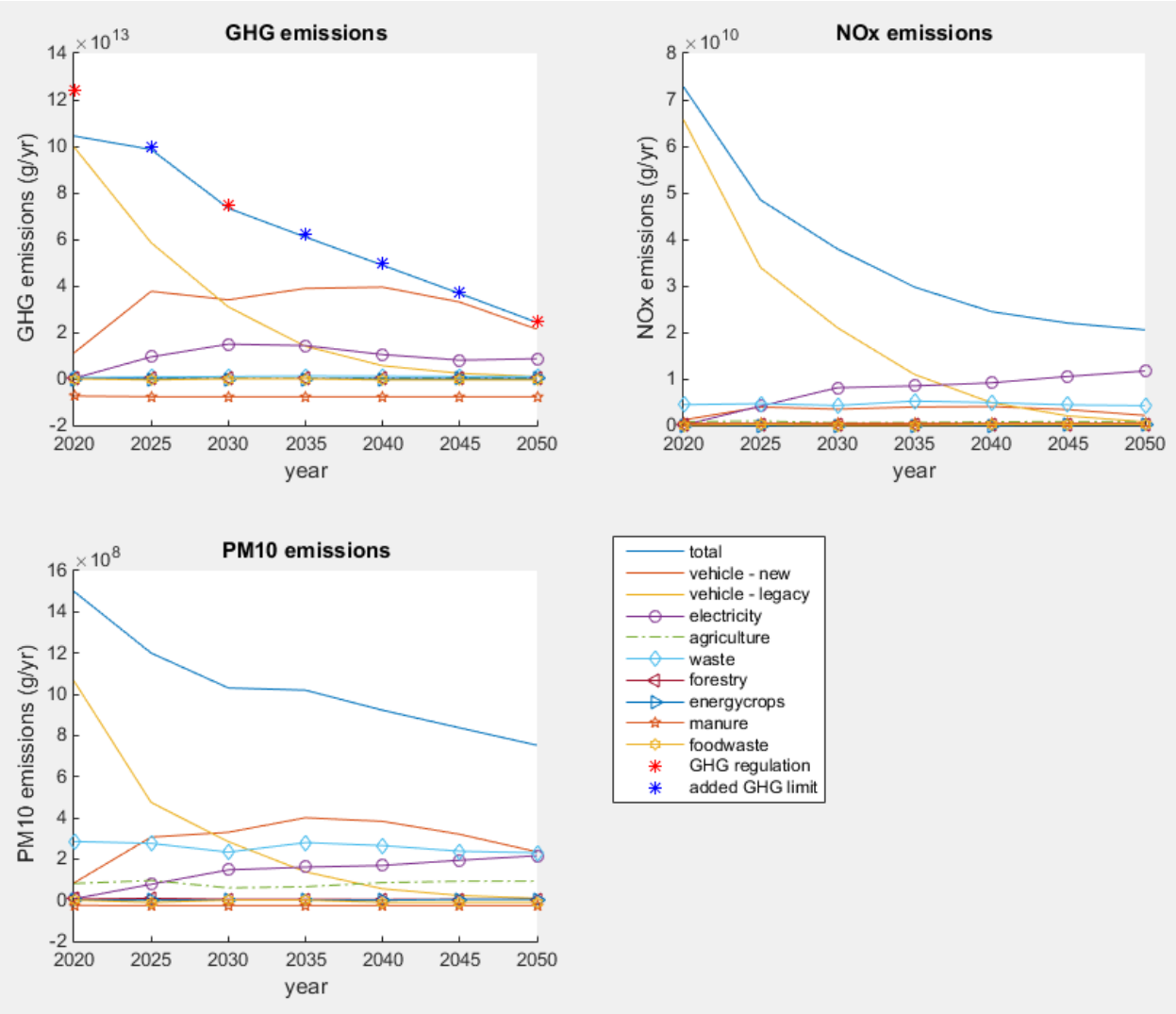

Figure 127. Increase in all VMT by 50% emissions

One last case to run for VMT change is to increase LDV VMT by 100% and HDV VMT by 50%, representing a major VMT increase noted by some of the previously-cited literature studying autonomous vehicles. This significant increase in VMT is not able to be met due to the feedstock constraints imposed, but an increase in the electricity feedstock constraint would allow for meeting the prescribed VMT increase. Instead, a 96% increase in LDV VMT and 50% increase in HDV VMT is the largest increase that can be supported by the feedstock availability modeled. This case increases total cumulative cost by 105% in 2050. Similar to the previous

scenario with a 50% increase in VMT for all vehicles, this scenario projects significant adoption of ZEVs and other alternative vehicle types to meet GHG emissions goals.

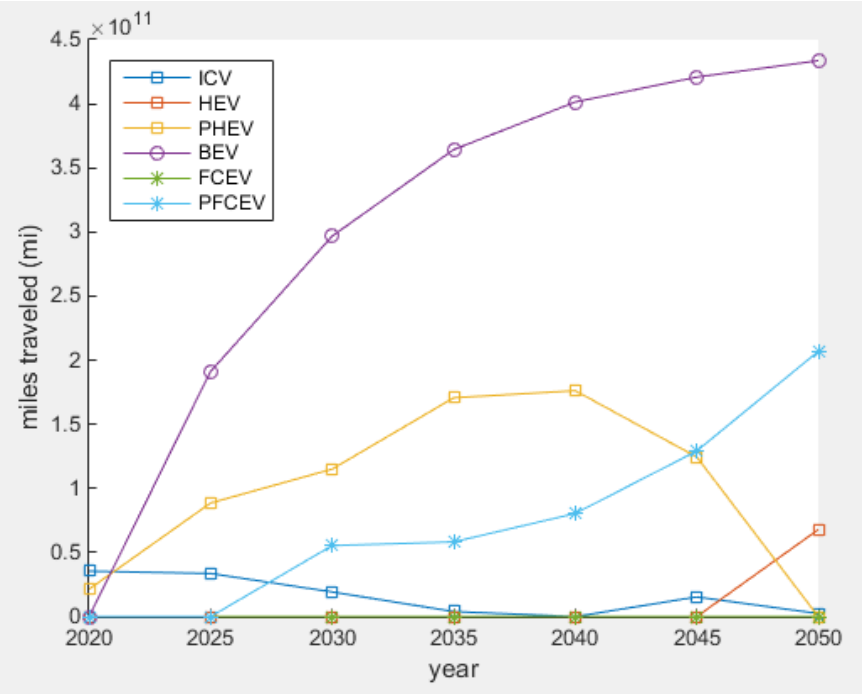

Figure 128. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% LDV miles traveled

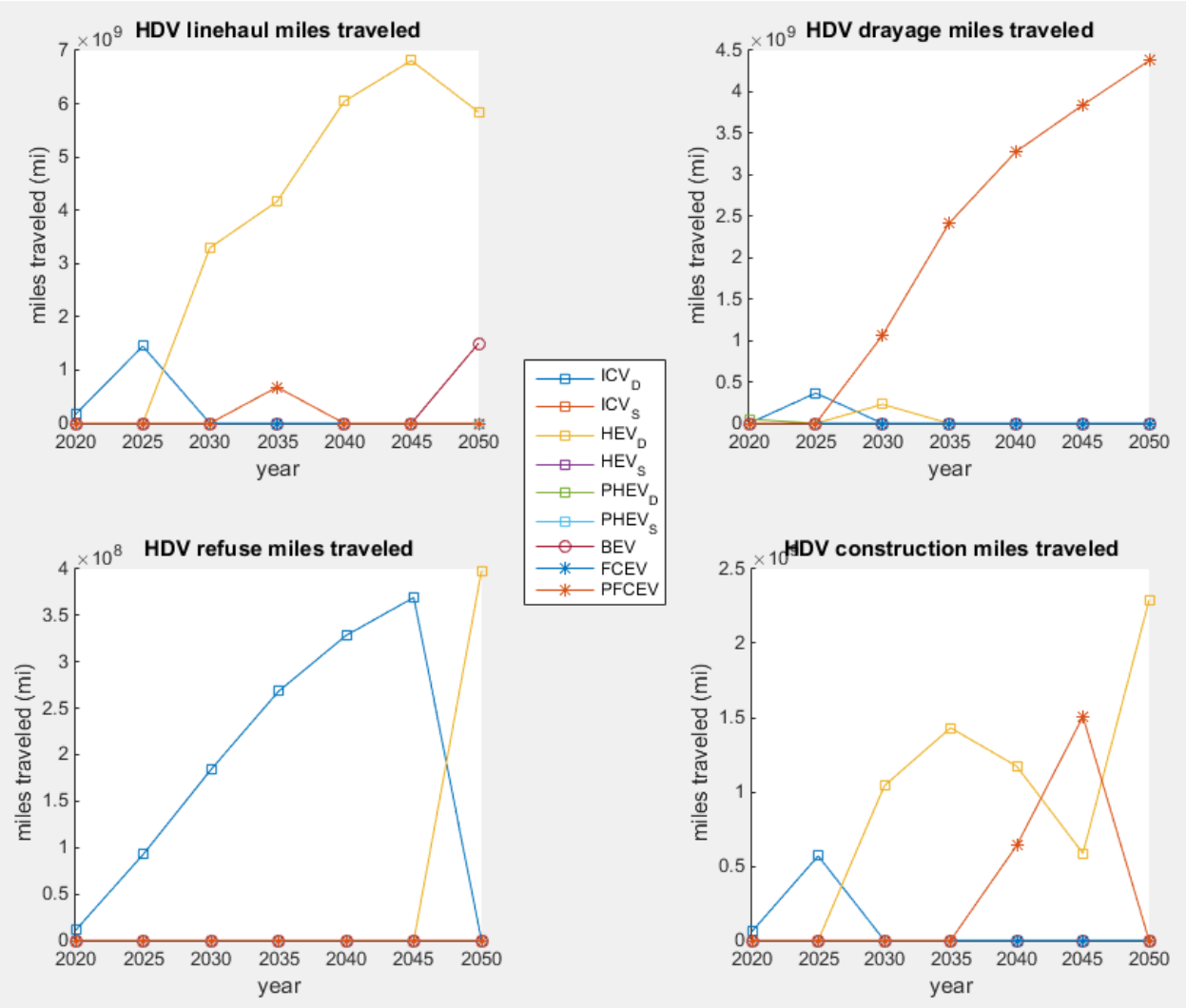

Figure 129. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% HDV miles traveled by vocation

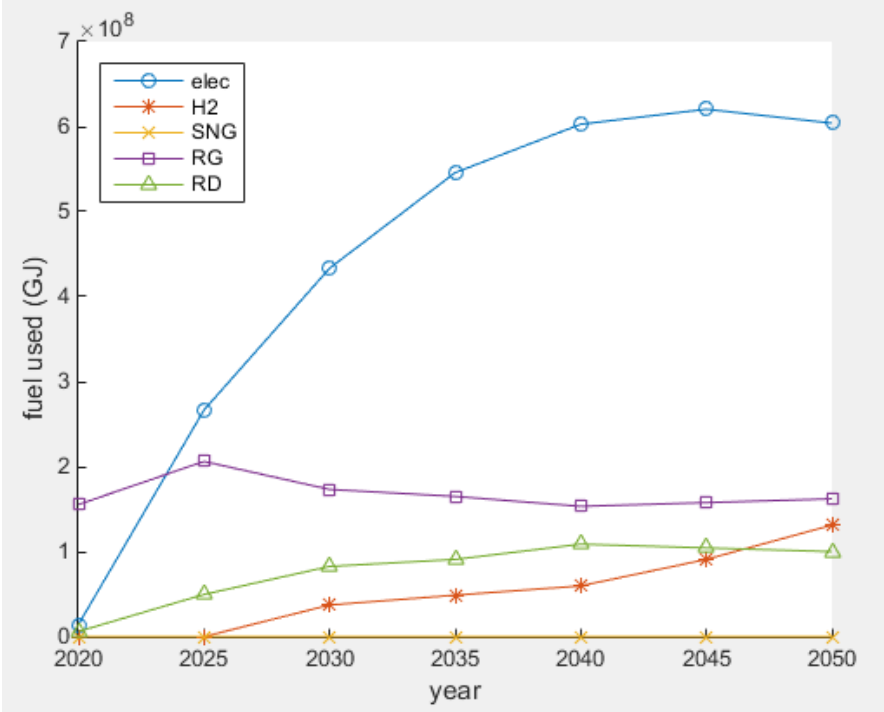

Figure 130. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% fuels used

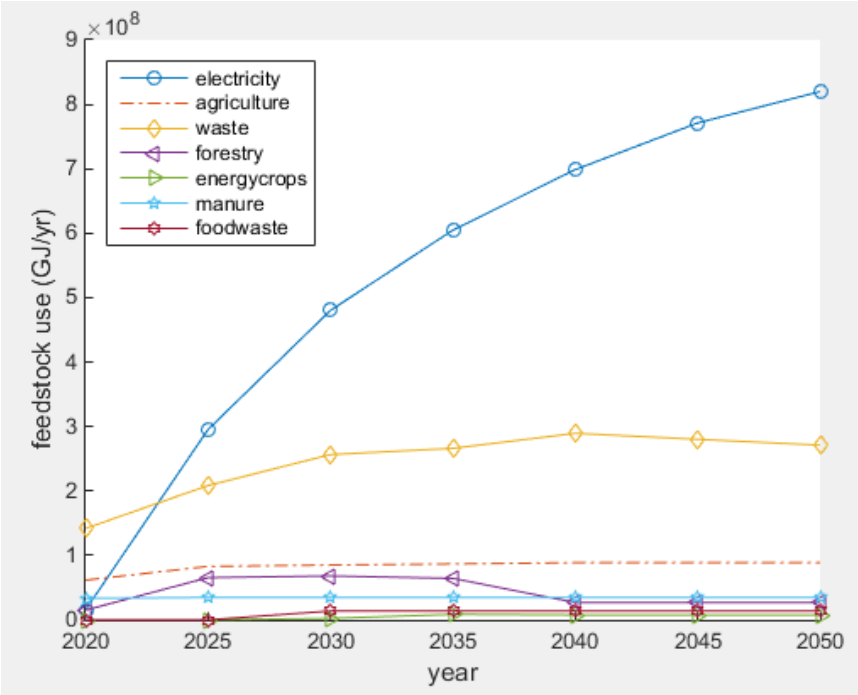

Figure 131. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% feedstocks used

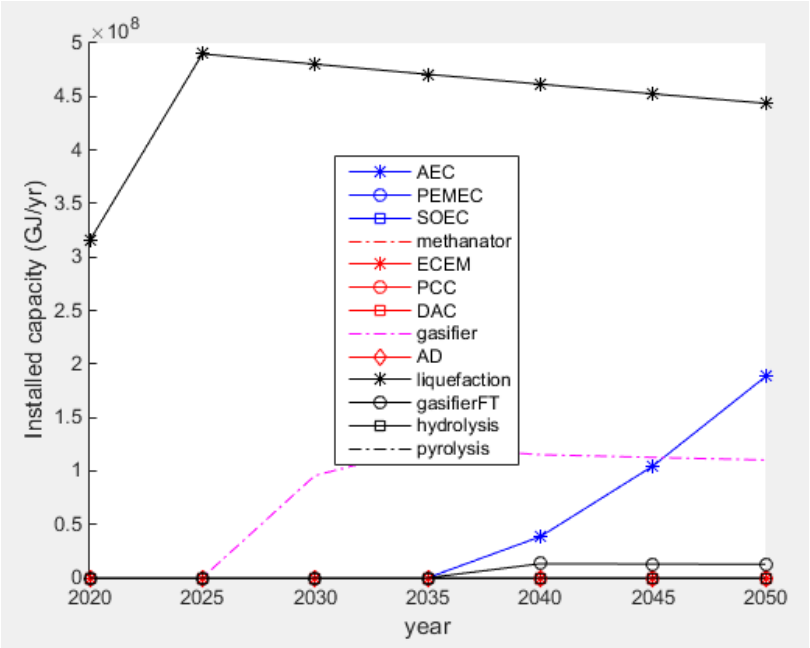

Figure 132. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% fuel production equipment used

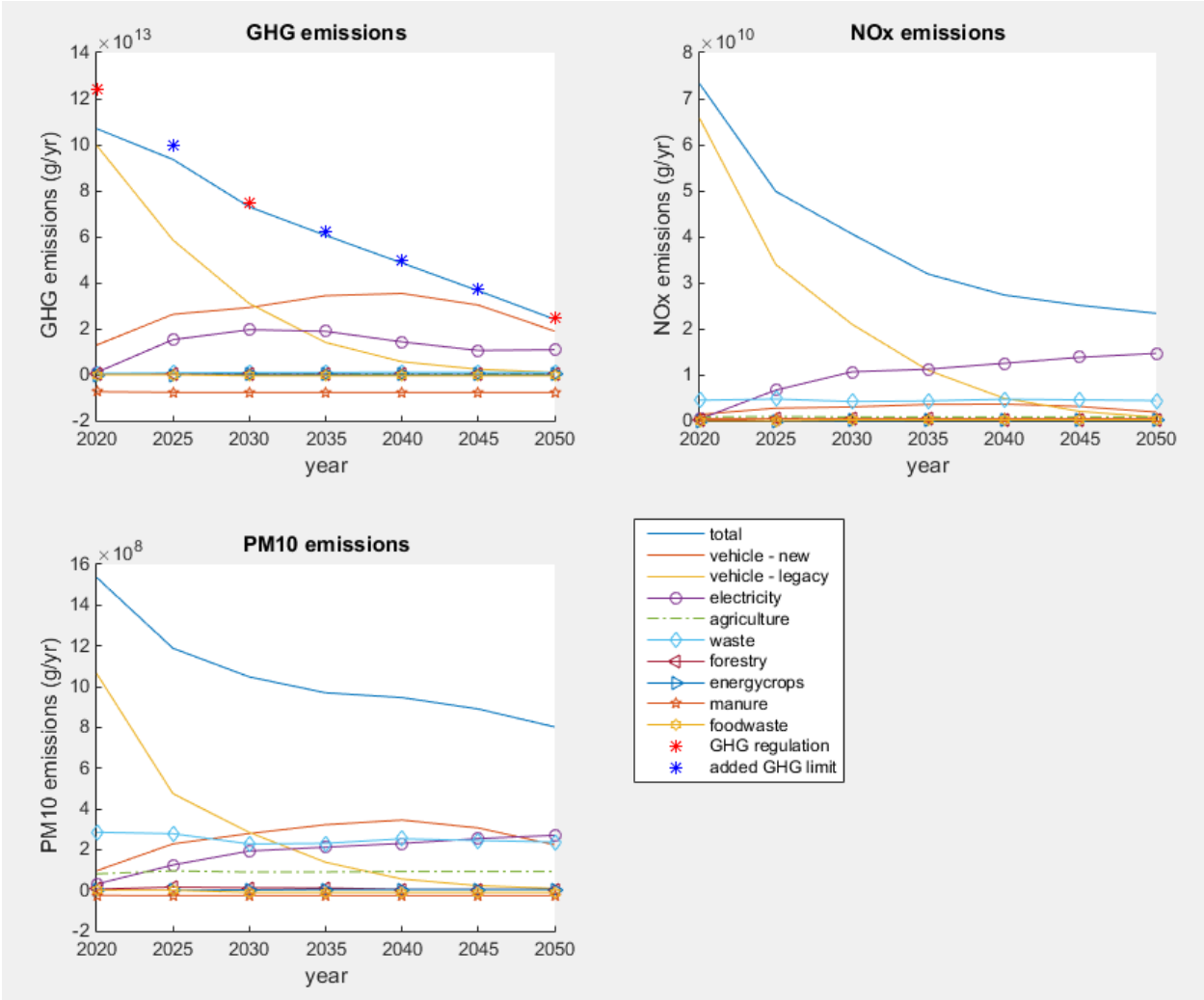

Figure 133. Increase in light-duty VMT by 96% and heavy-duty VMT by 50% emissions

9. SUMMARY AND CONCLUSIONS

9.1 Summary

The goal of this dissertation is to establish viable fuel pathways and powertrain configurations for LDVs and HDVs that meet environmental constraints at the lowest cost. Achieving this goal was accomplished through reviewing related literature, finding major research gaps, and formulating a methodology to fill those gaps. The literature review uncovered two gaps relevant to the goal of this dissertation: 1) techno-economic study of alternative fuel pathways and alternative vehicles is extensive, but studies that consider the combined fuel and vehicle pathways with the various electricity and biomass feedstocks are absent; and 2) no work has been conducted an optimization analysis of the various alternative fuel and vehicle powertrain options that can be used to meet emissions goals. Addressing these two research gaps formed the goal of this dissertation in order to project the optimal evolution of the transportation sector to meet environmental and technical constraints.

Techno-economic analysis for the fuel pathways and powertrain configurations started with data from the literature. Fuel production efficiencies and vehicle efficiencies obtained from the literature were extrapolated when needed for advanced alternatives not yet on the market. Technology costs from the literature were used with Wright's Law and learning rates to project future costs based on cumulative installed capacity. Fuel feedstock emission factor data from the literature and emissions inventories combined with fuel pathway efficiency were used to determine total fuel emissions. Vehicle emissions factors were sourced from emissions inventories and vehicle testing certification.

Model constraints are GHG emissions, VMT, technology deployment rates, and fuel feedstock availability. GHG emissions constraints come from California legislation and an

Executive Order, and CAP constraints from California Air Resources Board's Mobile Source Strategy. VMT projections, as well as the amount of VMT met by new vehicles included in the present modeling, are from emissions inventories. Technology deployment constraints come from various literature sources and U.S. Department of Energy future energy scenarios. Fuel feedstock availability is from modeling in the literature and extensive U.S. Department of Energy biomass characterization.

With the intention of using the preceding techno-economic data and constraints described, an optimization problem was formulated using linear programming. This model, named Transportation Rollout Affecting Cost and Emissions (TRACE), selects from available fuel feedstocks, fuel production equipment technologies, fuel distribution methods, fuel dispensing methods, and vehicle powertrain configurations that can use those fuels. TRACE has the objective of selecting the lowest cost option of meeting transportation needs, both LDVs and four major HDV vocations (linehaul, drayage, refuse, and construction), while meeting the environmental and technical constraints previously detailed. The technology adoption choices reduce future costs of those technologies based on Wright's Law, affecting the results of the proceeding optimization steps.

With the vast number of inputs to TRACE, including numerous efficiencies, costs, learning rates, and emissions factors, sensitivity analyses provide insight into the major components that have the largest impact on results. Some of these components include fuel production technology costs, fuel distribution costs, vehicle costs, P2G plant capacity factors, fuel feedstock costs, technology learning rates, and VMT projections. Note that all of the previous factors are supply-side factors except for VMT projections which are demand-side

factors. Additionally, further constraints such as drayage CAP emissions and ZEV requirements provide insight into the effect of these key scenarios that may face California in the near future.

9.2 Conclusions

9.2.1 LDV Conclusions

- **For the TRACE Non-ZEV Constrained Case, BEVs are a preferred LDV type in 2030 and beyond due to high fuel and vehicle pathway efficiency and moderate fuel distribution and dispensing costs, while PFCEVs begin significant adoption in 2050.**

  While relatively high GHG emission factors generally discourage BEV use in early years of modeling, SB 100 forces electric grid GHG emissions reductions in later years. These emissions reductions, combined with very high fuel and vehicle pathway efficiency, make light-duty BEVs a common choice in many of the cases run without a ZEV constraint. PFCEVs have similar characteristics with higher overall costs, but can use carbon-negative biomass while also providing driver conveniences such as long driving range and short fueling time.

- **With constraints requiring ZEVs, PFCEVs as well as BEVs emerge as the preferred options for LDVs.**

  A ZEV requirement that precludes the sale of any vehicle with an internal combustion engine results in PFCEVs as well as BEVs being preferred for LDVs. PFCEVs achieve the range and fueling times typical of today's ICVs, and, along with BEVs, reduce GHGs an additional 18% and CAPs up to an additional 40%.

9.2.2 HDV Conclusions

- **In the absence of ZEV constraints, ICVs, using renewable diesel produced by liquefaction of biomass, are the preferred HDV until 2045 due to low vehicle cost, low fuel feedstock cost, low fuel distribution and dispensing costs, and lower efficiency benefit of alternative powertrains compared with LDVs. By 2050, HEVs and PFCEVs are adopted for all modeled HDV vocations except refuse due to tightening GHG emissions constraints.**

  HDVs travel significantly fewer miles than LDVs and therefore have less impact on GHG emission reduction. Furthermore, efficiency benefits of alternative powertrains are less significant for HDVs than LDVs, so the cost per mile is lower with the less expensive conventional HDV powertrains than for much more expensive alternative powertrains. In addition, the use of low cost distribution and existing dispensing infrastructure for diesel fuel make renewable diesel-fueled ICVs a common choice for HDVs in most of the cases run. By 2050, due to significantly tightened GHG emissions constraints, all modeled HDV vocations except refuse begin adopting alternative powertrains including HEVs and PFCEVs.

- **With additional constraints requiring ZEV options, PFCEVs are preferred for HDVs due to efficiency and cost.**

  Imposing a ZEV requirement on HDVs leads to an HDV fleet of only PFCEVs. PFCEVs offer high vehicle efficiency and are also modeled to have the lowest cost of heavy-duty ZEVs. This is due to the powertrain specifications of a moderately sized battery and a fuel cell that can be sized smaller than that for a FCEV due to the sizing of the battery.

- **While additional constraints on drayage NO_x and PM_{10} tailpipe emissions do not have a significant effect on the level of CAP emissions, the health impact of such constraints may be significant.**

  Due to the relatively small number of miles traveled by drayage HDVs compared to LDVs and other HDV vocations, the NO_x and PM_{10} tailpipe emissions constraints from California Air Resources Board's Mobile Source Strategy for drayage trucks do not have a significant impact on the total CAP emissions. NO_x emissions reductions are 1.81% and PM_{10} emissions reductions are 4.51% by 2050. However, CAPs are a local issue. Therefore, the importance of utilizing PFCEVs for drayage should not be determined by the percentage reduction of statewide CAPs they enable, but instead by the local CAP reduction they enable at the ports, along freight corridors, and in nearby communities. These local reductions lead to health improvements by those living in affected areas.

9.2.3 General Conclusions

- **Spending more money on alternative transportation technologies in early years can lower total cumulative cost by 2050.**

  TRACE shows that spending more in the early years on alternative transportation technologies can reduce the total amount of money spent in the future. It should be noted that TRACE optimizes on each time step and not for total cost spent in the time horizon of interest and, as a result, it is conceivable that even more money could be saved compared to the Reference Case.

- **The TRACE Non-ZEV Constrained Case that meets environmental goals is 10% less expensive than the Reference Case (i.e., business-as-usual fossil gasoline-fueled**

light-duty ICVs in combination with a majority of fossil diesel-fueled heavy-duty ICVs augmented with some fossil natural gas-fueled heavy-duty ICVs) by 2050.

Adoption of alternative fuels and alternative vehicle types can lead to lower cumulative costs by 2050. The TRACE Non-ZEV Constrained Case LDV and HDV rollout case is projected to cost $1.28 trillion by 2050, 10% less than the Reference Case. This would require additional spending in early years, up to the year 2035, after which the alternative choices using cleaner and significantly renewable fuels as well as alternative vehicles reduces the cost of the transportation sector. While policy makers do not have to choose between saving money and reducing emissions, they have to agree to spend more money upfront.

- **Liquefaction is the preferred fuel production process due to a relatively high efficiency, low VOM cost, and a low cost of accompanying fuel distribution and dispensing as well as vehicle types.**

Most TRACE cases select liquefaction as either the sole or major fuel production process technology. As a method of producing liquid fuels from biomass, liquefaction takes advantage of low-cost fuel distribution, existing fuel dispensing infrastructure, and low-cost conventional ICVs. Compared with the other liquid fuel production technologies, liquefaction has moderate capital cost but low VOM cost and high efficiency.

- **Battery cost has a significant impact on total cumulative cost of the transportation sector.**

Assuming no reduction in battery cost with increased production (a pessimistic but realistic assumption if the same battery technologies are used in the next 30 years), total

cumulative cost of the modeled transportation sector increases by 22%. Therefore, if projections for future battery costs do not predict much decline, this would mean significantly higher cost for the transportation sector to meet emissions goals.

- **Both decreasing and increasing VMT have the potential to substantially change adopted technologies depending on the amount of change in VMT.**

If the future bodes a reduction in VMT for any number of reasons, the result is more reliance on ICVs for LDVs and only ICVs for HDVs due to. An increase in VMT, which could be spurred by the projected lower cost of transportation projected by TRACE among other reasons, pushes the system to react to more VMT that must be met while also complying with emissions constraints. This causes a shift in technology adoption toward more expensive but also cleaner options such as electrolyzers, gasifiers, PFCEVs, and BEVs.

- **The implementation of ZEV requirements results in adoption of light-duty PHEVs as well as BEVs, and adoption of heavy-duty PFCEVs for all vocations with a net result of 18% in additional GHG reductions, 6.6% reduction in NO_x reductions, and 40% in PM_{10} reductions.**

When imposing additional constraints to require only ZEV adoption, it is assumed that heavy-duty ZEV options are available in 2020, which is optimistic for some powertrain configurations and vocations. With such an imposition of constraints, LDVs are projected to be BEVs and PFCEVs, and all HDVs of all vocations are projected to be PFCEVs. The result is an overall increase in cost of 59% compared to without the ZEV requirement by 2050. This strategic adoption of ZEVs leads to 18% lower GHG emissions, 6.6% lower

NO_x emissions, and 40% lower PM_{10} emissions compared to the absence of a ZEV requirement. The resulting scenario yields GHG emissions levels 72.4% lower than Executive Order S-3-05 requires in 2050.

- **TRACE determines the viability of alternative vehicle technologies and identifies the contribution of each technology to meet environmental goals based on a set of constraints. While the constraints analyzed in this dissertation are examples of viable scenarios selected to demonstrate the utility and applicability of TRACE, the results may vary for other scenarios selected for examination. TRACE is thereby a tool for planning by identifying the portfolio of LDV and HDV vehicle technologies and associated fuel supply streams required to meet, on an economic and emissions basis, specific greenhouse gas and criteria air pollutant targets.**

  TRACE is a methodology that provides the means for identifying the portfolio of vehicle technologies and fuel supply streams required to meet environmental goals, as well as analyzing the cost and emissions impacts of any pre-determined scenario. The results of this dissertation are based on the constraints that have been introduced to demonstrate TRACE. Other sets of constraints may result in different fuel production and vehicle technology rollouts. Furthermore, due to the nature of optimization, the results shown are not necessarily the only viable options for meeting a given set of environmental targets.

9.3 Future Work

In general, future work should continue to update cost and efficiency projections as more accurate and up-to-date data are determined. As more accurate data are made available, projections into the future can also be made more accurate.

Further work on CAP emissions would benefit the results as well. More detailed emission factors for the various biomass feedstocks, in particular those that are categorized as straws and

residues in this work that would ideally be individually specified, would allow for more accurate CAP emissions calculations. Deeper investigation on the CAP emissions from the various fuel production processes, fuel distribution, and fuel dispensing, instead of relying on feedstock CAPs, would add greater detail and accuracy to CAP accounting. Lastly regarding CAPs, a spatial accounting and air quality analysis would better capture the impact of resulting CAP emissions changes compared to the CAP accounting of the present work.

The current talk of forestry biomass projections should be further investigated. The Billion Ton Report projects a decline of forestry biomass in 2040 [31], while some forecast an increase in dead and dying trees due to a number of issues such as wildfires and problematic beetle infestations [313].

Similar to the technology rollout constraints for fuel production, there should be analogous vehicle powertrain rollout constraints to ensure there is no unreasonable or impractical increase of any vehicle technology. Some of the TRACE results recommend rapid switching of vehicle technologies. While it may be true that vehicles generally have a shorter lifetime than some fuel production plants, there should not be too drastic of changes in a five-year period of time.

Additionally, material availability, particularly for batteries, fuel cells, and electrolyzers, should be further studied and implemented as additional constraints. These would nicely complement the technology deployment rate constraints and ensure that technologies recommended are feasible to adopt.

The option to optimize with foresight (i.e. optimize the entire window of analysis at once instead of optimizing each individual timestep) would change results and give the pathway with the lowest total cumulative cost. This would also remove the need to apply artificial GHG

emissions constraints for the years that are not legislation or Executive Order. Additionally, this foresight would better take advantage of Wright's Law as currently, the cheapest option that meets constraints is chosen even if choosing another may lead to lower cumulative cost in the future. Both methods of optimization (that of the work of this dissertation as well as the proposed method) have value, and adding the capability to do both would allow for other desired options and further insight into the impact of these adoption choices.

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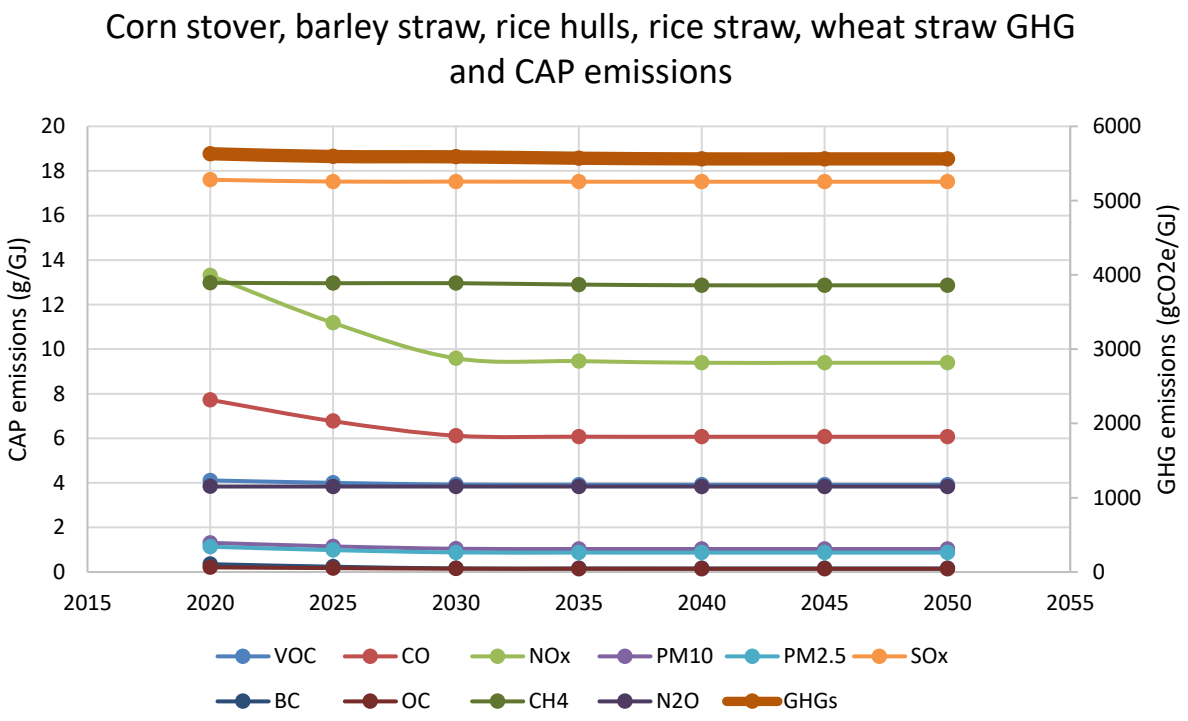
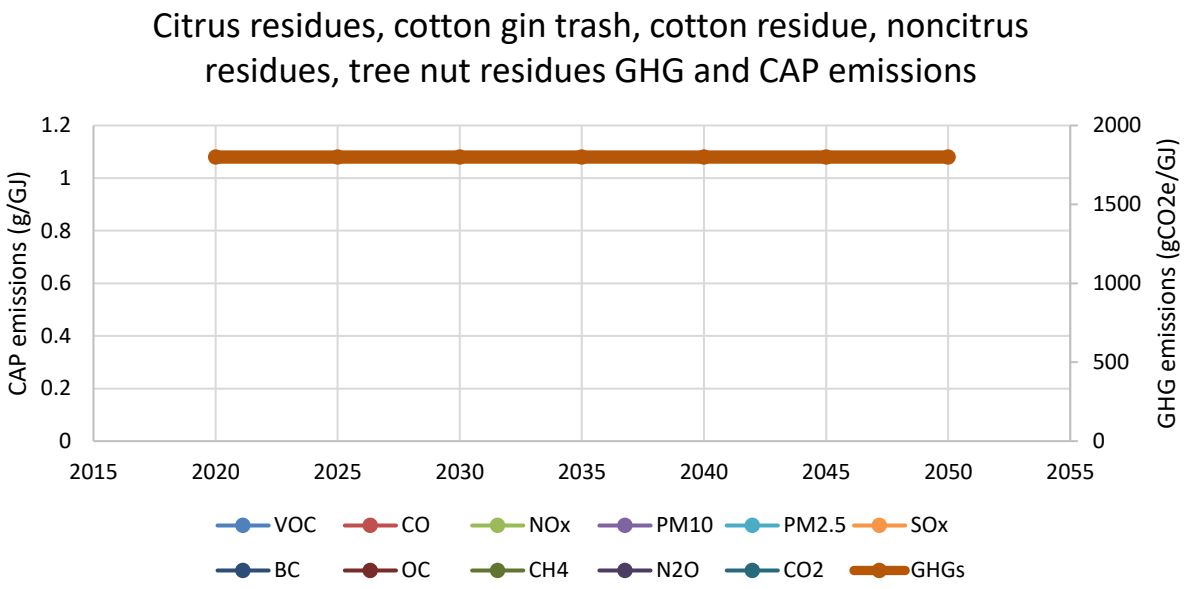
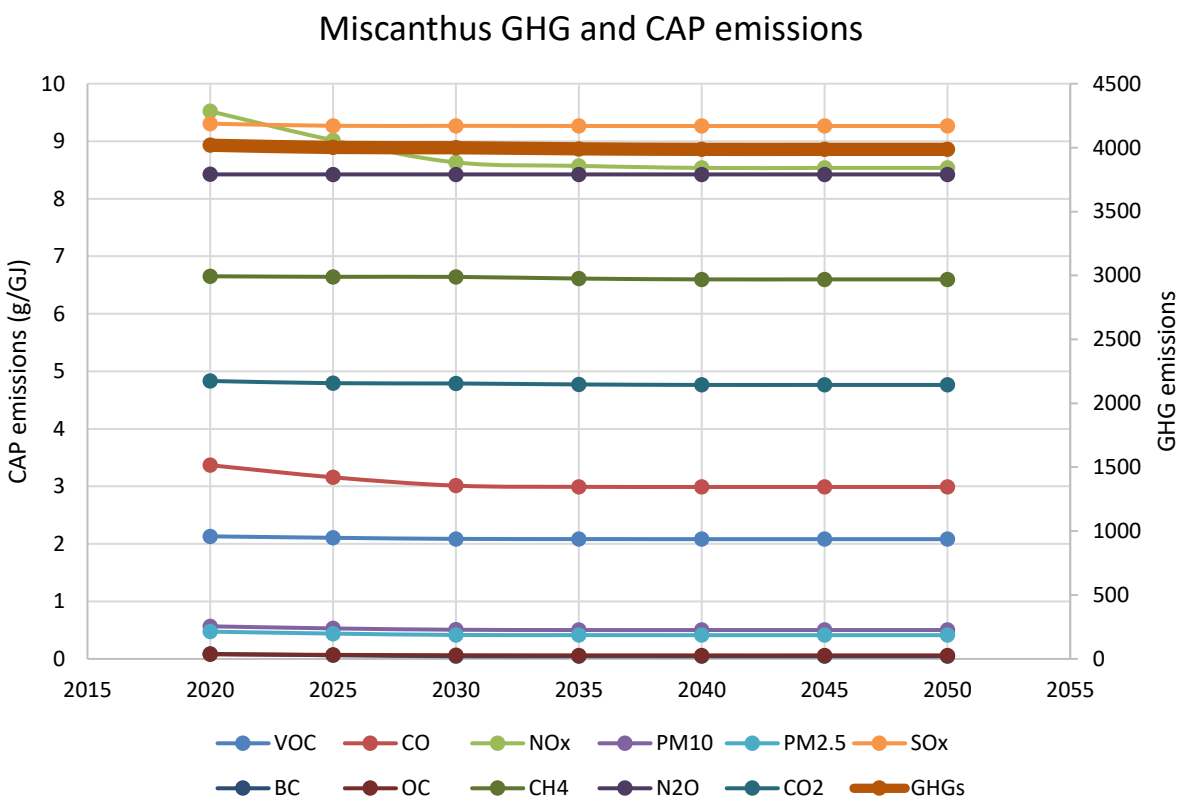
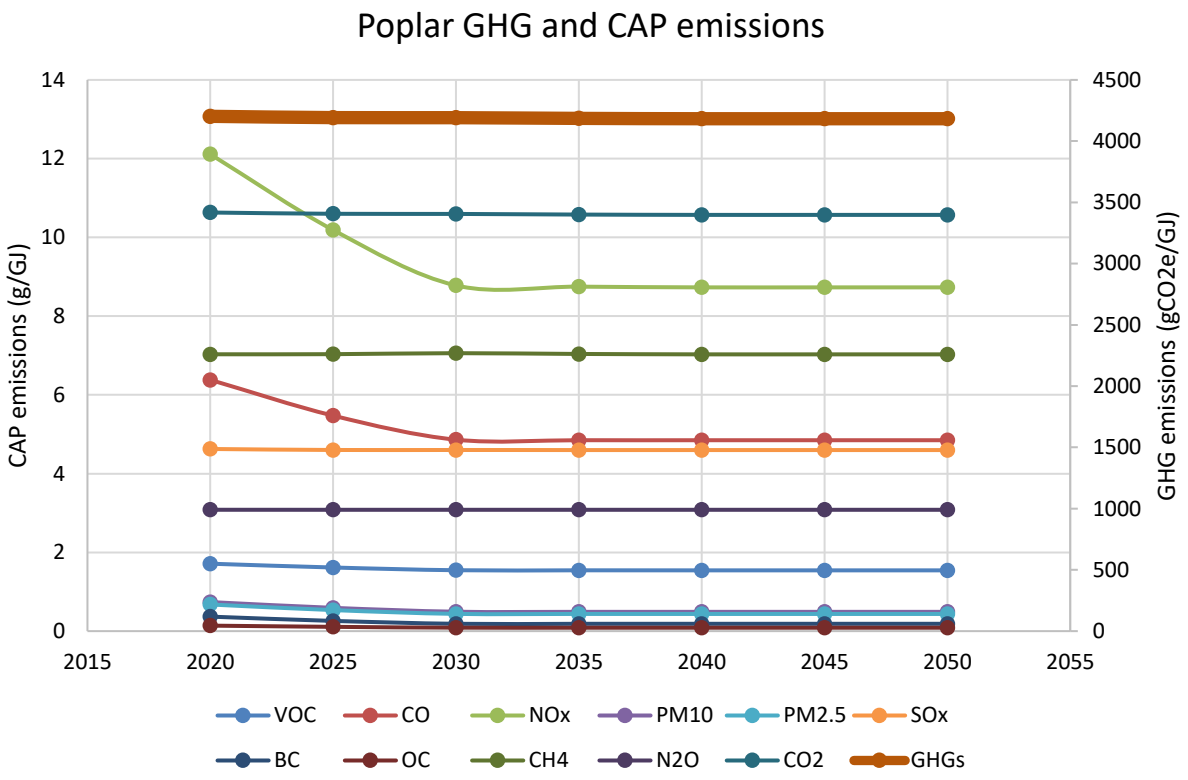
11. APPENDIX A

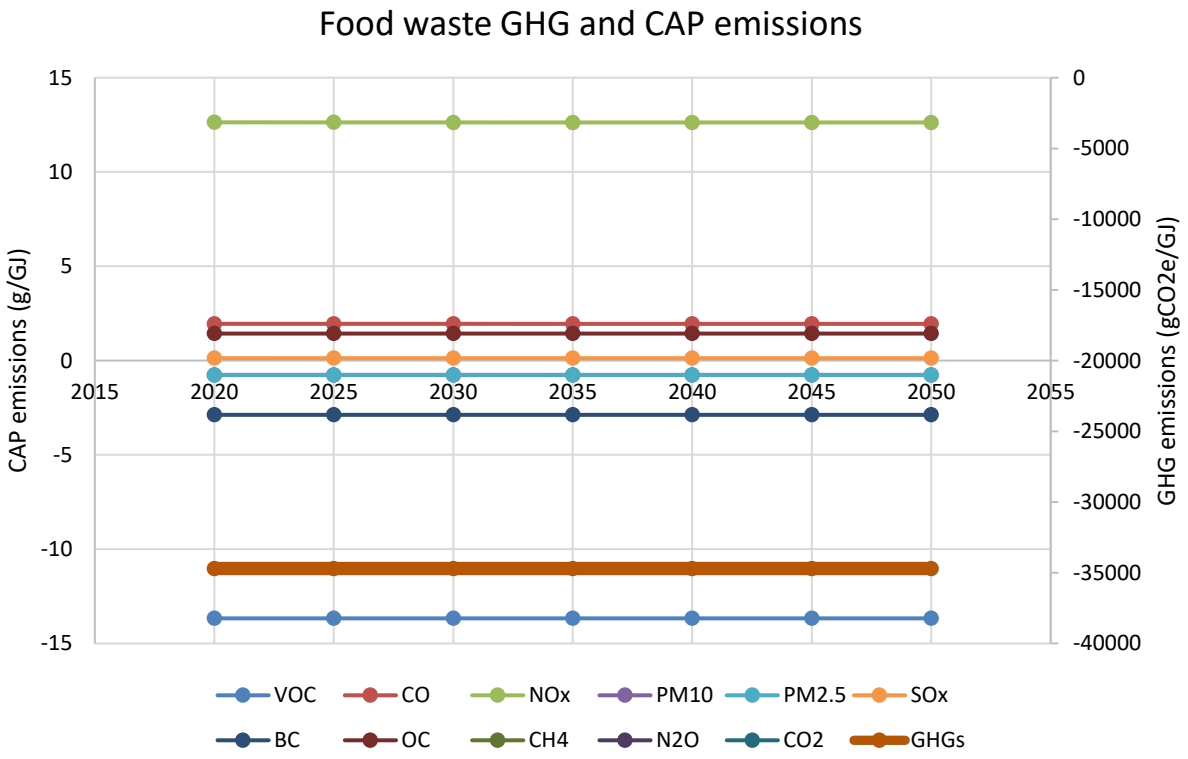
The following are the GHG and CAP emission factors for the various biomass feedstock categories. CAP emission factors are shown on the left y-axis, and GHG emission factors are bolded on the plots and shown on the right y-axis. Recall that not all have CAP emissions found in the literature, and in such scenarios the CAP emission factors of the closest-related category is used in modeling.



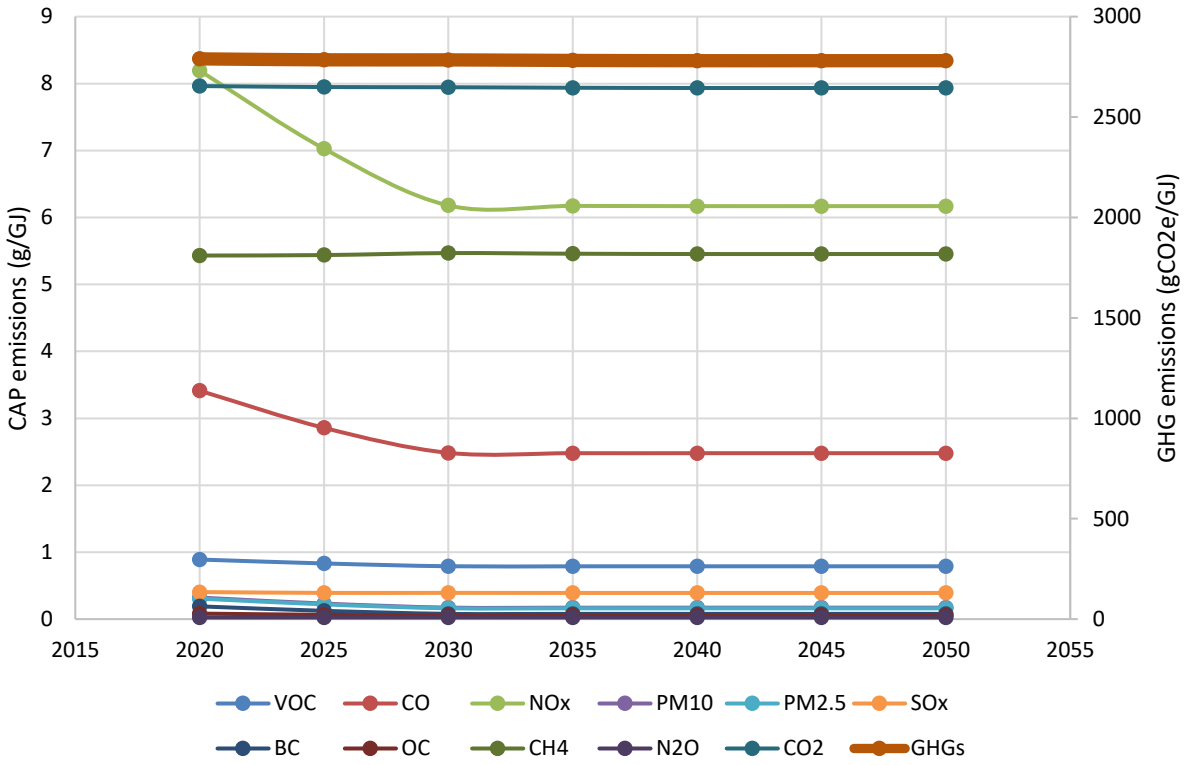

Citrus residues, cotton gin trash, cotton residue, noncitrus residues, tree nut residues GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
1.2
1
0.8
0.6
0.4
0.2
0
2000
1500
1000
500
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs


Miscanthus GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions
10
9
8
7
6
5
4
3
2
1
0
4500
4000
3500
3000
2500
2000
1500
1000
500
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs

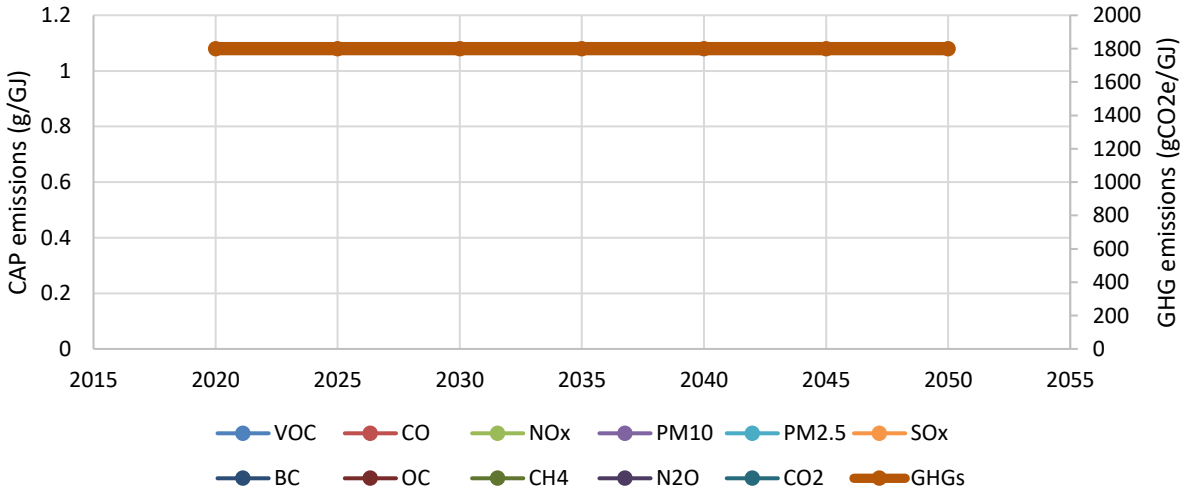

Poplar GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
14
12
10
8
6
4
2
0
4500
4000
3500
3000
2500
2000
1500
1000
500
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs

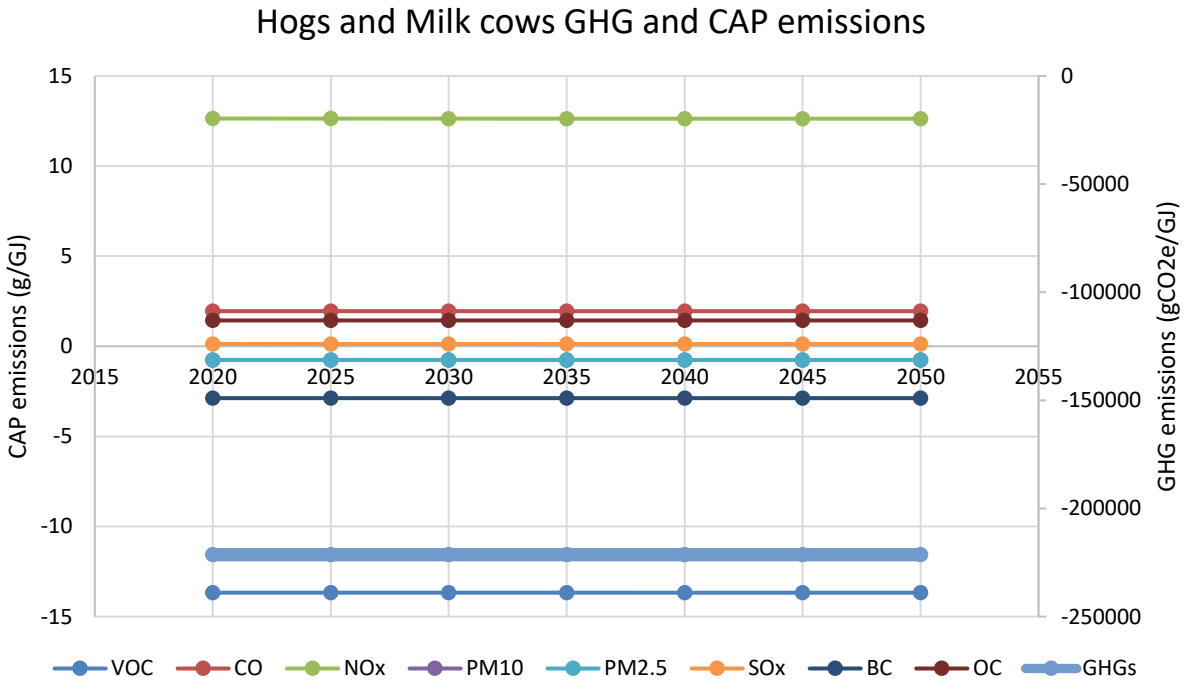

Food waste GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
15
10
5
0
-5
-10
-15
0
-5000
-10000
-15000
-20000
-25000
-30000
-35000
-40000
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs

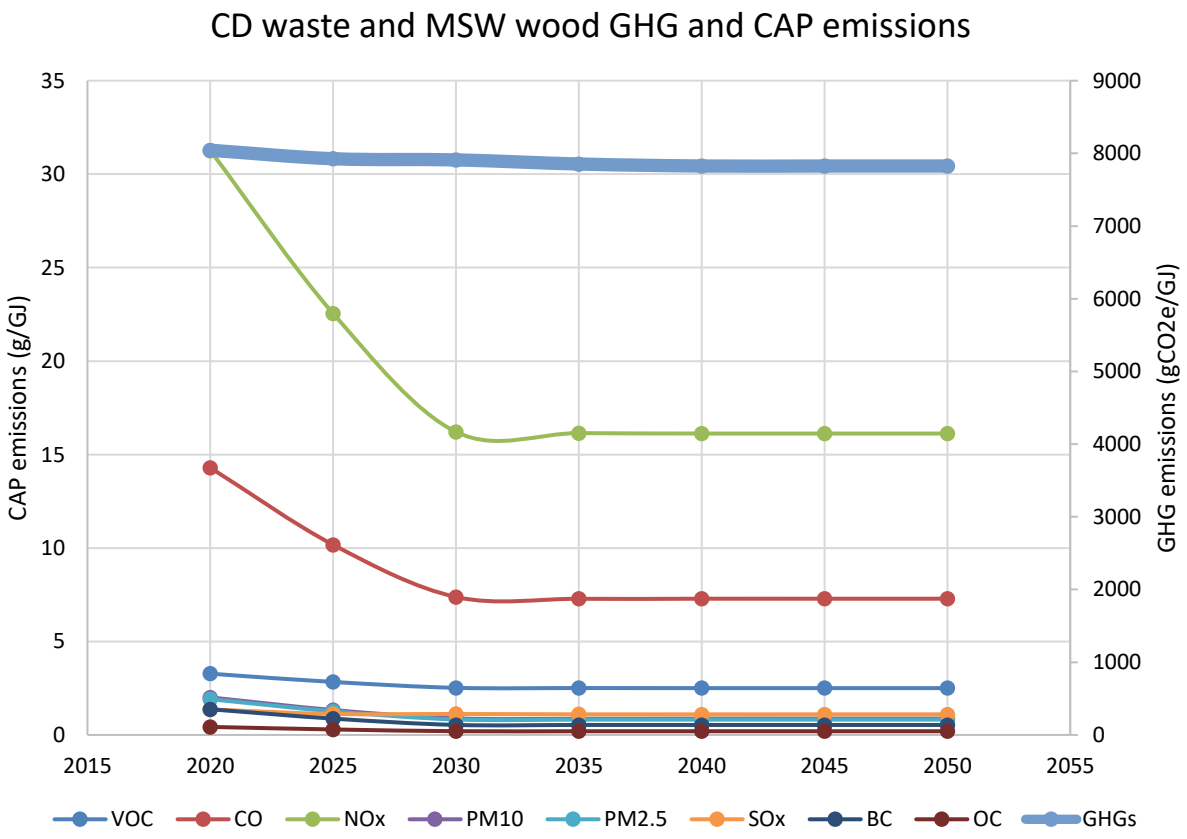
Hardwood, lowland, residue; hardwood, lowland, tree; softwood, natural, residue; softwood, natural, tree; softwood, planted, residue; and softwood, planted, tree GHG and CAP emissions

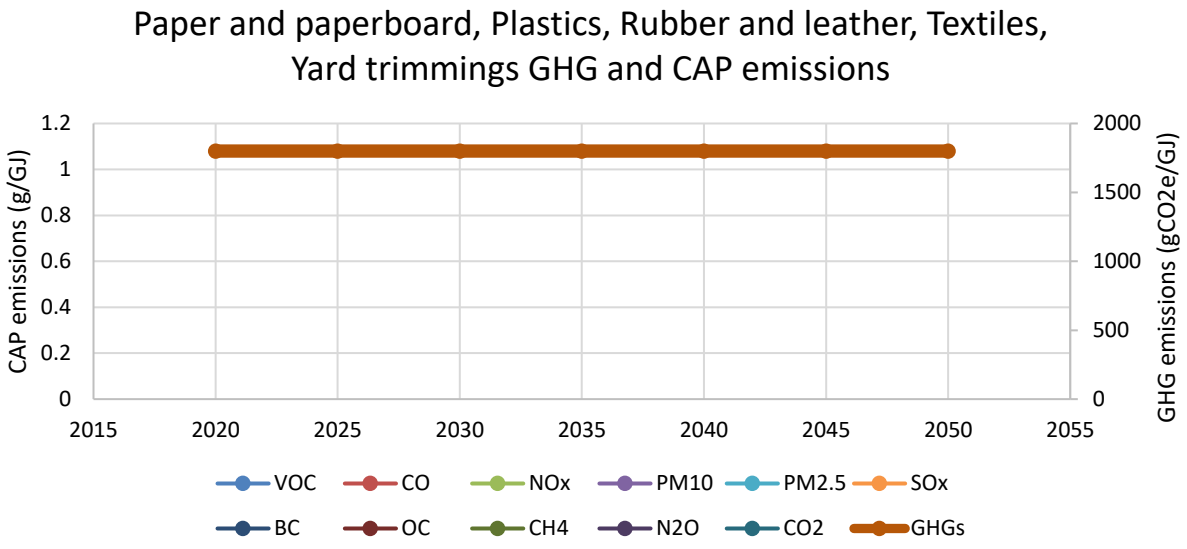


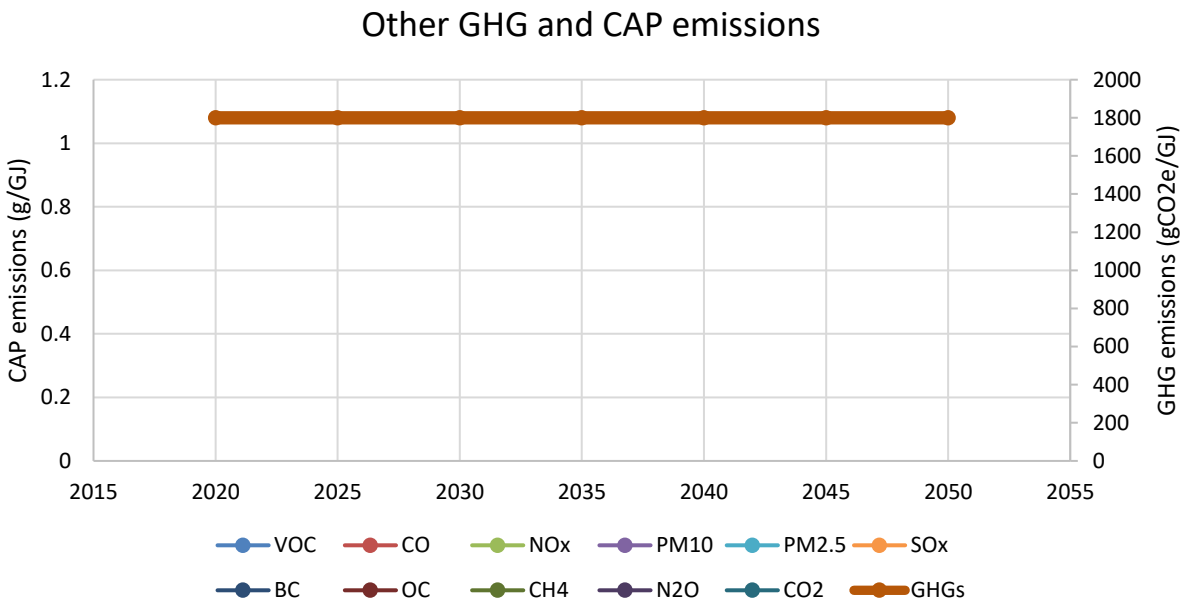
Primary mill residue and Secondary mill residue GHG and CAP emissions




Hogs and Milk cows GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
15
10
5
0
-5
-10
-15
0
-50000
-100000
-150000
-200000
-250000
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
GHGs


CD waste and MSW wood GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
35
30
25
20
15
10
5
0
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
GHGs


Paper and paperboard, Plastics, Rubber and leather, Textiles, Yard trimmings GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
1.2
1
0.8
0.6
0.4
0.2
0
2000
1500
1000
500
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs


Other GHG and CAP emissions
CAP emissions (g/GJ)
GHG emissions (gCO2e/GJ)
1.2
1
0.8
0.6
0.4
0.2
0
2000
1800
1600
1400
1200
1000
800
600
400
200
0
2015
2020
2025
2030
2035
2040
2045
2050
2055
VOC
CO
NOx
PM10
PM2.5
SOx
BC
OC
CH4
N2O
CO2
GHGs

12. APPENDIX B

The following are the vehicle specifications for each of the vehicles modeled, including LDVs, linehaul HDVs, drayage HDVs, refuse HDVs, and construction HDVs.

Table 34. LDV Specifications

Component	ICV	HEV	PHEV	BEV	FCEV	PFCEV
Glider, LDV (ea.)	1	1	1	1	1	1
ICE, gasoline (kW)	98.43	70.84	70.84			
Fuel cell (kW)					114.00	75.00
Traction battery (kwh)		2.16	8.80	60.00	1.60	13.00
Electric motor and inverter (kW)		53.00	53.00	200.00	113.00	112.00
Liquid fuel tank (GJ)	1.74	1.49	1.50			
Hydrogen tank (GJ)					0.61	0.48
Hybrid cost, LDV		1			1	
Plug-in hybrid cost, LDV			1			1

Table 35. Linehaul HDV Specifications

Component	ICV, diesel	ICV, SNG	HEV, diesel	HEV, SNG	PHEV, diesel	PHEV, SNG	BEV	FCEV	PFCEV
Glider, HDV (ea.)	1	1	1	1	1	1	1	1	1
ICE, diesel (kW)	324.00		233.18		233.18				
ICE, SNG (kW)		324.00		233.18		233.18			
Fuel cell (kW)								363.00	238.82
Traction battery (kwh)			15.00	15.00	88.44	89.58	500.00	2.28	15.72
Electric motor and inverter (kW)			120.00	120.00	120.00	120.00	400.00	400.00	400.00
Liquid fuel tank (GJ)	12.61		12.61		11.38				
SNG tank (GJ)		15.86		15.86		14.49			
Hydrogen tank (GJ)								10.91	7.33
Hybrid cost, HDV			1	1				1	
Plug-in hybrid cost, HDV					1	1			1

Table 36. Drayage HDV Specifications

Component	**ICV, diesel**	**ICV, SNG**	**HEV, diesel**	**HEV, SNG**	**PHEV, diesel**	**PHEV, SNG**	**BEV**	**FCEV**	**PFCEV**
Glider, HDV (ea.)	1	1	1	1	1	1	1	1	1
ICE, diesel (kW)	232.09		167.04		167.04				
ICE, SNG (kW)		232.09		167.04		167.04			
Fuel cell (kW)								247.00	162.50
Traction battery (kwh)			30.32	30.32	165.22	169.85	443.26	4.61	31.02
Electric motor and inverter (kW)			85.96	85.96	85.96	85.96	286.53	286.53	286.53
Liquid fuel tank (GJ)	11.20		11.20		9.35				
SNG tank (GJ)		14.09		14.09		12.08			
Hydrogen tank (GJ)								9.69	6.36
Hybrid cost, HDV			1	1				1	
Plug-in hybrid cost, HDV					1	1			1

Table 37. Refuse HDV Specifications

Component	ICV, diesel	ICV, SNG	HEV, diesel	HEV, SNG	PHEV, diesel	PHEV, SNG	BEV	FCEV	PFCEV
Glider, HDV (ea.)	1	1	1	1	1	1	1	1	1
ICE, diesel (kW)	237.66		171.04		171.04				
ICE, SNG (kW)		237.66		171.04		171.04			
Fuel cell (kW)								273.00	179.61
Traction battery (kwh)			30.00	30.00	115.87	123.84	428.57	4.56	25.63
Electric motor and inverter (kW)			88.02	88.02	88.02	88.02	293.41	293.41	293.41
Liquid fuel tank (GJ)	3.60		3.60		2.13				
SNG tank (GJ)		4.53		4.53		2.86			
Hydrogen tank (GJ)								2.66	1.71
Hybrid cost, HDV			1	1				1	
Plug-in hybrid cost, HDV					1	1			1

Table 38. Construction HDV Specifications

Component	ICV, diesel	ICV, SNG	HEV, diesel	HEV, SNG	PHEV, diesel	PHEV, SNG	BEV	FCEV	PFCEV
Glider, HDV (ea.)	1	1	1	1	1	1	1	1	1
ICE, diesel (kW)	172.68		124.27		124.27				
ICE, SNG (kW)		172.68		124.27		124.27			
Fuel cell (kW)								139.00	91.45
Traction battery (kwh)			18.19	18.19	85.81	89.04	299.20	2.76	16.62
Electric motor and inverter (kW)			63.95	63.95	63.95	63.95	213.18	213.18	213.18
Liquid fuel tank (GJ)	5.01		5.01		3.62				
SNG tank (GJ)		6.30		6.30		4.72			
Hydrogen tank (GJ)								3.68	2.54
Hybrid cost, HDV			1	1				1	
Plug-in hybrid cost, HDV					1	1			1