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Viable Pathways in the Energy Sector to Meet California Climate Goals with an Emphasis on Heavy-Duty Transportation and Refinery Emissions

THESIS

Submitted in partial satisfaction for the requirements
for the degree of

MASTER OF SCIENCE

in Civil and Environmental Engineering

by

Margaret Houck

Thesis Committee:
Professor G. Scott Samuelsen, Chair
Professor Diego Rosso
Professor Russell Detwiler

Dedication

To the bears who raised me, the sister who has become a best friend, and the best friend who is more like a sister.

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Abstract of the Thesis

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Master of Science in Civil and Environmental Engineering

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Professor Scott Samuelsen, Chair

According to the State of California progressive climate goals, the energy sector power generation technology mix must evolve by 2045 into a renewable, zero-emissions system. Planning and evaluating options for the technology mix are needed to achieve a cost-effective and timely result. To this end, the State's electric grid is modeled utilizing a least-cost optimization platform with the goal to identify the profile of technologies that fulfills the projected 2045 demand and while achieving both 100% carbon neutrality and minimal criteria air pollutant (CAP) emissions. Heavy-duty vehicles (HDVs) and refineries are prioritized due to their large contribution to emissions in the two highest emitting economic sectors: transportation and industry, respectively. For each of those subsectors, viable electrification scenarios are established and modeled to identify subsector-specific effects on the least-cost technology mix output. Then, the subsector scenarios are combined to evaluate the cost, air quality, and electric grid implications of the multi-sector electrification in the context of a 100% renewable grid.

Using an optimization tool, HiGRID+, two multi-sector scenarios were identified that achieve California 2045 environmental targets. These scenarios implement heavy-duty battery electric vehicle (BEV) and fuel cell electric vehicle (FCEV) deployments along with the substitution of fuel cell systems for refinery processes. Emissions and air quality analyses reveal sufficient emission reductions across the board to meet the State goals. An optimistic versus conservative charging infrastructure analysis revealed that total cost of BEV deployment is driven by charging infrastructure buildout (vehicle to charger ratio) whereas the cost of FCEV deployment is driven by storage capacity assumptions and hydrogen fuel cost. The cost of the two scenarios, one BEV centric and one FCEV centric, are similar.

I. INTRODUCTION

In response to the global climate problem, it is essential that the framework of the electric grid evolves to zero emissions in order to adapt to a sustainable energy future. California has long been a leader in climate initiatives and legislation to address and plan for the goal of carbon neutrality. These state policies mandate goals for the emissions reduction of both greenhouse gases (GHGs) and criteria air pollutants (CAPs), both heavily tied to the generation and use of electric power. As a result, these policies are driving a transformation of the California grid over the next three decades.

The California policies on climate are more progressive and detailed than the rest of the country. A summary of the statewide emissions reduction goals is presented in Figure 1 in combination with the greenhouse gas (GHG) emission reductions over the time covered by each policy. In 2006, Assembly Bill 32 mandated that California reduce GHG emissions to the 1990 levels by 2020 [1]. Senate Bill 32, enacted in 2016, added an additional target past that of AB 32 to promote continued reductions past the 2020 deadline, requiring that the State reach a target 40% below 1990 GHG emission levels by 2030 [2]. In 2018, California Governor Jerry Brown enacted Executive Order B-55-18 which directs the State to be carbon neutral by 2045 and net negative thereafter with the help of carbon capture and storage technologies to outweigh the unavoidable emissions and reduce the concentration of carbon in the atmosphere [3].

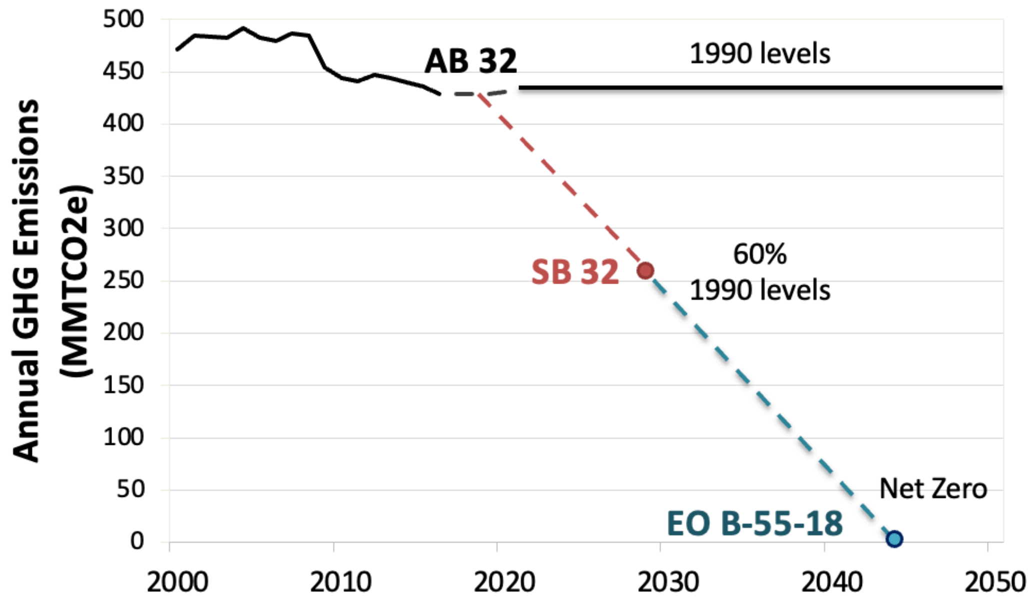

Figure 1: California legislative climate goals as a function of annual GHG emissions over time [4].

In support of statewide emission reduction goals, California has established comprehensive policies that target GHG-emitting sectors (Figure 2) [4]. In particular, reducing emissions from the electric grid has been of primary importance due to the desire to utilize renewable generation to offset emissions from other sectors. To achieve the legislative goals, the Renewables Portfolios Standard (RPS) was established in SB 1078, requiring load-serving entities like electric utilities to acquire a certain portion of their electricity sales from certified renewable sources [5]. The RPS drives the long-term goals by establishing the extent of progress that must be made each year, providing a framework thereby in which to create actionable steps.

In 2018, the State passed SB 100 which requires that all retail sales of electricity must come from renewable and zero-carbon energy sources by the year 2045 [6]. SB 100 also added the interim RPS targets of 44% by 2024, 52% by 2027, and 60% by 2030 (the 2030 target was previously 50% as set in SB 350 [7]). Each of these goals require a systematic restructuring of the grid to reduce if not eliminate the emission of carbon while minimizing system costs.

Specifically, solar and wind build rates need to at least triple and battery energy storage build rates must multiply by eight to accommodate SB 100 electricity and RPS goals [8]. At an hourly modeling level, which is useful for understanding specific technology buildout needs, it is difficult to identify the most practical, low-cost pathway to take to fulfill electric demand with renewables. For this reason, the 2045 targets are the primary focus of this investigation.

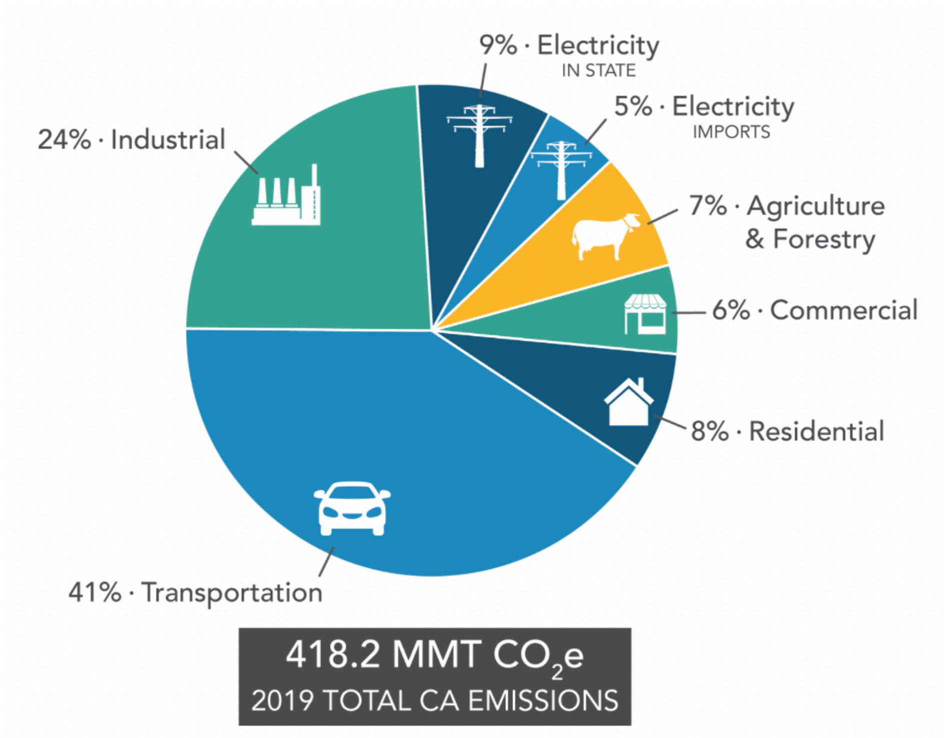

Figure 2: Sector breakdown of California greenhouse gas emissions from 2000-2019 [4].

As shown in Figure 2, the transportation sector accounts for about 41% of the state's greenhouse gas emissions, making it a priority for the reduction of carbon [4]. The State is also well-positioned to utilize renewable generation from the electric grid, either through the charging of battery electric vehicles (BEVs) or through the production and use of electrolytic hydrogen in fuel cell electric vehicles (FCEVs). The Advanced Clean Cars Program imposes multiple regulations designed to achieve GHG and CAP emissions reductions of 40% and 75%, respectively, by 2025 [9]. California also has codified targets for the implementation of electric vehicles (i.e., zero-emission vehicles, “ZEVs”) in order to contribute to large-scale emissions reductions. First, E.O. B-16-12 set the target of 1.5 million ZEVs by 2025 and E.O. B-48-18 set the target of 5 million ZEVs by 2030 [10], [11].Then, the Advanced Clean Trucks program promotes the use of zero-emission vehicles in the medium- and heavy-duty sectors, setting manufacturer sales requirements [12]. Finally, E.O. N-79-20 directs that 100% of new light-duty vehicle (LDV) sales in the state of California be ZEVs by 2035 and 100% of new medium- and heavy-duty vehicle (MHDV) sales be ZEVs by 2045, where feasible [13].

According to the California Air Resources Board (CARB), 24% of California’s GHG emissions come from the industrial sector. Of that, 29% is a result of petroleum refining and the steam reformation production of hydrogen [4]. While a state policy has yet to be established that sets deadlines and limits for GHG industrial emissions, efforts to monitor and regulate GHG emissions are ongoing. Cap-and-Trade is the main strategy that has been established to limit carbon emissions from industrial actors. Additionally, many of California’s 35 regional air quality regulatory agencies have set reduction targets for refinery emissions. For example, the South Coast Air Quality Management District (AQMD) updated its refinery regulations in 2021 to limit emissions of oxides of nitrogen and carbon monoxide generated by specific refinery processes [14], and the Bay Area AQMD recently updated 20 rules (Nov. 2021) under six different regulation categories, all addressing emissions and operations of petroleum refineries under their jurisdiction [15].

A challenge is to project a path, given the variety of existing and emerging clean energy technologies, to reach these goals in the most efficient and cost-effective manner. To this end, a recent study augmented an established California grid planning tool (the Holistic Grid Resource Integration and Deployment tool, HiGRID) with an optimization attribute [16]. The augmented tool (HiGRID+) is an hourly resolved electric grid optimization platform with single and multi-year capabilities that determines the least cost, viable pathway to meet a defined set of electric grid demands and installed renewable resources. HiGRID+ has been used previously to evaluate the optimal uses for otherwise curtailed renewable generation for a decarbonized electric grid [16]. However, sectors with a high rate of GHG and CAP emissions that portend to serve as a barrier to complete decarbonization and removal of criteria pollutants, specifically the heavy-duty transportation and industrial sectors, have yet to be systematically addressed.

The goal of this research is to:

Establish cost optimal pathways in the energy sector to achieve the reduction of carbon and criteria pollutant emissions while meeting the 2045 electric demand for the State of California with a focus on heavy-duty vehicle and industrial decarbonization.

In order to fulfill that purpose, the following objectives must be achieved:

1. Evaluate the current body of literature concerning large scale grid pathways to decarbonization, specifically in the State of California.
2. Develop expertise in the computational tools necessary for this investigation: MATLAB, optimization algorithms, and HiGRID+.
3. Test initial established scenarios created in the development of HiGRID+.
4. Finalize scenarios from the initial findings and additional scenario possibilities that have the most potential to reach the goals and explore each in depth.
5. Analyze results of final scenarios in order to identify best practices and viable pathways to simultaneously meet grid demand, achieve statewide climate goals, and minimize the cost of implementation.

II. BACKGROUND

A. Context

1. Statewide Emissions

The largest contributors to GHG emissions in the State of California are the transportation sector (41%), the industrial sector (24%), and electricity generation (14%) sector (Figure 2). The electrification of vehicles and industrial processes is a key strategy for emissions reductions in the first two sectors with a concomitant demand on the electric grid for which it is neither designed nor prepared to serve, either operationally or environmentally. Therefore, both an enhancement in the supply of electrical power in parallel with the decarbonization of the electric grid are required in order to support cleaner transportation and industrial sectors.

In addition to GHGs, CAPs pose a direct threat to human and ecological health. Figure 3 shows the most recent available (2017) breakdown of NO_x emissions sources in the state of California [4]. NO_x is only one of the six primary criteria air pollutants but, as a precursor to the generation of photochemical oxidant, is a useful indicator of air quality. Additionally, measures that limit NO_x emissions are also effective for limiting other CAPs [17]. According to the CARB inventory, aside from other mobile sources (ships, aircraft, etc.), HDVs are the primary contributor to anthropogenic NO_x in the atmosphere. As a result, the electrification of HDVs has high potential for contributing to overall transportation sector emission reductions.

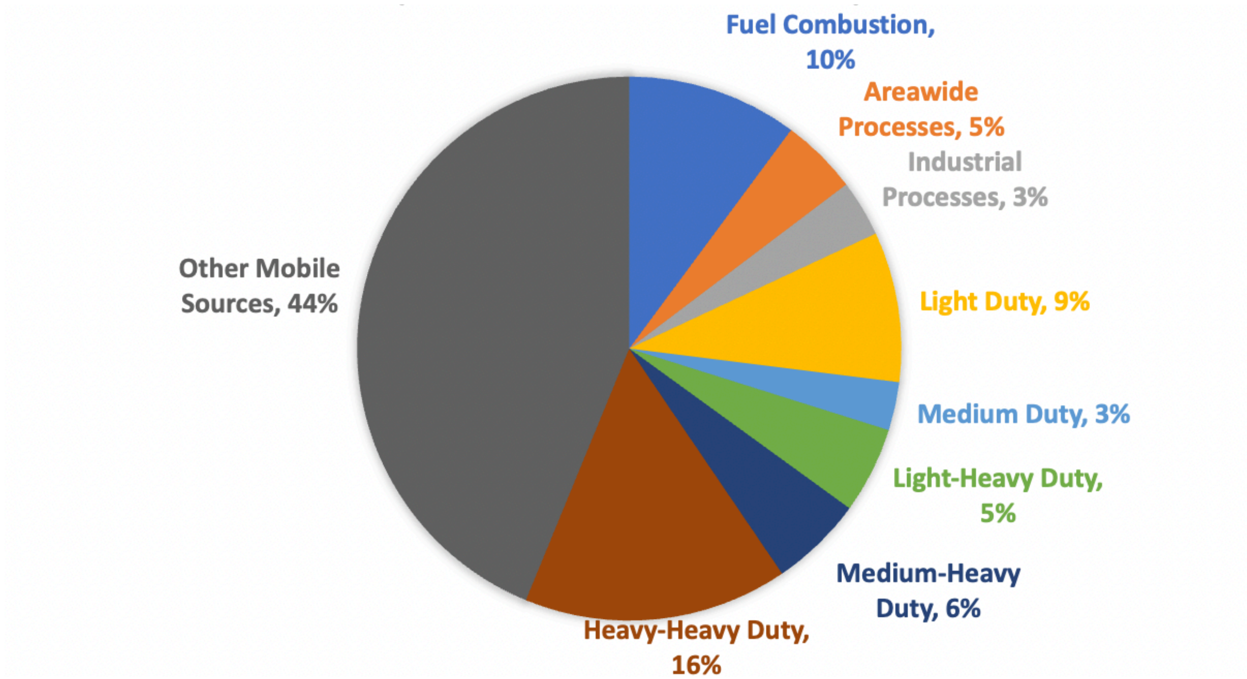

Figure 3: Sector breakdown of 2017 annual NO_x emissions. For reference, total NO_x emissions were about 1500 tons per day. Electric grid NO_x emissions are considered sourced from stationary Fuel Combustion. [4]

2. Electric Grid Composition and Challenges

The electric grid is inherently a source of a wide range of GHG and CAP emissions as a result of California's reliance on non-renewable energy services, primarily natural gas (48.3%) [18]. The distribution of electric generation sources used in 2020 can be found in Figure 4. California's climate goal deadlines have incentivized investments in alternative technologies and carbon offset strategies. According to the California Greenhouse Gas Emissions Inventory, the electric power system was the second largest contributor to GHG emissions until 2013 when it was surpassed by industrial emissions [4]. That drop was, and ideally will continue to be, driven by increased penetration of zero-carbon and renewable generation that offset the need for fossil fuel consumption.

As other sectors move to electrify, like the transportation sector's shift to zero-emission vehicles (ZEVs), pressure grows on the electric grid to supply power to those expanding end uses. As a result, the energy sector works as the nexus of cross-sector emissions reductions. As of 2016, the goal set forth by AB 32 (1990 emissions levels by 2020) was achieved largely due to the reduction of GHG emissions across the electric transmission system, showing that the State of California can adapt to climate goals and that the electricity sector is key in doing so.

Implementation of renewable power generation and storage technologies are essential to the future of a clean grid, but those technologies introduce new barriers that must be overcome through new grid management strategies. An urgent concern is grid resiliency due to the intermittent nature of renewable generation sources like wind and solar [19]. Both sources are subject to weather patterns and daily fluctuations, and solar is affected by hourly changes and cloud cover. In contrast, natural gas power plants function steadily to fulfill baseload, then dynamically by ramping power output up and down to balance the trend of daily consumer demand. Power plant ramping faces a new challenge with the introduction of variable renewable generation as it causes daily power plant demand to fluctuate more rapidly. This causes larger average rates of wear and tear, increasing plant emissions and necessitating grid adjustments. While this will no longer be a problem in a zero-emissions future with the elimination of natural gas power plants, it is an obstacle to the transition.

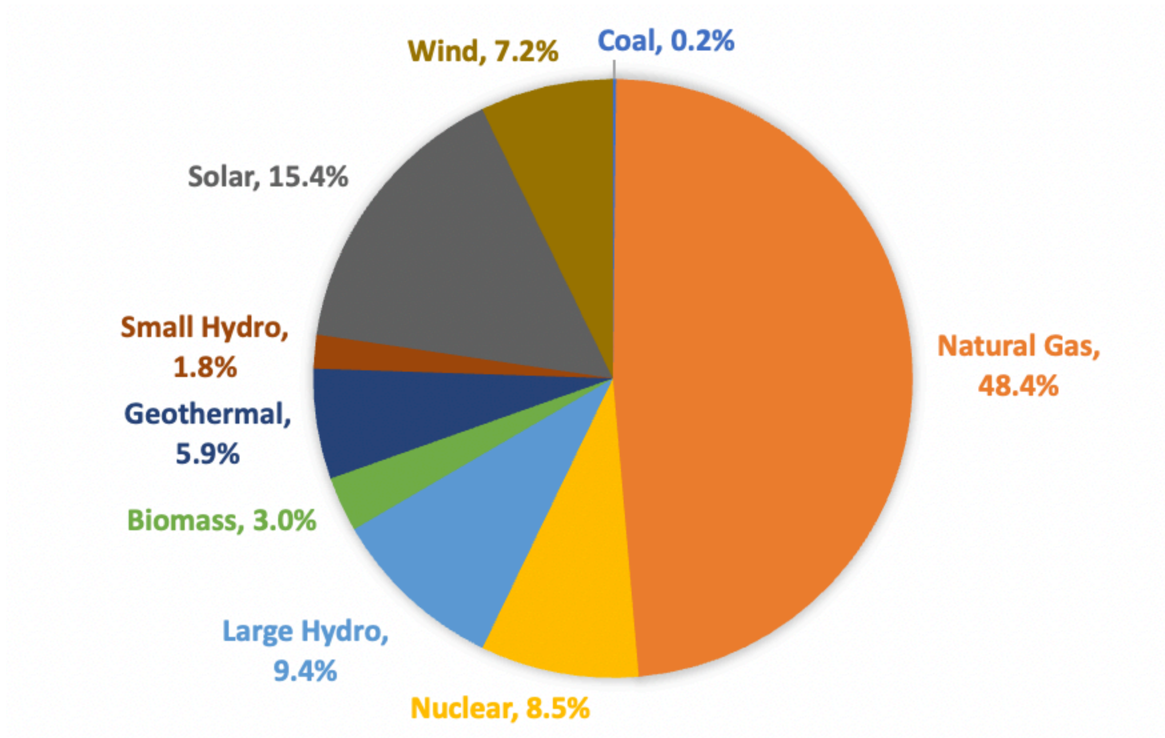

Figure 4: California in-state electric generation in 2020 by generation source. For reference, total system energy is about 191,000 GW. [18]

At times of day when renewable generation is particularly high, mostly from solar at mid-day, a large amount of excess renewable energy (ERE) cannot be used and is instead curtailed. As the statewide capacity of wind and solar resources increases, so does the amount of curtailed electricity from those sources at peak times until there is a technological solution implemented to capture it. Figure 5 shows how the amount of curtailed ERE has increased over the past few years. Energy storage technologies can act as a solution to that problem, storing ERE for use outside of peak renewable generation. However, energy storage is not always the most cost-effective option [20]. Due to the large quantity of ERE and the cost of energy storage (electrolyzers, pumped hydropower, battery technology), at times it is more cost-effective to curtail renewable generation at peak times [19]. Ultimately, curtailed ERE and previous studies into its end uses indicate that diversity in technology development and mix is a promising pathway to maximize reliability and minimize cost.

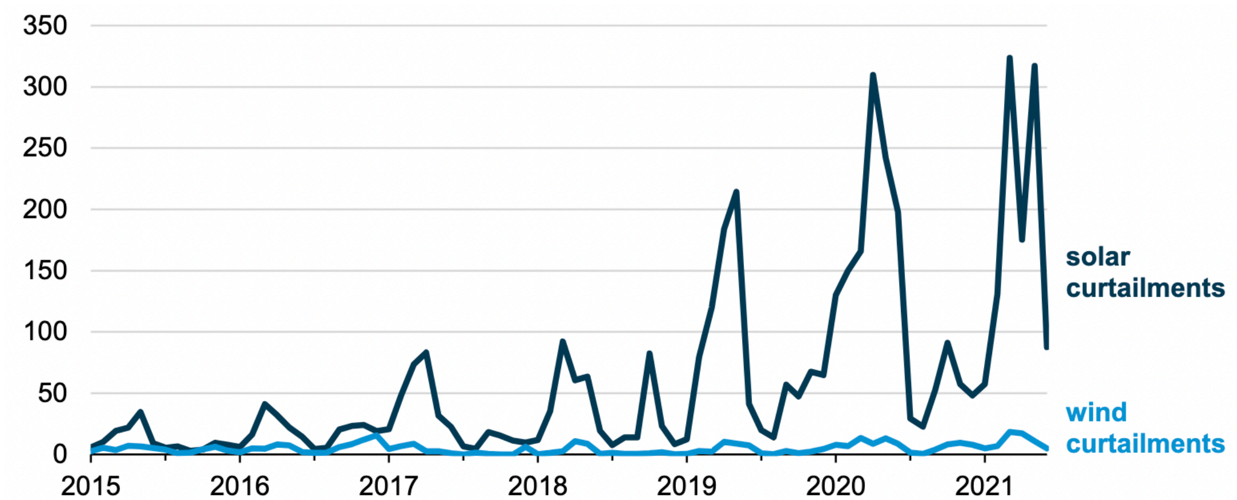

Figure 5: Monthly curtailment of wind and solar electricity in CA, Jan 2015-Jun 2021. [21]

B. Difficult to Decarbonize Sectors

Some sectors, due to the nature of the processes that emit the majority of the GHGs and CAPs, are more difficult to decarbonize. The difficult to decarbonize sectors and the highest emitting sectors (described in the previous section) are correlated due to the challenges they face in transitioning. This thesis focuses on the two highest emitting of these sectors, heavy-duty vehicles (HDVs) and industry, in the context of an electric grid transitioning to renewable and zero-emission technologies.

1. Heavy-Duty Vehicles

Electrification of the transportation sector has already begun, with more than 1 million light-duty ZEVs on the road in California as of 2021, consisting of 63% BEVs, 36% plug-in hybrid electric vehicles (PHEVs), and 1% FCEVs [22]. While battery-centric drive trains have dominated the LDV sector, battery powered HDVs have more obstacles because of battery size, battery and vehicle/payload weight, vehicle range, and charging times [23]. A number of HDV vocations (e.g., long-haul, public transit) have long distance travel applications, so their electrified powertrains have to accommodate trips with a long range. Other HDV vocations (e.g., drayage) have shorter ranges and are able to operate satisfactorily with battery power [24].

Charging infrastructure presents an additional challenge in the heavy-duty space for two main reasons. The first is that charging a high-capacity battery takes much longer than fueling a diesel truck. Some vocations only have one shift a day so can charge overnight, but the rest either must take longer stops for charging or companies must develop a robust cache of battery banks charged at warehouses [25]. The second charging infrastructure challenge is the availability of high-power chargers at the correct times of day. Current public vehicle charging infrastructure includes Level 2 AC chargers and DC fast chargers. While Level 2 chargers can be used for overnight charging of light-, medium-, and some heavy-duty vehicles, they are insufficient to charge the largest HDVs and therefore not a comprehensive option [25]. DC fast chargers can charge light- and medium-duty vehicles quickly, or some HDVs overnight but are not able to charge class 7-8 HDVs in short times [25]. Ultimately, in order to build a sustainable zero-emission HDV future that includes BEVs, an investment in higher power, shorter charge time charging infrastructure around the country is required.

Alternative fuels, more specifically FCEVs utilizing hydrogen fuel, also present a size-efficient solution [26]–[29]. They have emerged as a feasible option because hydrogen has a higher gravimetric energy density than gasoline, so it can be compressed and stored on board without imposing as much extra weight as a battery on an already heavyweight system [30]. FCEVs also have comparable fueling times and ranges to internal combustion engine vehicles, making them more competitive than BEVs on that metric in the heavy-duty space [31]. Implementation of FCEVs creates vehicle hydrogen demand (VHD) that motivates hydrogen infrastructure development, allowing for further development of a multi-end use hydrogen economy. Specifically, hydrogen converted to electricity by fuel cells for the electric grid, or electricity hydrogen demand (EHD), is a key part of the diversification of economy-wide uses of hydrogen.

However, FCEVs come with their own challenges. Like BEVs with charging infrastructure, hydrogen fueling infrastructure is a large barrier to FCEV penetration. According to the California Fuel Cell Partnership, 8 hydrogen stations in California are dedicated to heavy-duty refueling and over 50 additional open and online retail stations [32]. Compared to an estimated more than 10,000 diesel and gasoline stations in the state, that is very early infrastructure for a mode of transportation and severely limits the expansion of FCEV technology at all payloads [33]. In order for FCEVs to be truly zero-emission, the hydrogen production infrastructure must also evolve. As of June 2021, 95% of global hydrogen was gray hydrogen, or hydrogen produced from fossil fuels without the use of any carbon capture and storage (CCS) technology [34]. Gray hydrogen compromises the idea of life cycle zero-carbon transportation, so a transition including FCEVs requires investment in carbon-neutral green hydrogen production methods. Those methods include electrolytic hydrogen using electricity from renewable resources, biogas reformation, and artificial photosynthesis [34].

Once a ZEV fleet mix develops, the shift to electrification will have a notable effect on the grid. BEVs and FCEVs both increase grid demand profiles because BEVs draw power directly from the grid and green hydrogen production for FCEV fueling draws power from the grid for electrolysis albeit utilizing to some extent excess renewable resources.

Electrification will increase peak demand, which is a good indicator of system cost because it defines the maximum capacity at which the grid must be able to comfortably operate [35]. Even though generation does not have to constantly meet peak demand, the transmission system must be able to accommodate it to prevent outages. Fortunately, BEV charging and electrolysis for hydrogen fuel can be considered flexible loads. BEV charging time and rate can be adjusted by the customer manually or smart charging systems can optimize when a network of BEVs charge to minimize cost and strain on the grid [35], [36]. Hydrogen production is even more flexible because the timing of production is not tied to the timing of vehicle fueling; fuel is produced ahead of time, transported to the fueling station, then extracted according to customer needs [37]. Ultimately, the capacity of the electric grid must increase as demand naturally increases over time in addition to the vehicle electrification load. With continued expansion and investment in renewable generation sources, compatible energy storage, and load shifting strategies, peak load can be met and rapid daily ramping managed.

2. Refineries

Industrial emissions account for 24% of 2019 California GHG emissions, making industry the second highest emitting sector in the state [4]. Of those emissions, Figure 6 shows the largest subsector contributors: petroleum refining and hydrogen production (29%), manufacturing (26%), and oil and gas production and processing (17%) [4]. For the purposes of this investigation, petroleum refineries are the primary target for decarbonization and CAP emissions reductions because of the unique challenges they face. Refineries are considered difficult to decarbonize due to the disperse nature of their internal pollution sources. Instead of there being one primary process responsible for emissions, refineries "may emit CO_2 from well over 100 point sources" [38]. Figure 7 describes the flow of fuel through a medium conversion refinery, and the red arrows indicating CO_2 emissions sources illustrate the complexity of refinery decarbonization. As a result, the solution must be equally complex, addressing the most egregious processes and pieces of machinery as possible to minimize emissions.

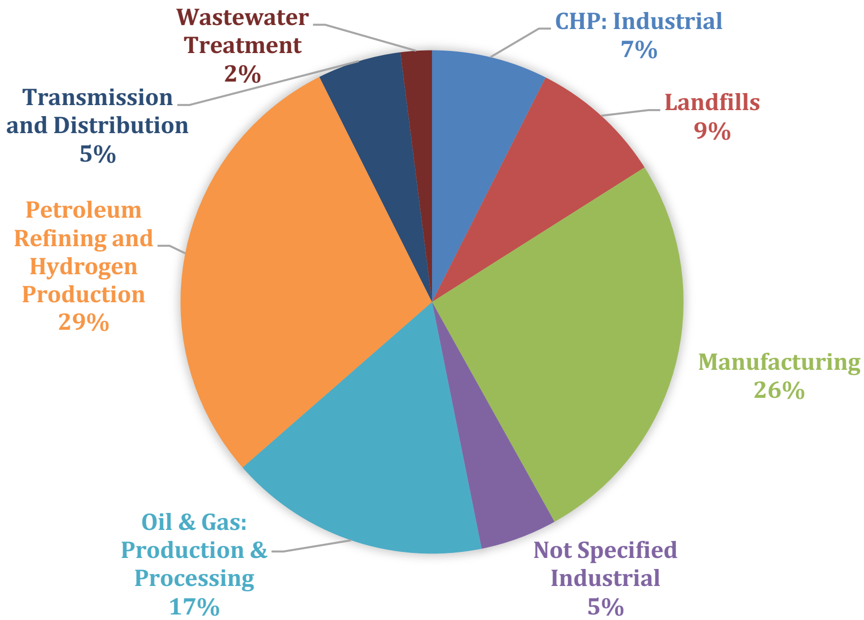

Figure 6: 2019 Industrial GHG Emissions by Subsector (Total = about 100 MMT CO2e). Data: [4]

There are, however, available strategies for combatting refinery emissions. Electrification of the full transportation system reduces demand for hydrocarbon fuels, therefore reducing the product and emissions output of refineries. While this is a benefit, a zero-carbon economy cannot rely on the eradication of refineries because of the market's need for non-fuel refinery products. Refineries produce a wide range of products including petrochemicals, plastics, asphalt, and a variety of hydrocarbon fuels primarily for transportation [39]. The approach to emissions minimization must include both the reduction of hydrocarbon fuel demand and refinery decarbonization.

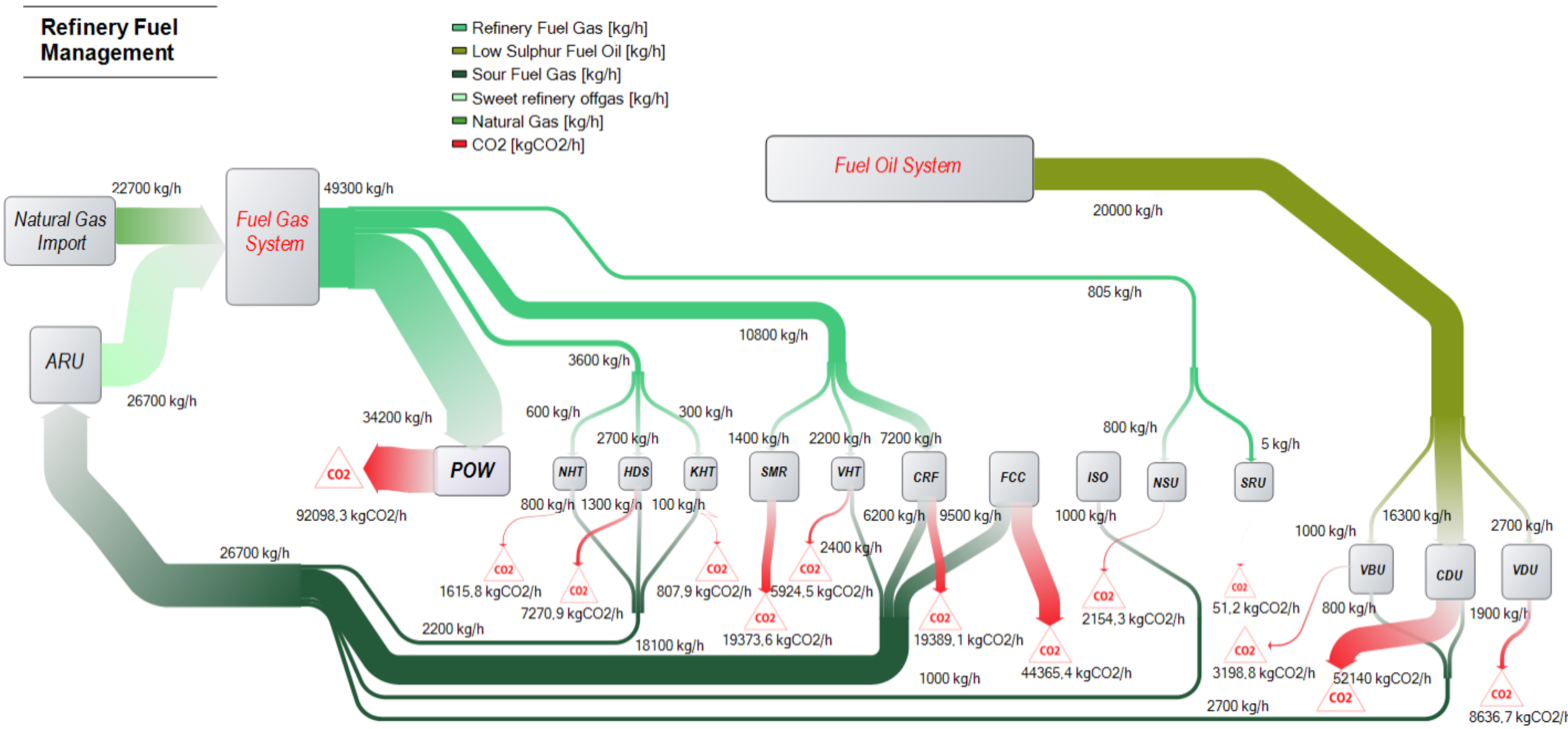

Figure 7: Sankey diagram of fuel management and primary CO2 emission point sources in a simplified medium conversion refinery. [40]

Fuel cells use electrochemical reactions to convert a fuel (e.g., natural gas, biogas, hydrogen) to electricity without using combustion, allowing them to be highly efficient and extremely low in pollutant emissions [41]. In a refinery, fuel cells can replace power plants, heaters and boilers, and steam methane reformation (SMR) units among other processes [40]. Operating on natural gas, the emission of carbon would be reduced, and the emission of CAPs reduced to virtually zero as a result of both the higher fuel-to-electricity efficiency of fuel cells and the capture of the high-quality exhaust heat to displace the use of fossil-fuels in heaters and boilers. Using green hydrogen as the fuel would further reduce the carbon, virtually to zero as well. Therefore, fuel cell systems are a viable substitute for the highest emitting refinery processes. Like the transportation system, the shift to zero-carbon operation at refineries requires the overhaul of the hydrogen production system to generate renewable green hydrogen instead of blue or gray hydrogen [34].

C. Thesis Positionality

This thesis seeks to fill the following four gaps in established literature with the goal to identify options for least-cost technology mixes in 2045 that minimize CAP emissions, achieve the 100% decarbonization target, utilize multi-sector integration, and meet the electric load demand:

First, many analyses of pathways to decarbonization are less stringent in that they target the previous policy goal of an 80% reduction of direct GHG emissions instead of the most recent goal of zero net emissions by 2045 [42]–[45].

Second, updated modeling is necessary to evaluate the technological shift options based on least cost to reach the 2045 target and thereby inform policymakers and agencies faced with the development of investment strategies and incentive programs that are required to achieve the 2045 mandate. Not all the current body of literature optimizes according to least cost [43], [45].

Third, an important characteristic of this investigation is that it prioritizes the reduction of both GHG and the emission of criteria air pollutants. The regulatory trend and trend in the literature has focused on decarbonization in the absence of air quality considerations, the latter of which is necessary to implement a just transition and protect communities [16], [42], [44]–[47]. This analysis aims to have the maximum possible impact by including considerations for both GHGs and CAPs.

Finally, this thesis conducts a multi-sector analysis by including changes to the electric grid, transportation sector, and industrial sector, while previous research in the field is either single-sector or limited multi-sector [16], [43], [45], [46], [48], [49].

The combination of these four attributes situates this thesis in a gap in literature that is valuable for audiences including policymakers, agencies, investors, sustainable energy academics, and non-government organizations (NGOs).

III. APPROACH

Task 1: Evaluate grid pathway literature.

This task investigates California policies and goals to ensure that the constraints of the HiGRID+ model include all the codified constraints provided by the State. Additionally, a review is conducted of previous and current approaches to designing a grid framework that achieves sustainability goals. That investigation requires evaluation of popular computational grid modeling tools, national and state policy plans, and an interdisciplinary understanding of grid dynamics and demands. Ultimately, this task serves to attain a familiarity with grid demand, load profiles, renewable and non-renewable generation technology, energy storage technology, and other steps in grid life cycle analysis. It also includes specific research into difficult to decarbonize sectors in order to choose what elements of decarbonization need to be prioritized.

Task 2: Computational tool expertise.

In order to achieve the technical skills to complete this investigation, this task requires the development of mastery of the MATLAB coding language through online resources and hands-on practice with the HiGRID+ script. For the HiGRID+ optimization extension, Task 2 explores the use of optimization algorithms in terms of their mathematical background and computational implementation. A comparison between the general framework of optimization algorithms and the HiGRID+ optimization structure is also a necessary element of this task. Finally, computational tool expertise includes becoming familiar with the structure and implementation of the HiGRID+ code in order to model a variety of specific scenarios, compare them, and evaluate their viability. HiGRID+ has the capability of incorporating additional constraints that are specific to the difficult to decarbonize sectors identified in Task 1, and Task 2 informs how those constraints can best and most accurately be applied.

Task 3: Interrogate established scenarios.

Using the background knowledge attained in Task 1, this task reevaluates the preliminary results relevant to the research developed using the HiGRID and HiGRID+ tools. Previous results were sourced from academic research (namely recent theses and dissertations) that informed the creation of the HiGRID and HiGRID+ models. Confirming previous results and exploring their significance in relation to a holistic grid framework allows this investigation to refine the methods of grid modeling and identify the gaps in current literature. This task involves identifying boundaries in the use of HiGRID+ and how these limits can be pushed to achieve new results. In order to put sector-specific results in the context of full-grid dynamics, this task also requires a deep dive into the chosen difficult to decarbonize sectors: heavy-duty vehicles and refineries. Ideally, it answers the question: where are carbon and criteria pollutant emissions coming from in these sectors, what technologies or strategies exist to mitigate those, and what are the cost implications of those solutions?

Task 4: Finalize scenarios for in-depth investigation.

Task 4 compiles a combination of previously explored and unexplored pathway scenarios based on the evaluation in Task 3 in order to investigate that shortened list in depth. The overall goal of the research comes to the forefront in this task, as it includes very specific, quantitative pathways to simultaneously clean the electric grid and electrify heavy-duty transportation and industrial sectors. Each scenario explores a different way of prioritizing technologies like BEVs, FCEVs, molten carbonate fuel cells (MCFCs), solid oxide fuel cells (SOFCs), etc. The goal of this task is to compare pathway scenarios, identifying strengths, drawbacks, and important across the board considerations that contribute to the viability of each option/modification.

Task 5: Analyze results.

Task 5 involves completing a final evaluation of pathways and the identification of a select few least-cost viable scenarios as recommendations for the state of California in meeting the 2045 (1) climate goals with an emphasis on heavy-duty transportation and refinery emissions, (2) electric grid demand, and (3) the CAP reduction target projected to achieve the level of urban air quality required to protect the health of the under-served as well as the general population.

IV. METHODOLOGY

A. HiGRID+

The Holistic Grid Resource Integration and Deployment tool, “HiGRID,” was developed to analyze the balance of baseload, dispatchable, and intermittent renewable generation technologies as renewables are increasingly introduced into the technology mix [50]. HiGRID takes hourly electric demand, technology-specific parameters, and operating constraints as inputs and generates an hourly operation profile of each installed generation and storage technology that meets demand, and outputs the GHG emissions of the technology mix. The four main modules include Renewable Generation, Dispatchable Load, Balance Generation, and Cost of Generation. Figure 8 lists the technologies modeled by each module along with a description of what they do [51]. This model is useful in assessing the performance of the electric grid in response to a portfolio of emerging technologies, particularly those essential to renewable power generation and decarbonization.

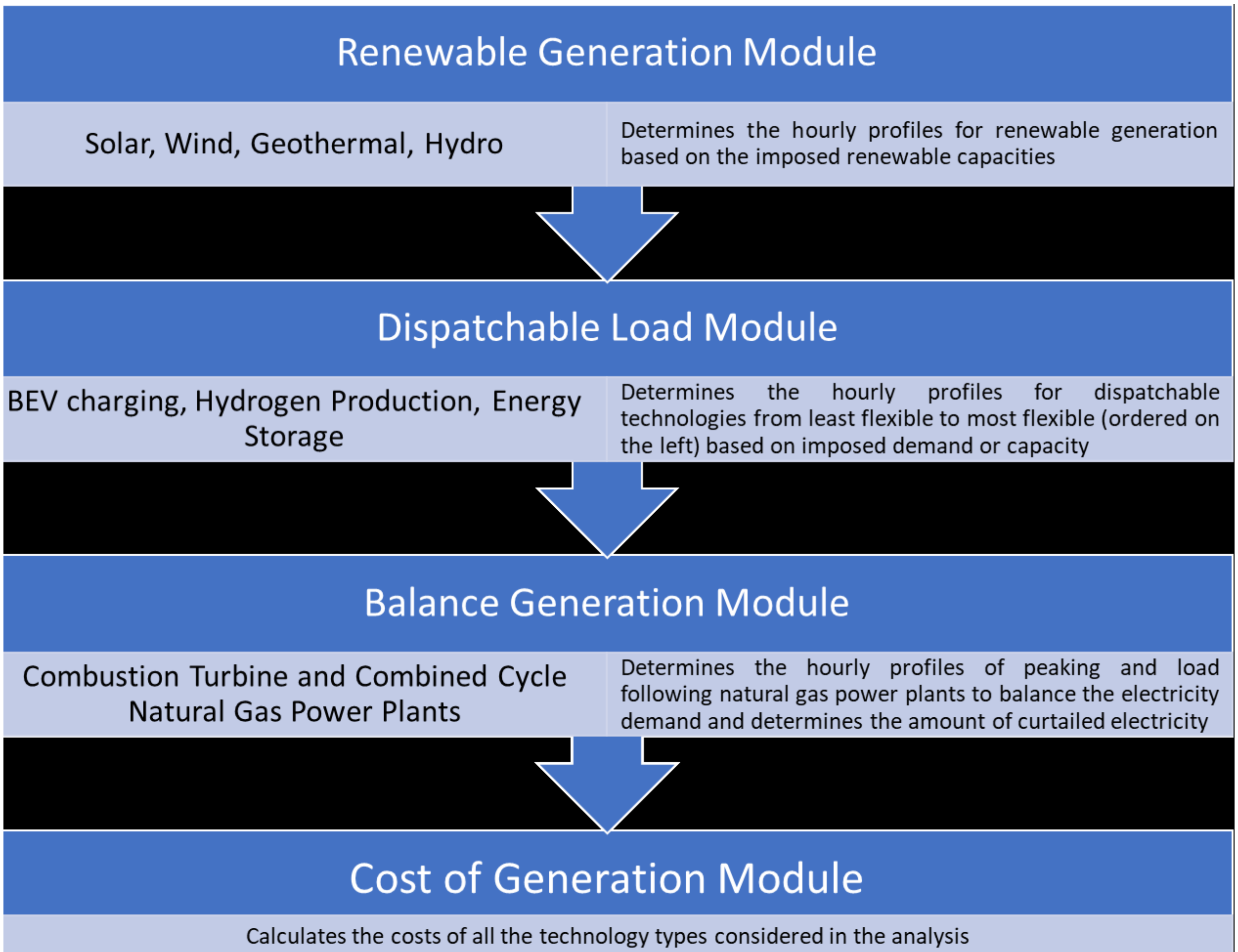

Figure 8: A description of the modules of the HiGRID model. [51]

The version of the tool used in this analysis (HiGRID+) uses the same framework of HiGRID with the addition of a cost-based optimization algorithm. The optimization effectively acts in place of the Dispatchable Load and Balance Generation modules of HiGRID, selecting the hourly profiles of each input technology that fulfill demand while minimizing system cost. The objective function is cost (instant cost and fixed/variable operation and maintenance) and the constraints that ensure all demands are met and the grid is balanced. For the purposes of this analysis, additional constraints include the elimination of natural gas power plants (NGPPs) and a zero-carbon electric grid.

The effects in 2045 of the shift to electrification and alternative fuels can be modeled in HiGRID+ by adjusting the input electric load profile. The 2045 electric load profile and individual sector loads are adopted from the Energy and Environmental Economics (E3) PATHWAYS study on reducing California's emissions [52]. Sector loads are then adjusted based on different decarbonization scenarios, altering the output of HiGRID+ and presenting potential technology mix pathways for the model year. The following sections outline methodology for analyzing single-sector pathways (for HDVs and refineries) to isolate sector-specific effects, then combines selected single-sector scenarios to design a multi-sector approach to net zero.

B. HDV Scenarios

The decarbonization scenarios for the HDV sector were adopted from scenarios established by Forrest [43] that include one base case scenario and four HDV pathway scenarios. The base case scenario is a current policy reference (CPR) case according to the E3 PATHWAYS model's 2045 emissions projections [52]. All four of the HDV pathway scenarios use the same LDV electrification assumptions as the base case scenario, while the four HDV allocation strategies with varying ZEV penetrations in Table 1 differentiate the four HDV pathway scenarios:

Scenario	Description
CPR Base Case	Current policy reference scenario.
40% HD ZEV	Conversion of 40% (by vehicle miles traveled, VMT) of the heavy-duty fleet to ZEVs,
73% HD ZEV	Conversion of 73% (by vehicle miles traveled, VMT) of the heavy-duty fleet to ZEVs,
High BEV	High BEV penetration scenario.
High H2	High hydrogen FCEV penetration scenario.

Table 1: Descriptions of the 2045 heavy-duty vehicle decarbonization scenarios.

The annual BEV charging and hydrogen demand associated with each HDV scenario are presented in Figure 9 and Figure 10, respectively.

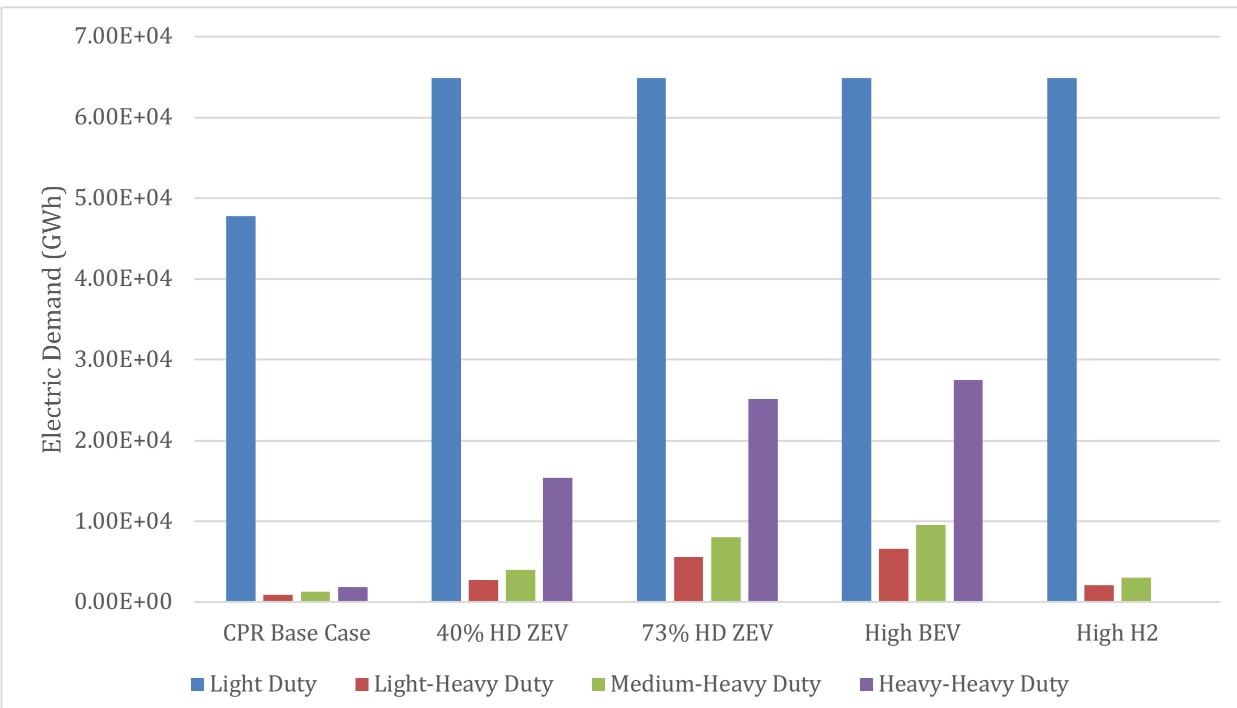

Figure 9: HDV scenario BEV charging demands in GWh.

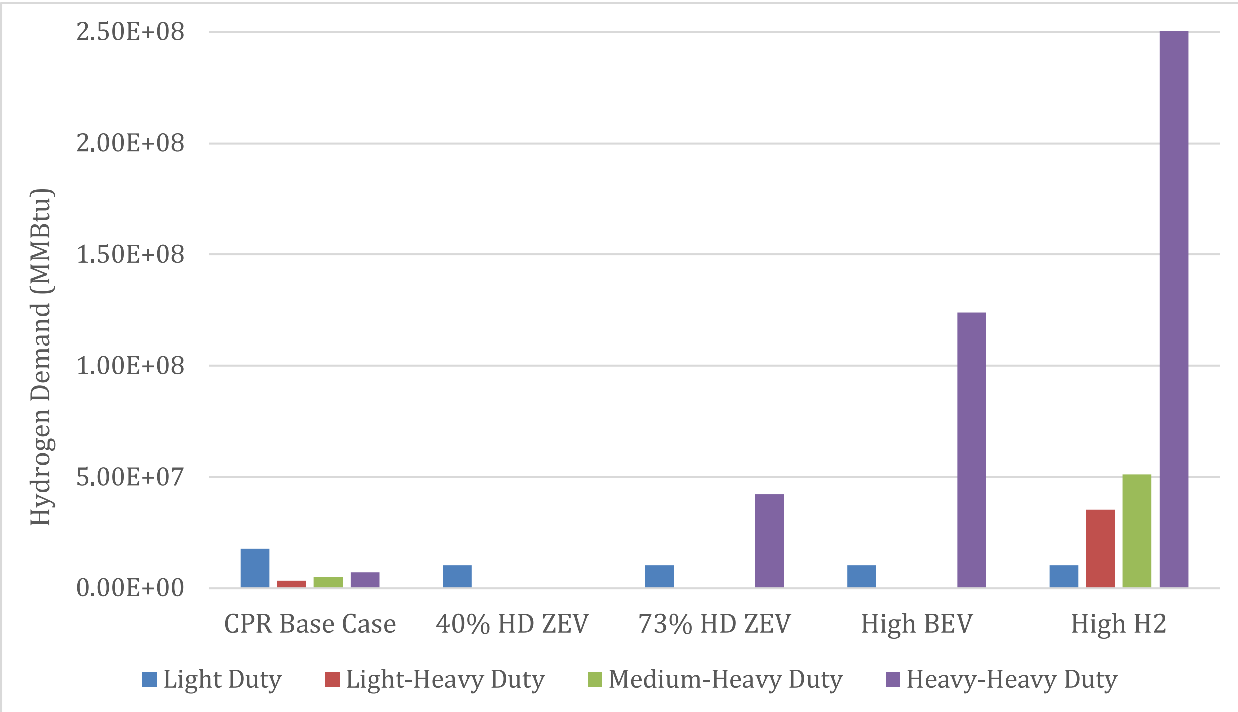

Figure 10: HDV scenario hydrogen demands in MMBtu.

The demand distributions indicate that, from left to right, the demand in both electricity (Figure 9) and hydrogen fuel use (Figure 10) increases. When compared to the CPR base case, all the HDV scenarios reduce demand for fossil fuels. While the High BEV and High H2 cases are the highest in ZEV deployment, their combination of BEV and FCEV deployment is the most ambitious. In fact, both of those cases involve an almost 100% shift to ZEVs on the heavy-heavy duty scale. In addition to meeting the mandate which requires that all retail sales of electricity must come from renewable and zero-carbon energy sources by the year 2045, every scenario meets or improves upon the target set by California EO S-3-05 to reduce GHG emissions to 80% of 1990 levels by 2050 [53]. The 40% HD ZEV case yields an 80% reduction in vehicle tailpipe GHG emissions, the 73% HD ZEV case yields a 90% reduction and the High BEV and High H2 cases yield a 95% reduction compared to 1990 levels [43]. Emissions reduction estimates were calculated based on historical data on vehicle tailpipe emissions [54] and projected VMT for the year 2045 from EMFAC [55].

Due to the difference in time constraints associated with BEV charging and FCEV fueling, different approaches were adopted for each vehicle type. For BEV charging, the annual electric demand values in [43] were adjusted into annual hourly resolved profiles for the year 2045 because of the immediacy of BEV charging demand. Normalized hourly profiles for LDVs and HDVs were adopted from [56] and scaled according to the annual demand. The normalized profiles for each vehicle type differ according to vehicle use. For example, LDV demand is higher on weekdays than weekends because they are often commuter vehicles. Figure 11 illustrates that fluctuation by showing a four-week sample of the normalized LDV profile. HDVs have more consistent day-to-day demand patterns but between sub-weight classes, there are small perturbations in the normalized profiles due to their wide range of uses (see Figure 12). The E3 load profile data include all sectors (residential, commercial, industrial, etc.) except transportation demand [52]. The scaled electric demand profiles for each of the HDV scenarios were added into the E3 non-transportation load, resulting in a suitable input electric load profile for HiGRID+.

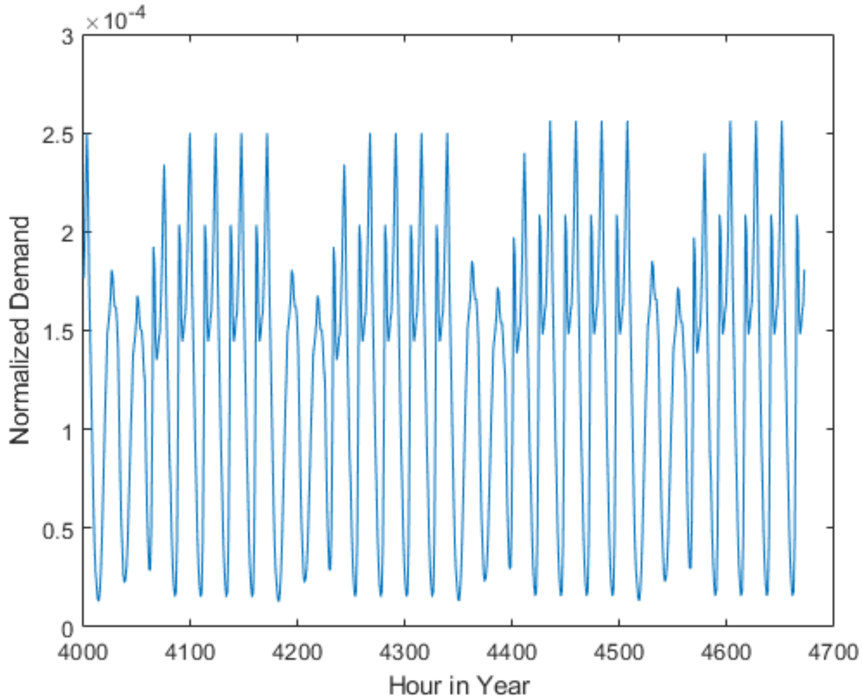

Figure 11: A four-week summer sample of the normalized LDV profile.

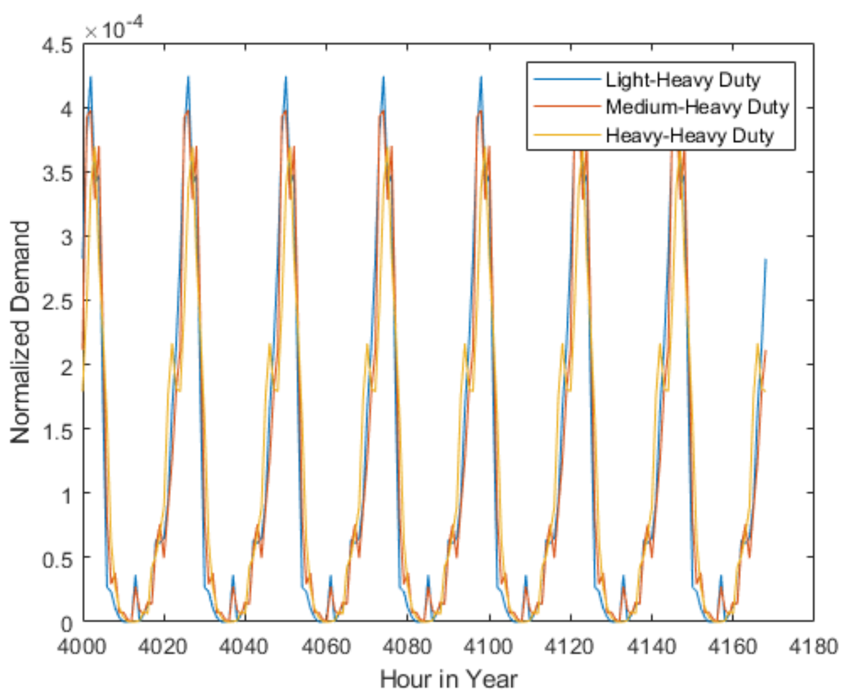

Figure 12: A one-week summer sample of the normalized hourly HDV profiles.

The hydrogen demands, however, are less time-sensitive since hydrogen can be produced via electrolyzers at any time preceding the fueling time. The hydrogen demands were incorporated into HiGRID+ by adjusting the existing FCEV hydrogen demand constraint. The optimization considers the hydrogen demand, allocating electrolyzer resources to generate the necessary fuel when carbon-neutral electricity is available any time preceding the fueling time window. A summary of electricity and hydrogen flows is mapped in Figure 13.

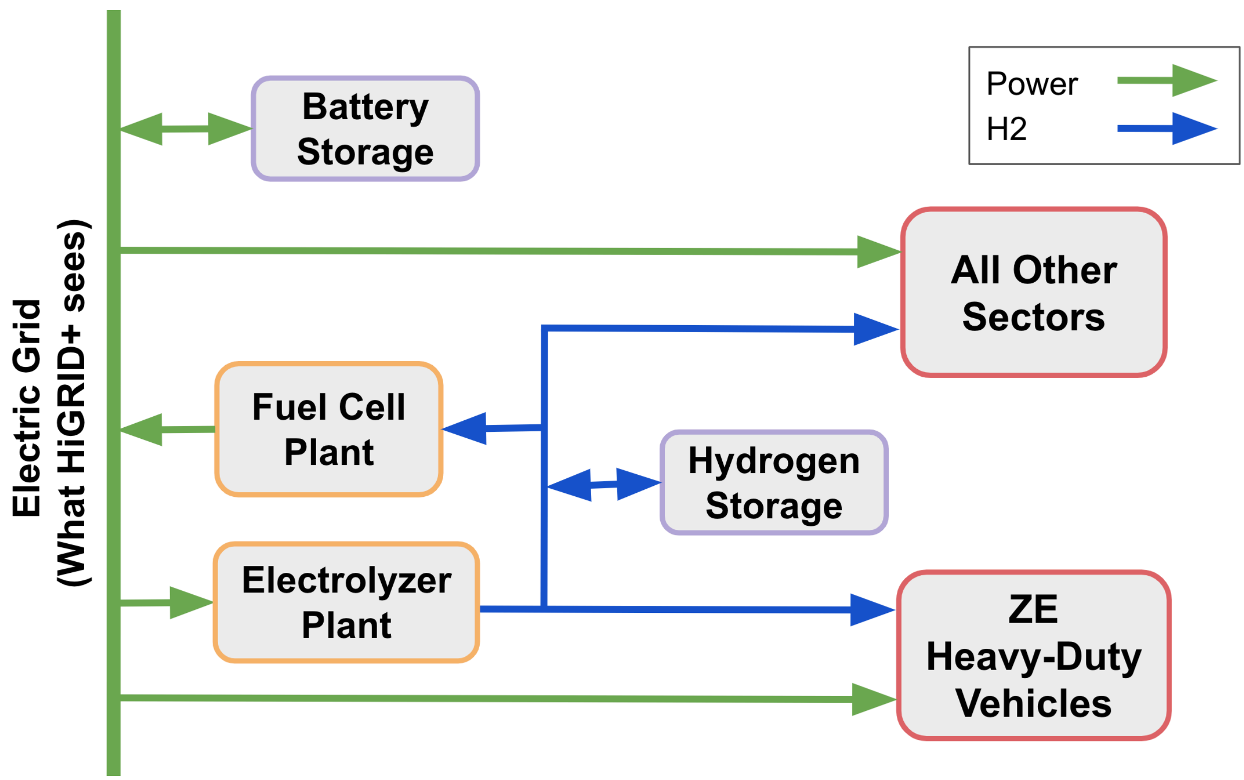

Figure 13: Simplified supply and demand flow map for the HDV scenarios.

C. Refinery Scenarios

The key to using HiGRID+ to analyze the effects of different refinery decarbonization pathways on the electric grid is to identify the processes that emit the most and retrofit them with zero-carbon technologies, as long as they achieve the same step in the refining process. Typically, a petroleum refinery has nonrenewable on-site power generation, usually a natural gas power plant, that provides a large portion of the electricity and steam needed to perform oil refining. However, that presents a challenge for emissions reduction from a grid modeling standpoint because the on-site power generation is not an installed element of the electric grid. In order to address emissions from currently on-site generation, the demand met by that generation was de-localized in the eyes of the HiGRID+ model and incorporated into the electric load balanced by the optimization. The model can then ensure that all the electric demand of California refineries is met by zero-emission sources.

Fuel, steam, and power were the three demands of concern for addressing refineries in the HiGRID+ tool. Solid oxide and molten carbonate fuel cells are fuel flexible, and the lowest emission fuel option is hydrogen. Fuel demand profiles can then be translated into the electric load profile necessary to produce electrolytic hydrogen. Multiple refinery units require steam to function, so a zero-emission steam source was necessary because current refineries use the steam byproduct of their electricity-generating natural gas turbines. Hydrogen boilers, the specifications of which were drawn from industry projections, were implemented to meet the total refinery steam demand [57]. The hydrogen boiler model from the specification uses a hydrogen combustion reaction to superheat steam that is then channeled to a heat exchanger to heat the working fluid (in this case, water) so that the system remains a closed loop. Figure 14 depicts the flow of power and steam in an example refinery in order to provide perspective on where those demands go in refinery processes [58]. The figure also includes a visualization of all the process units that were retrofitted in different combinations for the refinery HiGRID+ scenarios (among a few others that were left as is). Additionally, the process units that were eligible for retrofit and their shorthand abbreviations can be found in Table 2. The ultimate HiGRID+ input is electric demand, so a map of how different demands (H_2, steam) are back converted into electric demands for use in HiGRID+ can be found in Figure 15.

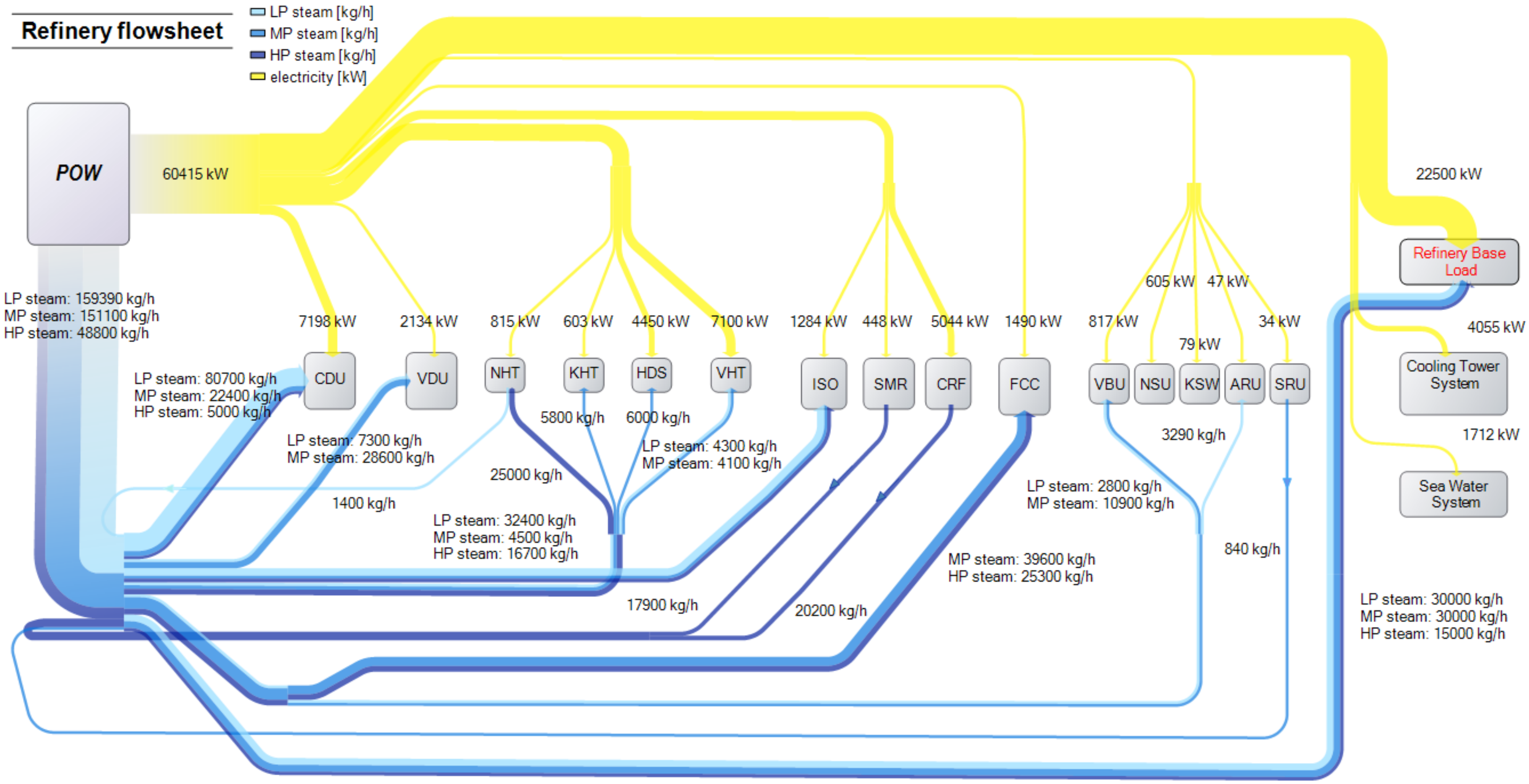

Figure 14: Sankey diagram of electricity and steam flow between reference refinery process units. [37]

Abbreviation	Unit Name
CDU	Crude Distillation Unit
CRF	Catalytic Reformer
FCC	Fluid Catalytic Cracker
HDS	Diesel Hydro-Desulfurization Unit
KHT	Kerosene Hydrotreater
NHT	Naphtha Hydrotreater
NSU	Naphtha Splitter Unit
POW	Electricity Generation
SMR	Steam Methane Reformer
SRU	Sulfur Recovery Unit
VBU	Visbreaker Unit
VDU	Vacuum Distillation Unit
VHT	Vacuum Gasoil Hydrotreater

Table 2: Refinery process units that are options for fuel cell retrofit and their abbreviations. [40]

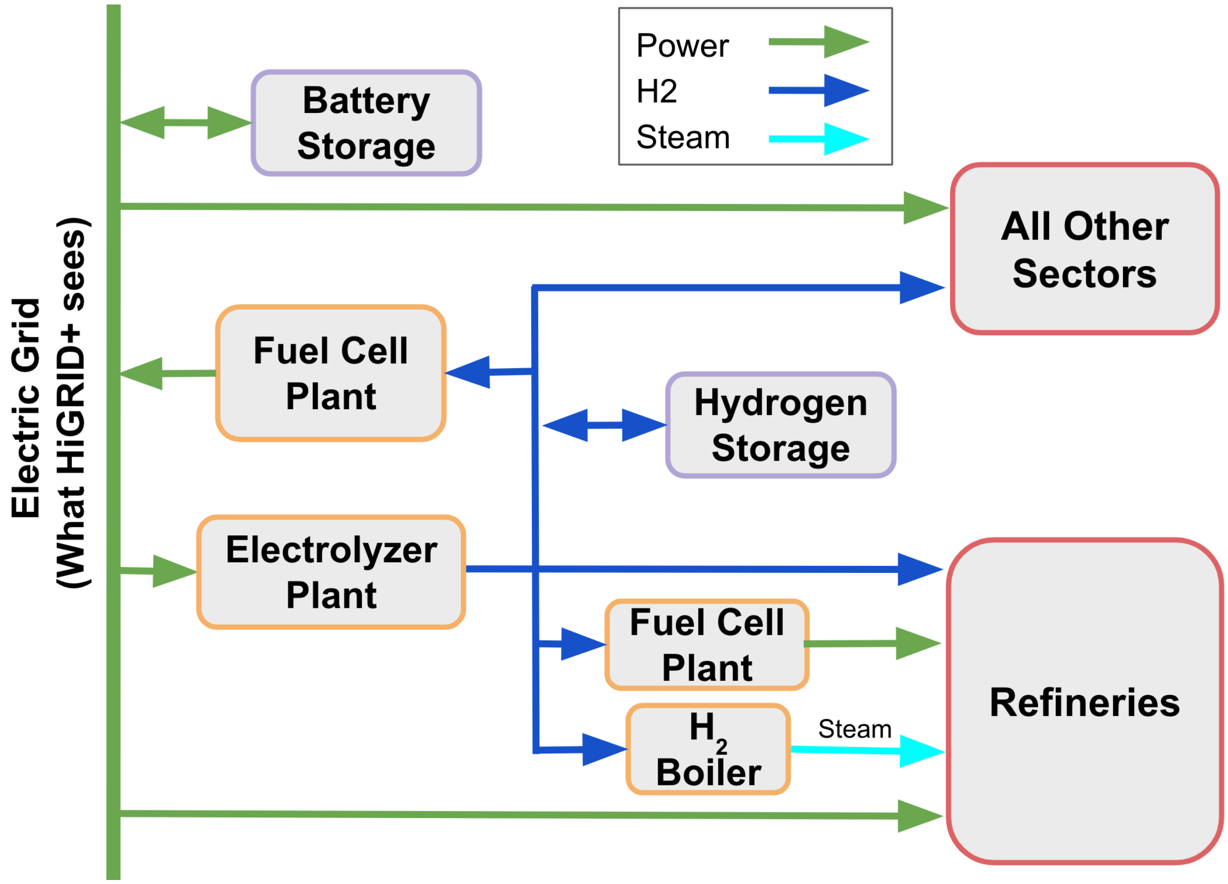

Figure 15: Simplified supply and demand flow map for the refinery scenarios.

Previous studies have conducted the thermodynamic analysis of a reference refinery, calculating the GHG and CAP emissions that occur when different refinery processes are replaced with a fuel cell system [40], [58]. The refinery scenarios for this investigation, described in Table 3, were adopted from a research study conducted by the UC Irvine Advanced Power and Energy Program (APEP) for the South Coast Air Quality Management District (AQMD) [58].

Scenario	Description
RZERO	Complete removal of emissions from refineries in California
RARO	(1) complete retrofit of applicable sources with MCFC post-combustion systems and (2) SMR retrofitted with an MCFC
RPWR	Substitution of the power plant with a SOFC+GT hybrid system
RSMR	Retrofit of the refinery's SMR with a tri-gen MCFC system.
RMCFC	Retrofit with MCFC in the SMR, Distillation Column, Vacuum Distillation Column, and Catalytic Cracker. In addition, the power plant is replaced with a SOFC+GT hybrid system

Table 3: Descriptions of the refinery scenarios. [58]

Each scenario in the APEP study is comprised of a different combination of retrofitted and existing technologies to compare the effects of different approaches to fuel cell integration. The RZERO case serves as an upper bound of emission goals and therefore does not have technical specifications. The RARO case retrofits all eligible process units with an MCFC and an SMR unit with an MCFC tri-generation system at 45% utilization factor (Uf). The RPWR case isolates the effects of power generation by only replacing the power plant with a SOFC/gas turbine hybrid system. Similarly, the RSMR case isolates the effects of SMR by replacing the SMR with a tri-generation MCFC system. Finally, the RMCFC case is a more eclectic combination of retrofit and replacement options. Some, but not all, units are retrofitted with an MCFC (listed in Table 3) and the electricity generation is replaced by the same SOFC/gas turbine hybrid unit as the RPWR case. The report data include annual fuel, hydrogen, steam, and electric demand values for each process unit version, and the four technical scenarios were assembled by combining the process units according to the case specifications.

Four reference refineries were modeled in the APEP study: a simple hydroskimming refinery with a capacity of 150,000 barrels per day (bpd), a medium conversion cracking refinery with a capacity of 220,000 bpd, a high conversion coking refinery with a capacity of 220,000 bpd, and a high conversion refinery with a capacity of 350,000 bpd. For the purposes of this investigation, the thermodynamic results of the medium conversion refinery were used as a starting point for the demand calculations. A 220,000-bpd medium conversion cracking refinery is the most representative of the 14 active refineries in California because almost all those refineries utilize catalytic cracking processes. The average capacity of California refineries is about 125,000 bpd, but the priority for model accuracy was the most representative combination of refining processes [59]. Otherwise, the electric, fuel, and steam demands can be scaled according to plant capacity and economy demand for the products. Annual electric demands for each scenario were compared to the CPR Base Case in Figure 16. The RARO case has no refinery-specific electric demand because all of the process units were converted to fuel cells, so the demand was shifted to hydrogen.

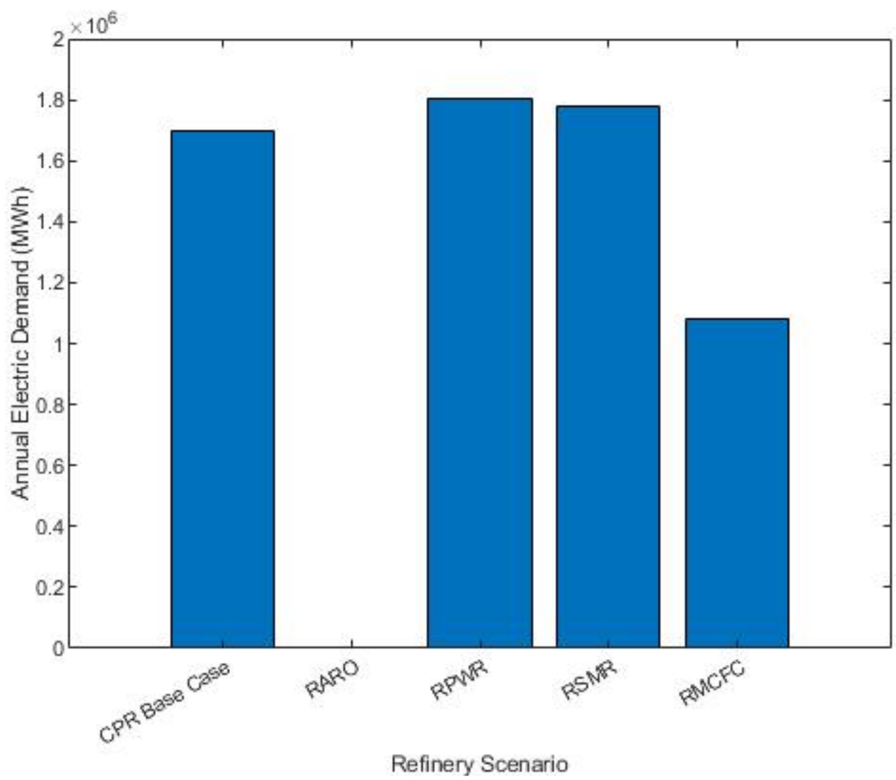

Figure 16: Refinery electric demand in MWh by scenario.

The main limit of the APEP study results' applicability to this analysis is its use of natural gas as the fuel cell fuel. Using natural gas, which is primarily made up of methane, renders it impossible for carbon emissions to be 100% removed. Therefore, conversion calculations were necessary to approximate the fuel demand in the case that natural gas fuel was replaced by hydrogen fuel. In order to make that approximation, the ratio of the lower heating values (LHVs) of natural gas and hydrogen was used as a scaling factor to convert tons/hour of natural gas to kilograms/hour of hydrogen (with proper unit conversions).

The total hydrogen demand for each scenario includes the fuel cell fuel demand and the hydrogen needed to generate the steam required for refinery processes in hydrogen boilers. The thermodynamic modeling results include annual steam demands, so a conversion factor of 62 kg hydrogen to 3000 kg steam was taken from Hydrogen Technology, Inc.'s Dynamic Combustion Chamber (hydrogen boiler) product specifications [57].

The refinery hydrogen demand values are plotted compared to the CPR Base Case and the US Energy Information Association's (EIA's) record of PADD 5 (west coast) refinery and blender net input of hydrogen in Figure 17 [60]. The EIA value was included to put into perspective the amount of hydrogen currently used by refineries in the region. The large difference between the PADD 5 value and the refinery hydrogen demands shows that hydrogen infrastructure must be built out and scaled up between now and 2045 to meet growing demand and achieve a least cost system. In the RARO case, all electric demand is shifted to hydrogen demand for fuel cell power. The other cases have higher hydrogen demands then RARO because they have steam demands that RARO does not, and steam generation in those scenarios has a higher hydrogen demand than complete fuel cell retrofits.

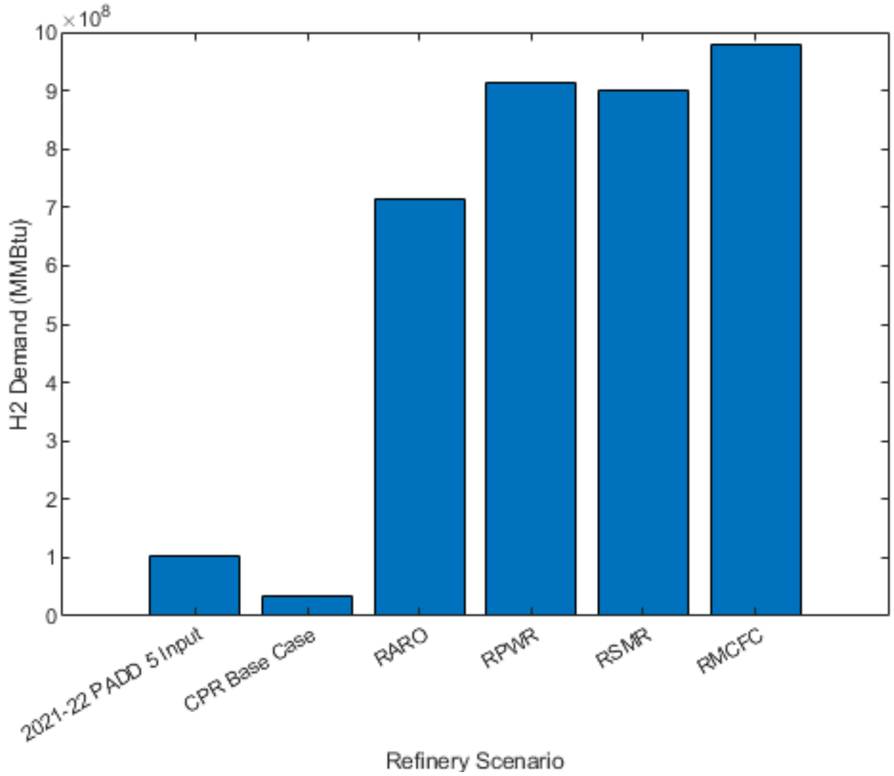

Figure 17: Refinery scenario hydrogen demand in MMBtu compared to the CPR Base Case and the June 2021 - May 2022 PADD 5 input.

Once annual values were calculated for hydrogen demand (fuel and steam) and identified for electric demand, the annual demand values needed to be transformed into annual hourly demand profiles. Therefore, normalized operation profiles for each process unit were required. Each process has a corresponding capacity factor (value 0-1) that indicates what portion of the year the unit operates. The downtime is used for system maintenance. This operation schedule is similar to a baseload generation unit on the grid, except that where baseload would ideally increase operation when electric demand is high, a demand side unit would increase operation when demand is low to maintain grid balance. Eichman developed a process for identifying the ideal baseload operation according to annual net load and technology capacity factor [61]. To use those calculations, the 2045 electric load profile was inverted and vertically shifted (Equation 1) to identify ideal normalized profiles for each refinery unit in the year of interest [52].

$$E_{inv} = -1 * (E_{load}) + \max(E_{load})$$

Equation 1

Where E_{inv} is the length-8760 inverted vertically shifted electric load and E_{load} is the original electric load profile. Using the adjusted load, the monthly average of the inverted load, avg_{month} was taken:

$$avg_{month} = \frac{\left(\frac{1 - E_{inv}}{\max(E_{inv})}\right)}{\sum_{i=1}^{N}\left(\frac{1 - E_{inv}(i)}{\max(E_{inv})}\right)}$$

Equation 2

where N is the number of months in the year, 12. Then, the monthly "available capacity," or maximum demand capacity in this analog (Cap_{avail}), of the process in question was calculated using its total capacity (Cap_{base}).

$$Cap_{avail} = \frac{E_{inv}}{\max(E_{inv})} * Cap_{base}$$

Equation 3

Next, the utilization/capacity factor for each process was applied to the Cap_{avail} by calculating how much demand needed to be reduced from each month to correspond with the defined capacity factor, CF_{base}. That value, Cap_{red}, is defined in Equation 4.

$$Cap_{red} = \sum Cap_{avail} - N * \sum_{i=1}^{N} Cap_{base}(i) * CF_{base}(i)$$

Equation 4

Finally, the monthly capacity setpoint for each industrial process was determined by removing the capacity reduction from the available capacity scaled by the inverted monthly average of electric demand:

$$Cap_{setpoint} = Cap_{avail} - avg_{month} * Cap_{red}$$

Equation 5

The process generates a profile that is batched monthly to correspond with a more consistent pattern than hourly variation. Figure 18 is an example profile for the electricity generation MCFC retrofit, which has a capacity factor of 65%. All the process operation profiles have the same shape because they are based on the same net load profile, but with different vertical shifts to account for varying capacity factors.

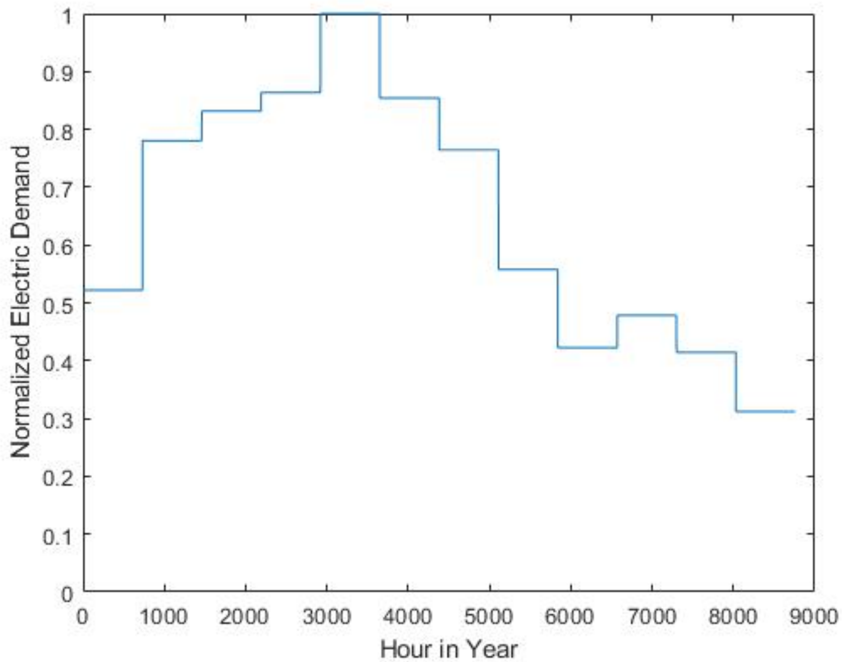

Figure 18: Annual normalized electric demand profile for an electricity generation unit retrofitted with an MCFC.

Finally, the annual electric load demands for each process were multiplied by their corresponding operation profiles. Retrofitted and original reference units of the same process had the same normalized profiles, but different electric demands according to their thermodynamics. The refinery demand assumptions from E3 were subtracted from total electric load profile used in the HDV CPR Base Case and for each scenario, the corresponding process profiles were combined and added to the total load. Then, the hydrogen demand, fuel and steam requirements combined, were added to the hydrogen constraints of HiGRID+. At that point, each scenario was ready to be input into the optimization.

D. Combined Scenarios

The combined scenarios are the goal of this analysis. They were constructed from the lowest emission HDV scenarios, High BEV and High H2, and the lowest CAP emitting refinery case, RARO. CAPs were the priority for refinery emissions because the switch to hydrogen fuel eliminates the CO_2 emissions predicted by the AQMD report [58], but there are still CAP emissions associated with fuel cell operations. The result is two multi-sector pathways for comparison, listed in Table 4.

Scenarios	**HDV: High BEV**	**HDV: High H2**
Refinery: RARO	High BEV + RARO	High H2 + RARO

Table 4: The combination of two HDV and one Refinery scenarios to construct the two multi-sector scenarios.

To build these scenarios into HiGRID, the techniques for the individual sector electric load profiles were combined to generate four new profiles that reflect the new multi-sector approaches. Similarly, the hydrogen demands were summed for the hydrogen constraint. The simplified demand flows that were used to define the HiGRID+ inputs of the combined scenarios are mapped in

Figure 19. The green arrows are the inputs that are combined to form HiGRID+'s input demand profile, while the rest of the figure shows how that translates to individual subsector demands. The HDV CPR Base Case was used as the overall reference base case.

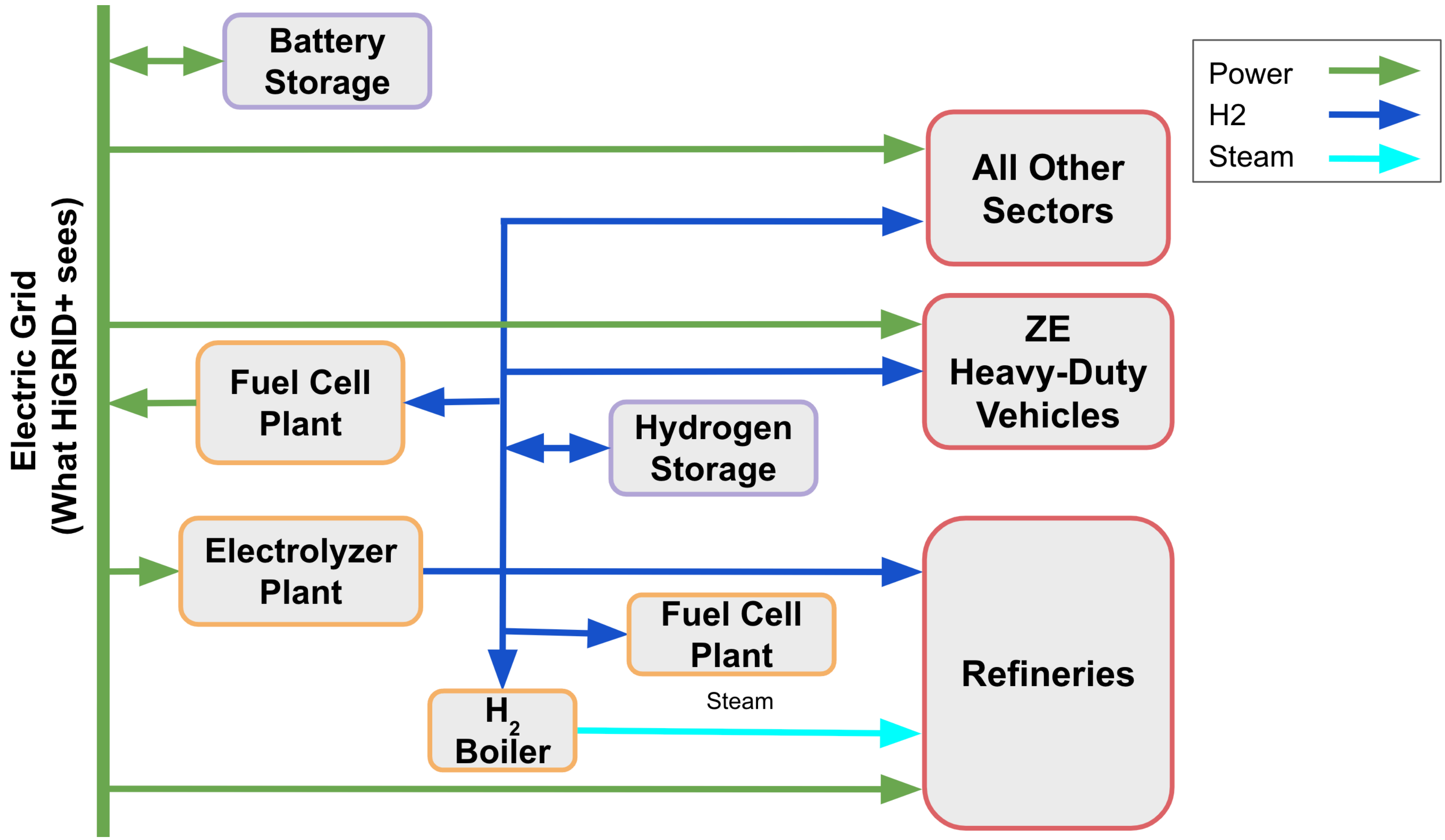

Figure 19: Simplified demand flow from electric power to ultimate subsector demands for the combined scenarios.

V. RESULTS

A. Heavy Duty Vehicle Scenarios

1. System Cost and Curtailed Electricity

For the HDV scenarios, the electric and hydrogen demands vary by a wide margin between the CPR Base Case (lowest demands) to the High BEV and High H2 cases (highest demands). As a result, the least cost renewable capacity for each scenario varies as well. With high electric and hydrogen demands, high wind and solar capacities are necessary to meet high peak demands. However, as the load demand decreases, a lower renewable capacity can reduce cost by reducing the deployment of new utility scale wind and solar and the total curtailed electricity. On the other hand, renewable capacity must also remain sufficiently high to fulfill load demand and, at the same time, provide sufficient flexibility to maximize the curve-flattening effect of energy storage. To illustrate the relationship between renewable capacity, electric demand, and system cost, the system cost was minimized for the High H2 scenario by changing wind and solar capacities by the same scaling factor. Then, each of the other vehicle electrification scenarios were run with their specific electric and hydrogen demands at the High H2 least cost wind and solar capacities. Figure 20 shows the cost outputs for those scenarios. The base wind and solar capacities were based on the 70% and 80% RPS capacities used by Wang [51] but scaled up slightly to account for the 100% RPS goal. Those base values are 174.1 GW solar (combined fixed and 1-axis) and 91.3 GW wind (regional).

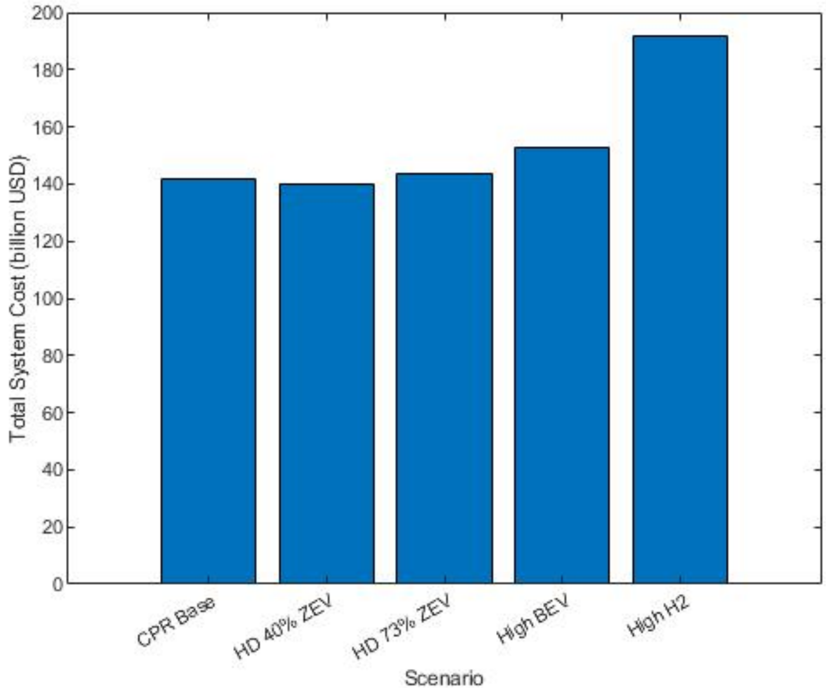

Figure 20: Total system cost of HDV scenarios using the least cost wind and solar capacities for the High H2 case.

In this set of runs, every scenario has a higher cost than the CPR base case because any degree of vehicle electrification increases grid generation demand and therefore generation technology cost. Vehicle charging demand at peak demand times of day is particularly expensive for two related reasons: the overall peak load demand is increased, thereby increasing the maximum generation capacity required, and utility electricity is more expensive to the customer at peak times. The model does not capture customer-side price dynamics, but it does reflect the increase in total renewable capacity needed to meet increased peak demand and the resultant cost of that technology buildout. In fact, there is an apparent lower limit on the cost at a constant renewable capacity. The set generation exceeds the demand of the two CPR cases and the HD 40% ZEV case such that the cost of renewable deployment dominates the total system cost.

The target metric of this investigation is least cost, so the wind and solar capacities associated with the approximate least cost for each scenario were determined by spanning *renewable capacity for all scenarios. Figure 21 serves as an example of the cost results from spanning renewable capacity for the HD 73% ZEV scenario. From 10% above the base capacity value (set here as the minimum cost capacities for the CPR Base Case), the cost decreases with increasing capacity because the additional renewable capacity allows for more efficient utilization of energy storage technologies. until it hits the inflection point where additional wind and solar are no longer cost effective.*

Table 5 lists the least cost wind and solar capacities for the HDV scenarios found using this strategy.

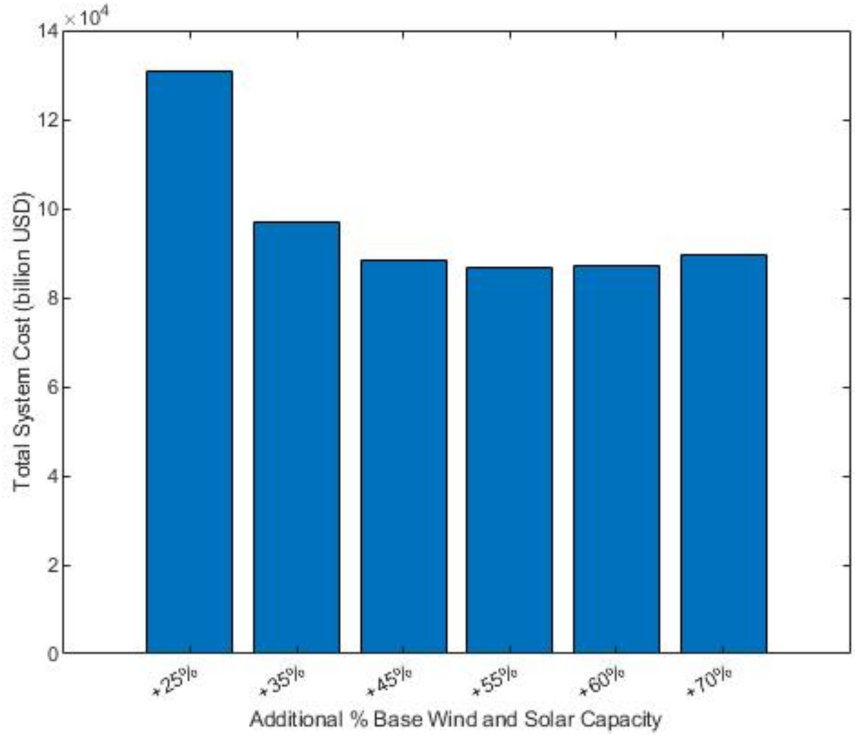

Figure 21: Cost output of wind and solar capacity spanning for the HD 73% ZEV scenario.

(MW)	CPR Base Case	HD 40% ZEV	HD 73% ZEV	High BEV	High H2
Wind Capacity	109,598	109,598	141,564	182,664	273,996

Solar Capacity	208,936	208,936	269,876	348,228	522,342

Table 5: The wind and solar capacity values for each HDV scenario associated with the approximate least cost. The precision is attributed to the strategy of beginning with values on the order of those used in [51] *but scaled up to account for a 100% RPS instead of 70-80%.*

The total electric grid system cost for each HDV scenario at least cost can be found in Figure 22. The higher ZEV penetration of the High BEV and High H2 case is reflected in their higher costs as the demand for gasoline shifts to a grid-related demand. It is of note that the increased cost from demand shifting to the grid is in part offset by cost associated with the decreased gasoline demand and therefore production. That offset is not modeled by HiGRID+ and therefore does not affect the system cost output.

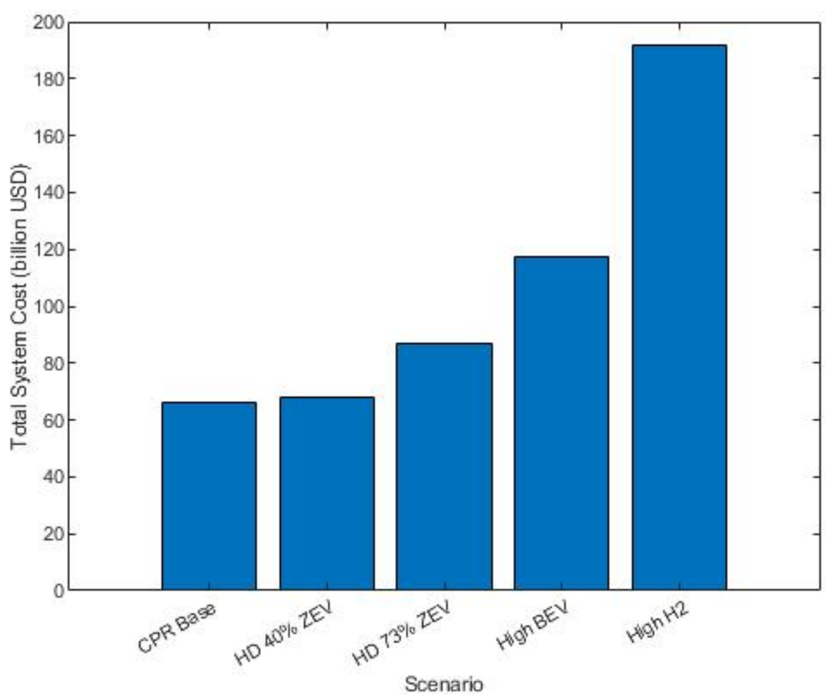

Figure 22: Total system cost of minimized cost HDV scenarios in billions of USD.

Figure 22 also shows that the 40% zero-emission HDV scenario has a slightly lower system cost than the CPR case. This is likely because the loads associated with that case correspond more consistently with complementary technologies. For example, charge demand that temporally corresponds with a peak in installed renewable generation prevents the need for additional technology operation elsewhere in the grid. Additionally, the 40% scenario has a small amount of hydrogen demand from LDVs and none from HDVs, the least of all the scenarios, so there is less need for hydrogen infrastructure. In this case, less hydrogen demand correlates to lower grid system cost, but some cost would be incurred elsewhere in the economy for gasoline production, which is not captured in this model.

2. Technology Selection

a) Electrolyzer and Energy Storage Mix

The mix of electrolyzer and energy storage technologies is an indicator of least cost pathways for managing increased electric and hydrogen demand. The electrolyzer technologies from which to select by the optimization model are alkaline, solid oxide, and proton exchange membrane. The energy storage options are Li-Ion batteries, Zn-Br batteries, pumped hydro, and compressed air. Figure 23 contains the output for each vehicle electrification scenario for electrolyzer and storage technology capacity. If a technology is not represented in a plot, it was not selected by the model in any of the scenarios.

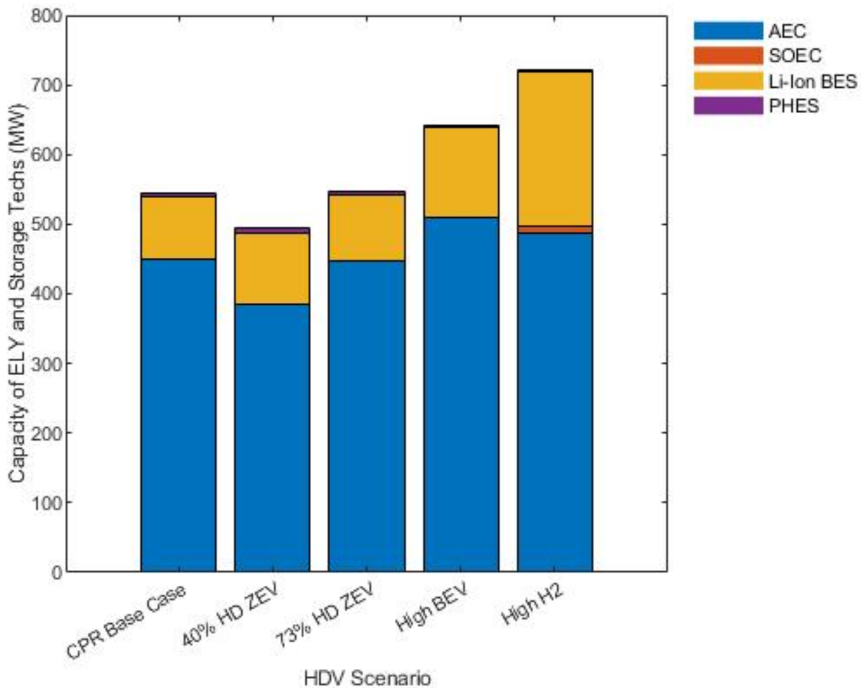

Figure 23: Minimized cost HDV scenario electrolyzer and energy storage technology capacity results.

With a correlation coefficient of 0.9561, there is a direct relationship between VHD in MMBtu and total combined electrolyzer and energy storage capacity in GW. In the High H2 scenario, with the highest hydrogen demand by far, the electrolyzer capacity decreases relative to that of the High BEV case while Li-ion capacity more than doubles. It is important to note that the High Hydrogen case reaches the maximum capacity of available underground storage of 3.5 x 107 MWh, which equates the current storage capacity available in California's salt caverns. Figure 24 and Figure 25 show the hourly demand profile and constituent load demands overlaid with the renewable generation profile from the same period of approximately nine days for the High H2 and High BEV scenarios, respectively. The general trends in demand are similar, but due to the lower overall demand associated with the High BEV case, the peak load is about 200 GWh lower and the LDV/HDV load profile shapes are more apparent.

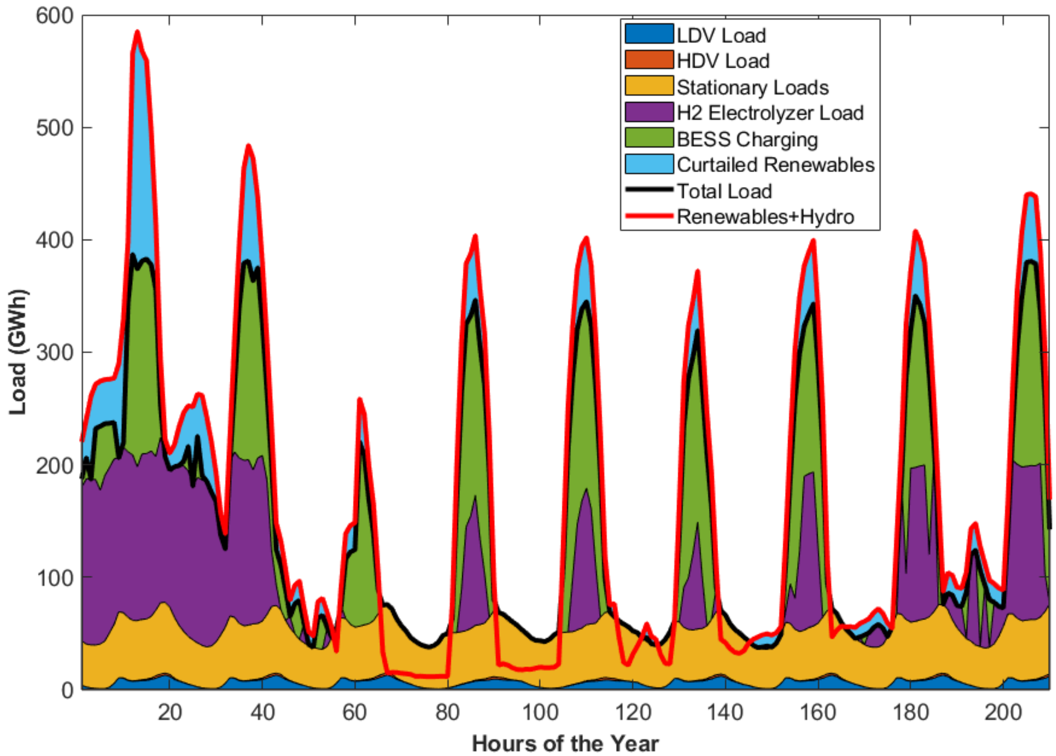

Figure 24: 210 hour sample generation and load time series from High H2 results (roughly Jan 10-18).

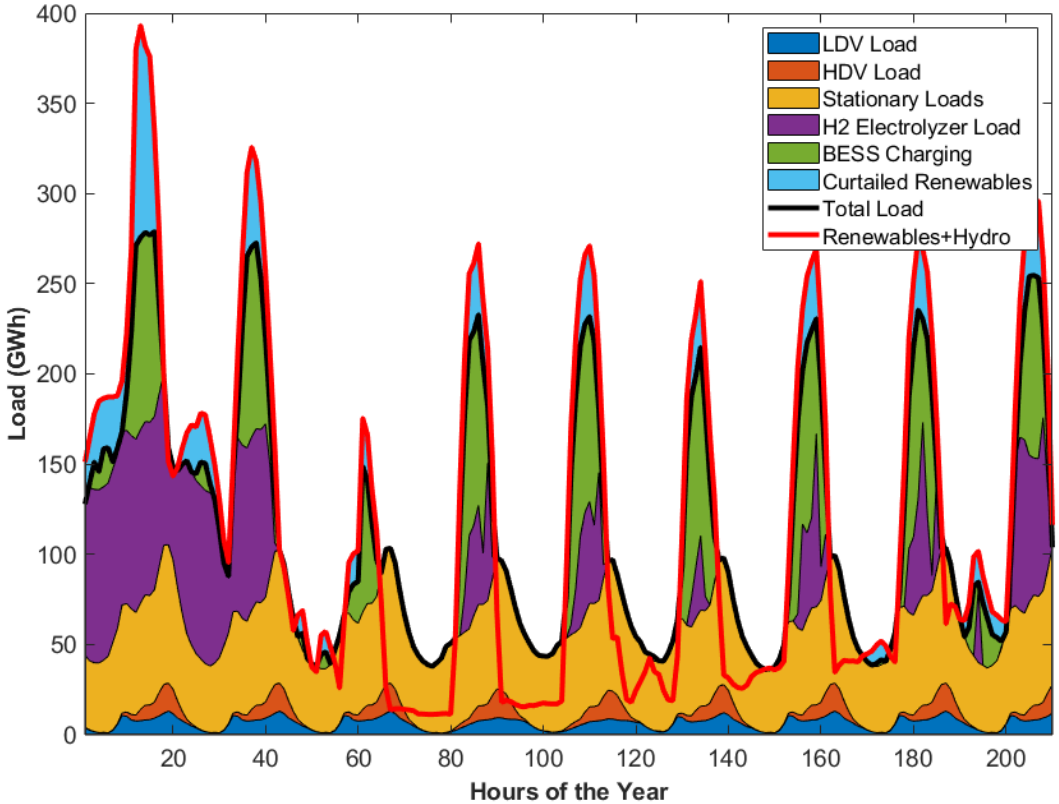

Figure 25: 210 hour sample generation and load time series from High BEV results (roughly Jan 10-18).

Figure 26 plots the energy storage charge and discharge hourly profiles by technology, the total electrolyzer demand, and renewable generation during the same window of 210 hours. Here, it is clearer that the energy storage charging trend (specifically Li-ion batteries, orange) and the electrolyzer demand (dark blue) both correlate with the peaks in renewable energy generation (light blue) and energy storage discharges at low renewable generation. Electrolyzer demand specifically operates at maximum capacity as much as possible in higher renewable generation peaks, seen in the early hours of the figure, and closely follows the drops in generation. For example, the electrolyzer demand dip around hour 275 mimics the generation dip at the same time. As a result, these technologies are likely utilizing otherwise curtailed renewable generation for energy storage and electrolytic generation of hydrogen fuel. Energy storage and electrolyzers act as complimentary technologies that help minimize cost in FCEV-heavy vehicle electrification scenarios like the High H2 case.

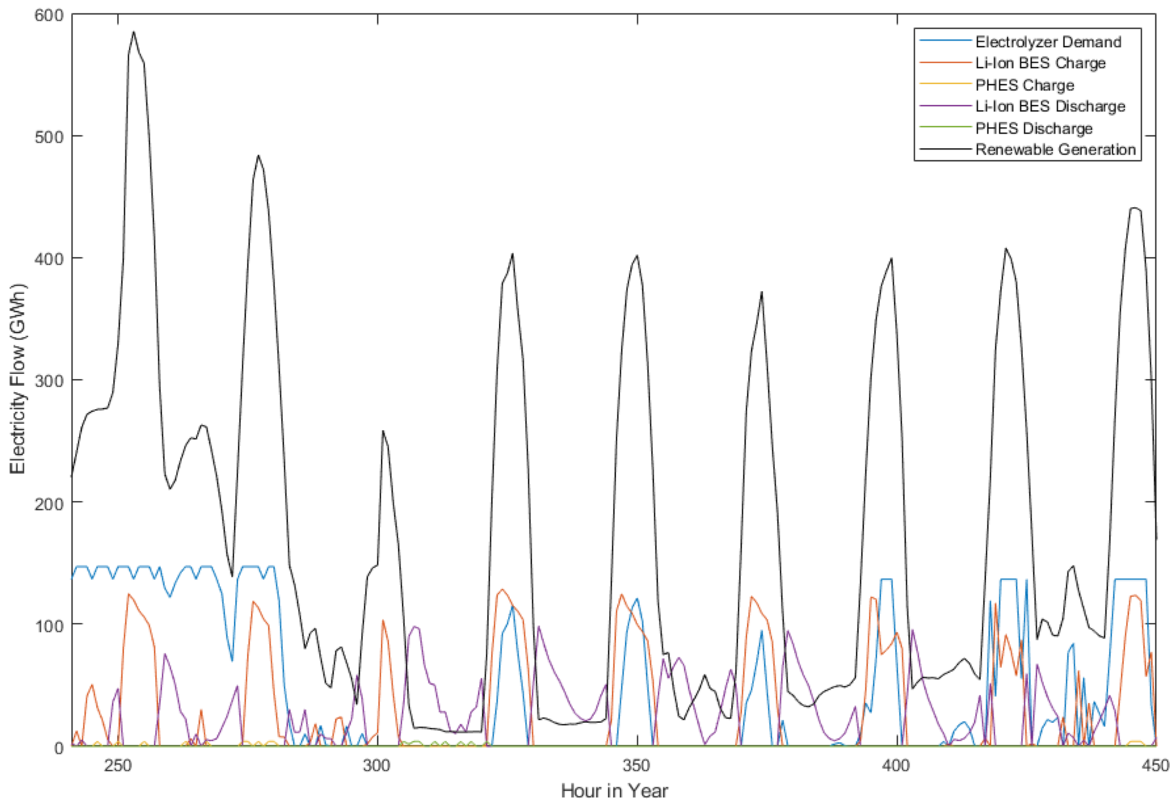

Figure 26: Energy storage discharge, electrolyzer demand, and renewable generation for the same sample timeseries in the High H2 results (roughly Jan 10-18).

With regard to the increase in battery energy storage capacity in place of electrolyzer capacity, further investigation into the results reveal that the optimization did not select hydrogen for energy storage due to the maximum underground storage limit. As a result, battery storage systems are prioritized at high hydrogen. The battery energy storage selected, provided short-duration load shifting as shown in Figure 26. The hydrogen produced and stored for FCEVs showed a more seasonal pattern. The seasonal behaviors of hydrogen production and storage are explored further in the next section. Potential drivers for not selecting hydrogen as an energy storage medium are high cost, limits on hydrogen underground storage set in the model, and seasonal variability patterns. These interdependences should be explored more in future work.

b) Vehicle Hydrogen Storage

Hydrogen can also be used in the context of the electric grid as a form of seasonal, long-duration energy storage. Hydrogen energy storage is included in the HiGRID+ algorithm, and the resultant annual state of charge profiles are found in Figure 27. For all scenarios, the overall shape of each curve is similar, ramping up the amount of stored energy in the middle of the year for discharge (use) in the mid-late winter. This storage pattern is driven by vehicle fueling demand and the changing availability of renewables throughout the year. Vehicle fuel demands are consistent year round, while renewable generation peaks in summer and is lowest in winter. Hydrogen storage allows for electrolytic hydrogen to be generated during the peak renewable generation months and stored for use during winter. The largest difference between each of these plots is the magnitude of maximum state of charge, which increases with overall electric and hydrogen demand. Higher load systems result in more seasonal energy storage.

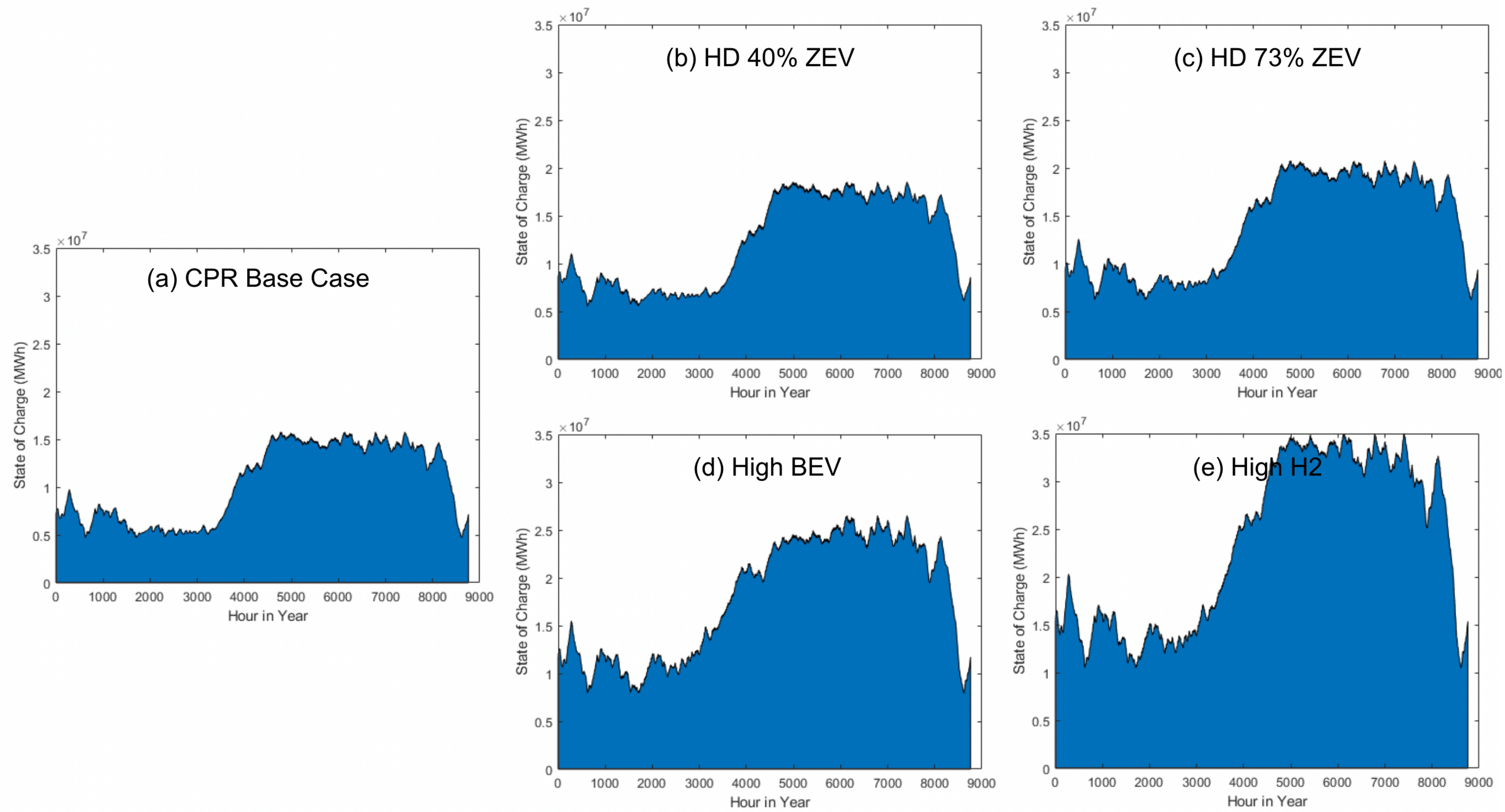

Figure 27: Minimized cost HDV scenario Hydrogen Energy Storage annual state of charge in MWh for (a) the CPR Base Case, (b) HD 40% ZEV case, (c) HD 73% ZEV case, (d) High BEV case, and (e) High H2 case.

3. Emissions and Air Quality Analysis

The purpose of this analysis, for the HDV scenarios, is to evaluate the impact on emissions and air quality associated with the transportation section assuming a zero-emission electric grid. The emissions analysis for the HDV scenarios was conducted by Forrest [43], providing a foundation from which multi-sector emissions analysis could be possible. This section summarizes those results and explains the significance of them in the context of a multi-sector analysis built around grid modeling.

a) GHG Emissions

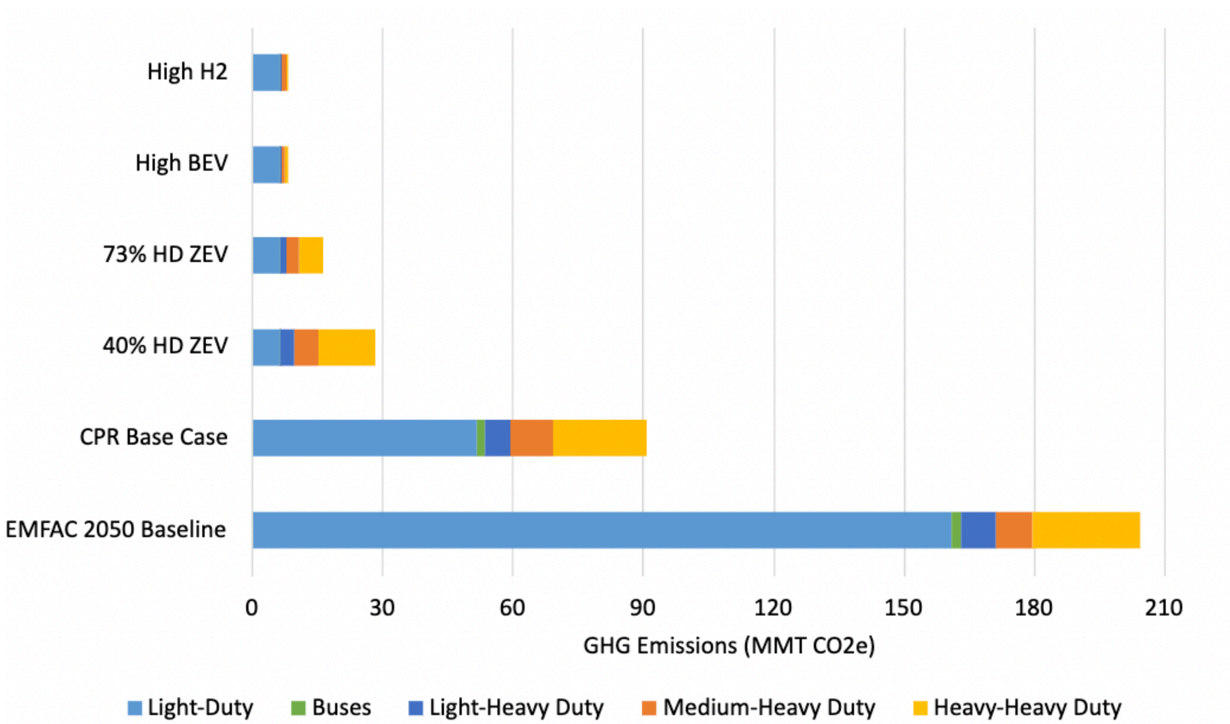

Figure 28: GHG emissions by HDV scenario in MMT CO2e. EMFAC 2050 Baseline represents a business-as-usual case with no electrification shift.[43]

The GHG emissions associated with each of those scenarios can be found in Figure 28 [43]. For reference, the figure includes the California Emissions Factor tool's (EMFAC) baseline for

2050, representing a “business as usual” scenario [55]. All the HDV scenarios meet the 80% below 1990 levels reduction goal, but none reach zero emissions due to the assumption that some legacy internal combustion engine vehicles will remain on the road.

b) Air Quality

As the lowest emissions scenarios with the highest electrification penetration, the spatial air quality modeling of the High BEV and High H2 scenarios were prioritized. They focus on $PM_{2.5}$ and ozone concentrations during summer months, as both pollutants of concern have peak events in the summer months. Spatial air quality analysis is crucial to understand the implications of criteria air pollution because of the negative health effects associated with poor air quality. Atmospheric chemistry modeling is also necessary because in addition to primary pollutants directly from vehicles, secondary pollutants form in the atmosphere that complicate further the health and environmental implications of emissions.

Figure 29 shows the air quality modeling results from the High BEV case from [43] generated with the Environmental Protection Agency’s Community Multiscale Air Quality modeling system (CMAQ). Due to the nature of Forrest’s investigation, the assumptions for the High BEV scenario simulated in the figure do not include a 100% renewable electric grid. Because this is at odds with the 100% renewable grid assumption of these analyses, these air quality results are considered a lower limit or conservative estimate as a renewable grid would only further reduce emissions and improve air quality outcomes. The map indicates an almost statewide reduction in 8-hour ozone concentrations as a result of vehicle electrification. The effect is largest in magnitude in the Los Angeles area, likely because of the large population of people who commute for work, school, and leisure. Maximum 8-hour ozone reductions in the state would occur up to 10 ppb, 14% of the state 8-hour ozone standard.

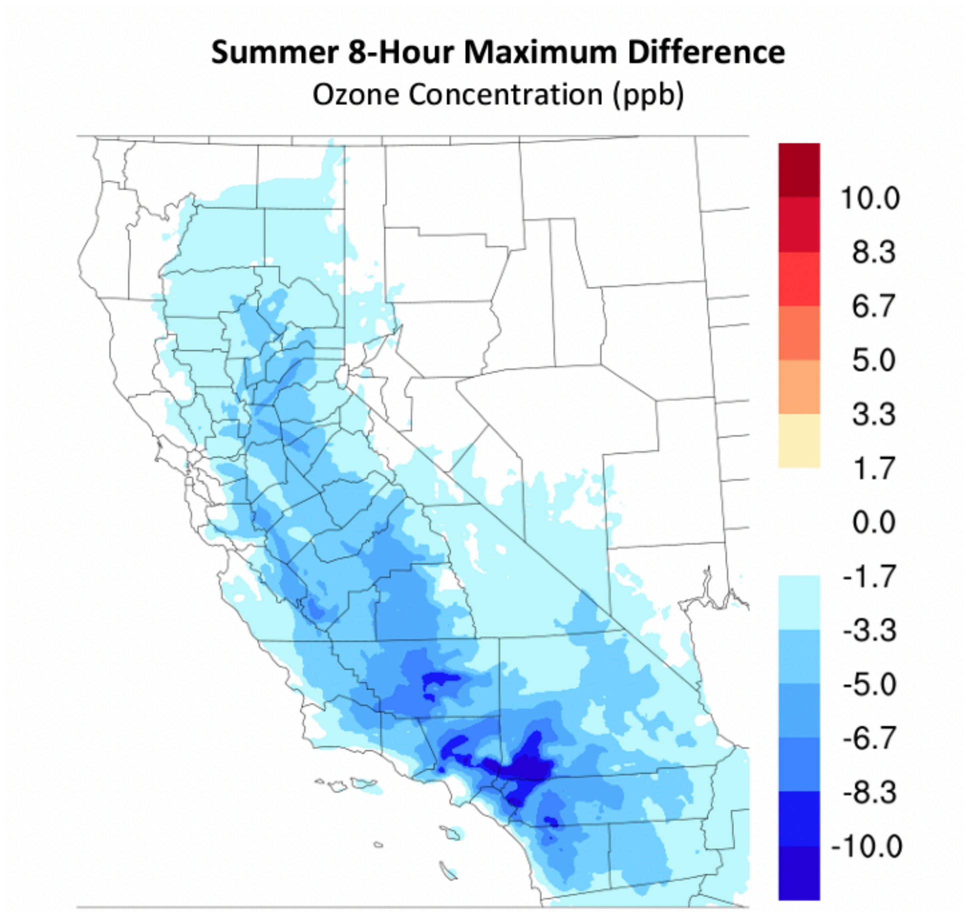

Figure 29: Changes in the ozone 8-hour concentration as a result of the High BEV case. [43]

Figure 30 shows the change in $PM_{2.5}$ concentrations, another good indicator for air quality due to its health effects. It also is a good indicator for vehicle emissions changes because gasoline vehicles emit tailpipe $PM_{2.5}$ from their combustion process, while electric vehicles (BEVs and hydrogen-operated FCEVs) do not. The CMAQ results show reductions of 24-hour $PM_{2.5}$ emissions throughout the state, particularly in the San Joaquin Valley and the Los Angeles area. The maximum reduction is about 2 $\mu g/m^3$.

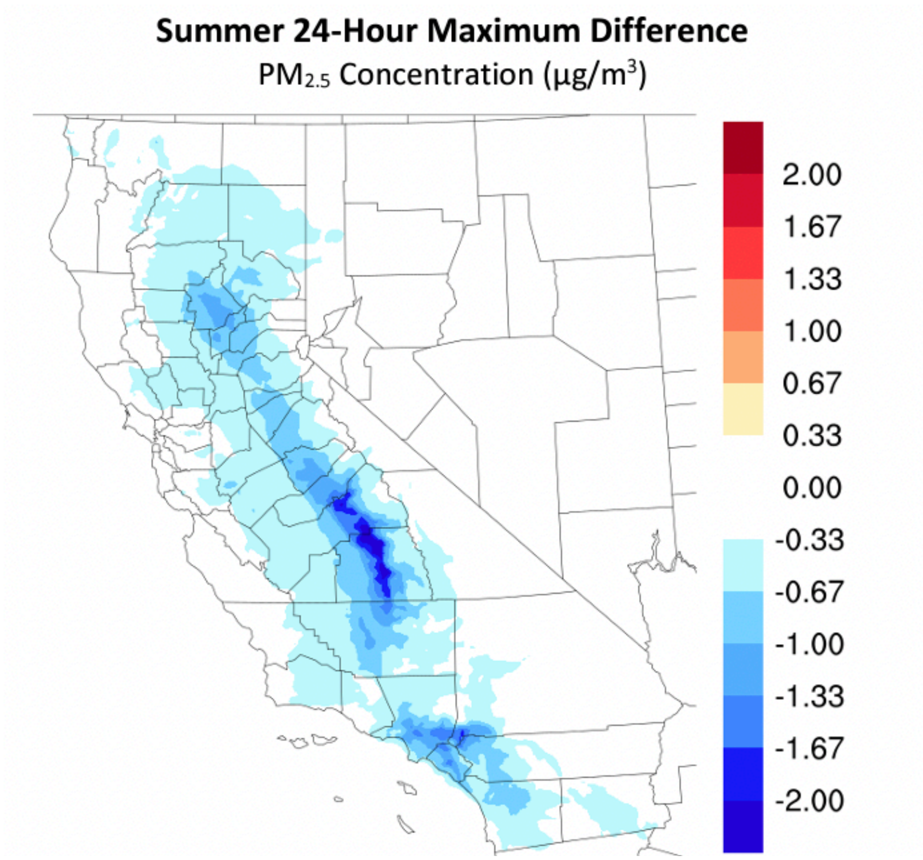

Figure 30: Changes in the 24-hour $PM_{2.5}$ concentration in summer as a result of the High BEV case. [43]

The High H2 scenario maps show the difference between air quality outcomes with a 100% renewable grid and without one. That means the maps do not show the total change from the base case but do indicate that a 100% renewable grid can add to the positive effects of vehicle electrification. Since a 100% renewable electric grid is an assumption for this thesis, these results are more representative of the scenarios modeled in HiGRID+. For example, Figure 31 shows the reduction in 8-hour ozone concentrations exclusively due to a complete renewable portfolio. Reductions go up to 3.0 ppb, 30% of the maximum concentration reductions achieved by the High BEV case without a fully renewable grid.

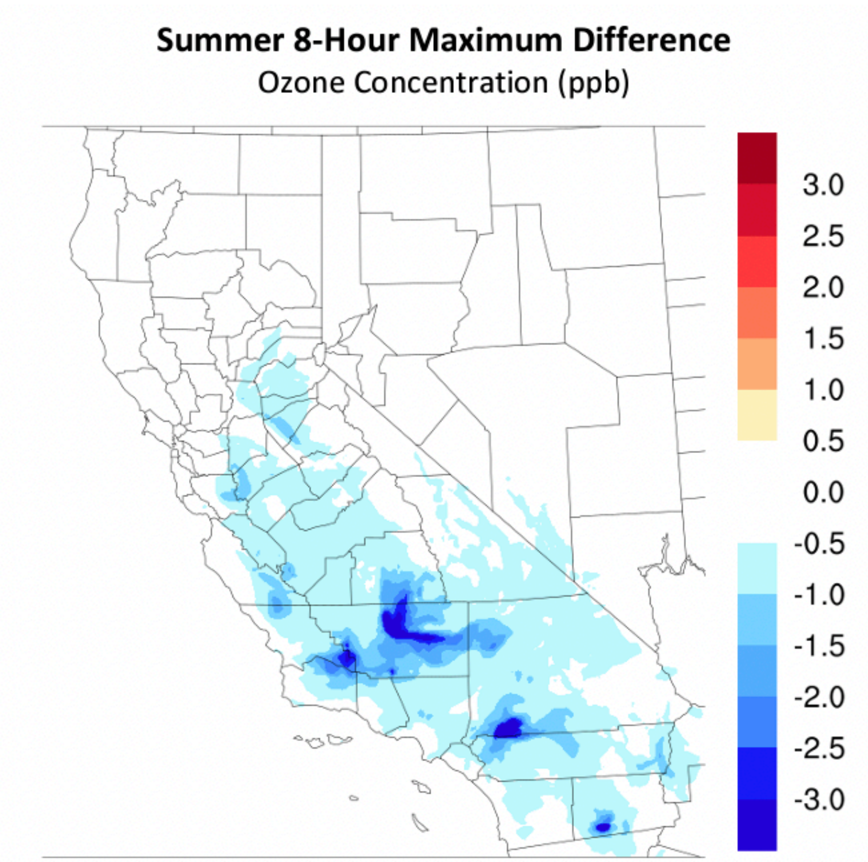

Figure 31: Changes in the 8-hour ozone concentration in summer as a result of combining the High H2 case with a 100% renewable electric grid. [43]

Similarly, Figure 32 depicts the change in $PM_{2.5}$ concentration that renewables cause in addition to the benefits of vehicle electrification. In the same way as in the High BEV results, these reductions would be more widespread in winter due to the weather patterns.

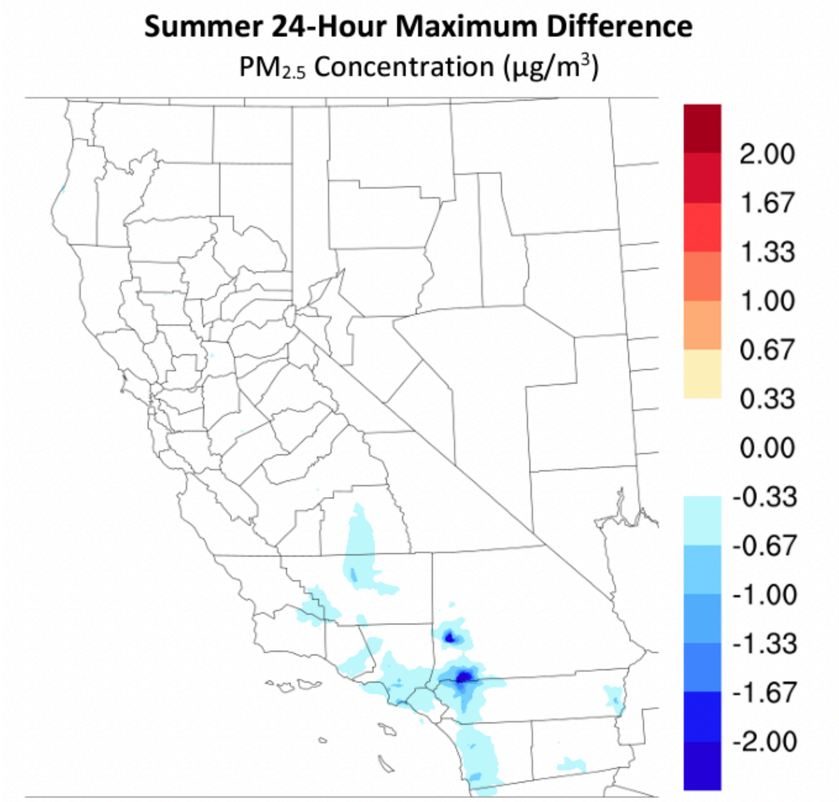

Figure 32: Changes in the 24-hour $PM_{2.5}$ concentration in summer as a result of the High H2 case.

Ultimately, the High BEV and High H2 cases present the lowest emissions options in terms of GHGs, and therefore were the cases of choice incorporated into the multi-sector scenarios. In winter, the reductions would be more widespread because the stagnant air allows for the concentration of primary $PM_{2.5}$ and more production of secondary $PM_{2.5}$. Therefore, the base value is higher and ZEV penetration has more of an effect.

4. Charging Infrastructure Analysis

The HiGRID+ tool calculates total charging infrastructure capacity by setting it as the peak charging demand. Since the vehicle population is constant across all scenarios, this results in a different vehicle to charger ratio for each of the HDV scenarios (listed in Table 6 according to a Level 2 charger power capacity of 7.2 kW).

	CPR Base Case	40% HD ZEV	73% HD ZEV	High BEV	High H2
Total Capacity (MW)	1.3668e4	2.4548e4	3.0418e4	3.2152e4	1.8330e4
Vehicle to Charger Ratio	47.2 to 1	84.8 to 1	105.1 to 1	111.1 to 1	63.3 to 1

Table 6: The total BEV charging infrastructure capacity calculated in the original HiGRID runs according to maximum electric vehicle demand. Vehicle to charger ratio calculated assuming a Level 2 charger power capacity of 7.2 kW and a total vehicle population of 40,205,297 [62]

Ultimately, the values in Table 6 do not consider spatial distribution of vehicles and charging stations, resulting in optimistic to the point of unrealistic vehicle to charger ratios. Additionally, HiGRID+ calculates the cost of BEV infrastructure with exclusively Level 2 charger cost assumptions. As a result, this charging infrastructure analysis was necessary to identify more accurate BEV infrastructure costs by implementing a more realistic vehicle to charger ratio and mapping LDV and HDV demands to Level 2 and DC fast charging cost assumptions, respectively. Since LDV and HDV demands were a controlled input, these cost assumptions would not change the optimization output and therefore could be calculated post-optimization. The load on the grid is the same no matter the vehicle to charger ratio.

This analysis took an optimistic and conservative approach to the vehicle to charger ratios. For both LDVs and HDVs, a 1:1 conservative ratio supplied an upper limit for the number of chargers necessary to accommodate the projected vehicle population [63]. The optimistic ratio reflects a more favorable scenario in which multiple vehicles can use a single charger to fulfill their electric demand. The optimistic ratios are different for LDV and HDVs due to the difference in demand volume and vehicle function. For LDVs, AB 2127 projects the need for

700,000 BEV chargers for 5 million vehicles, a vehicle to charger ratio of 7.14 to 1 [64]. For HDVs, a California Energy Commission presentation indicated a vehicle to charger ratio of 1.7 to 1 as an optimistic assumption [65]. The vehicle to charger ratios for the conservative and optimistic assumptions are summarized in Table 7.

Conservative		**Optimistic**	
Level 2	DCFC	Level 2	DCFC
1:1	1:1	7.14:1	1.7:1

Table 7: Vehicle to charger ratio assumptions for the conservative and optimistic charging infrastructure analyses.

Original BEV infrastructure costs were subtracted from the total cost and replaced with the cost associated with the calculated charging capacities for each HDV scenario using the listed vehicle to charger ratios. The resultant costs for all scenarios are plotted in Figure 33 with their original HiGRID+ cost calculation included for reference. Additionally, the percent differences between the original cost calculations and the charging infrastructure analysis outputs are plotted in Figure 34 to highlight the specific implications of the more realistic vehicle to charger ratios.

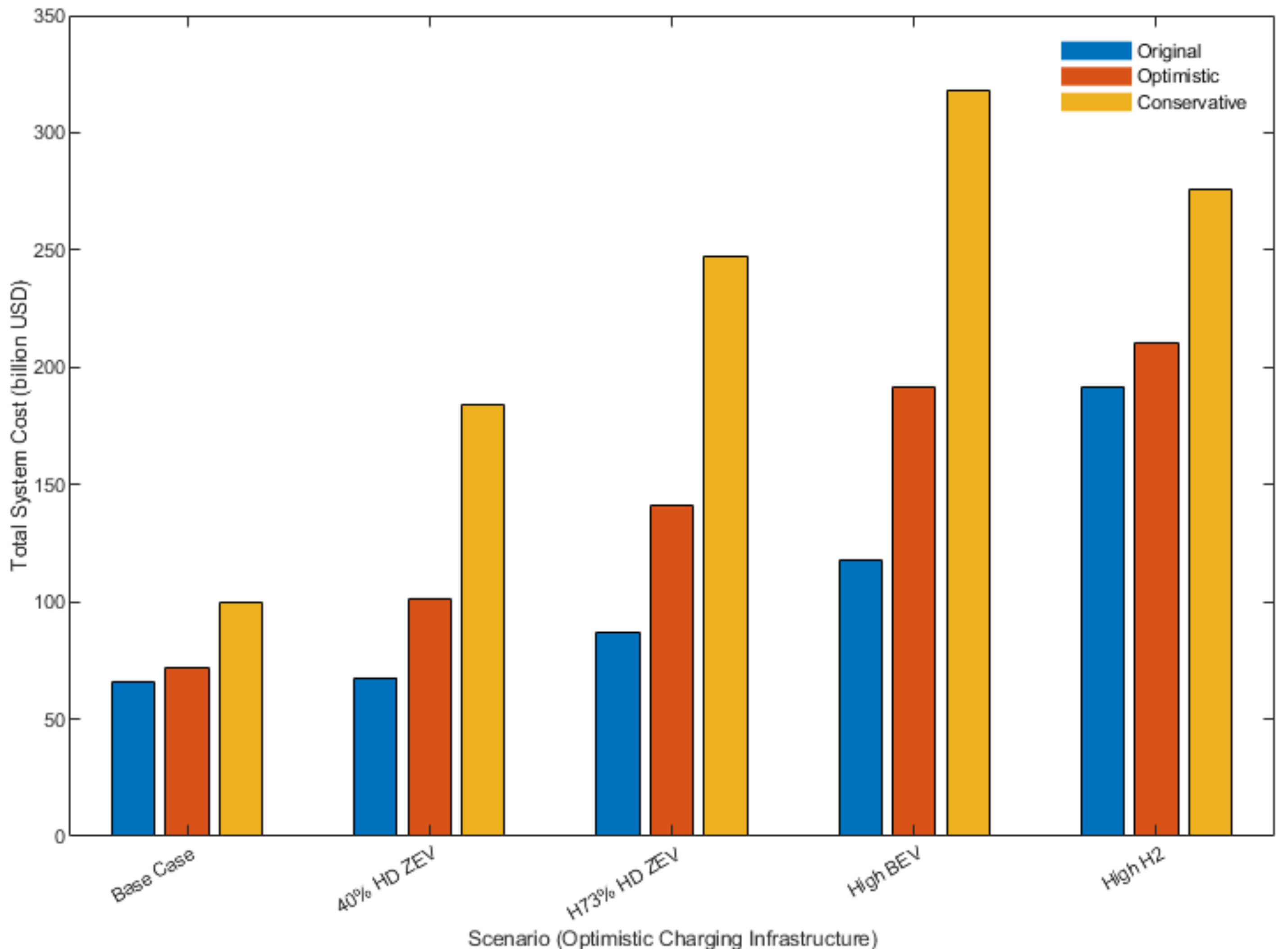

Figure 33: A direct cost comparison of the original HiGRID+ cost calculation and the conservative and optimistic charging infrastructure analysis adjusted costs.

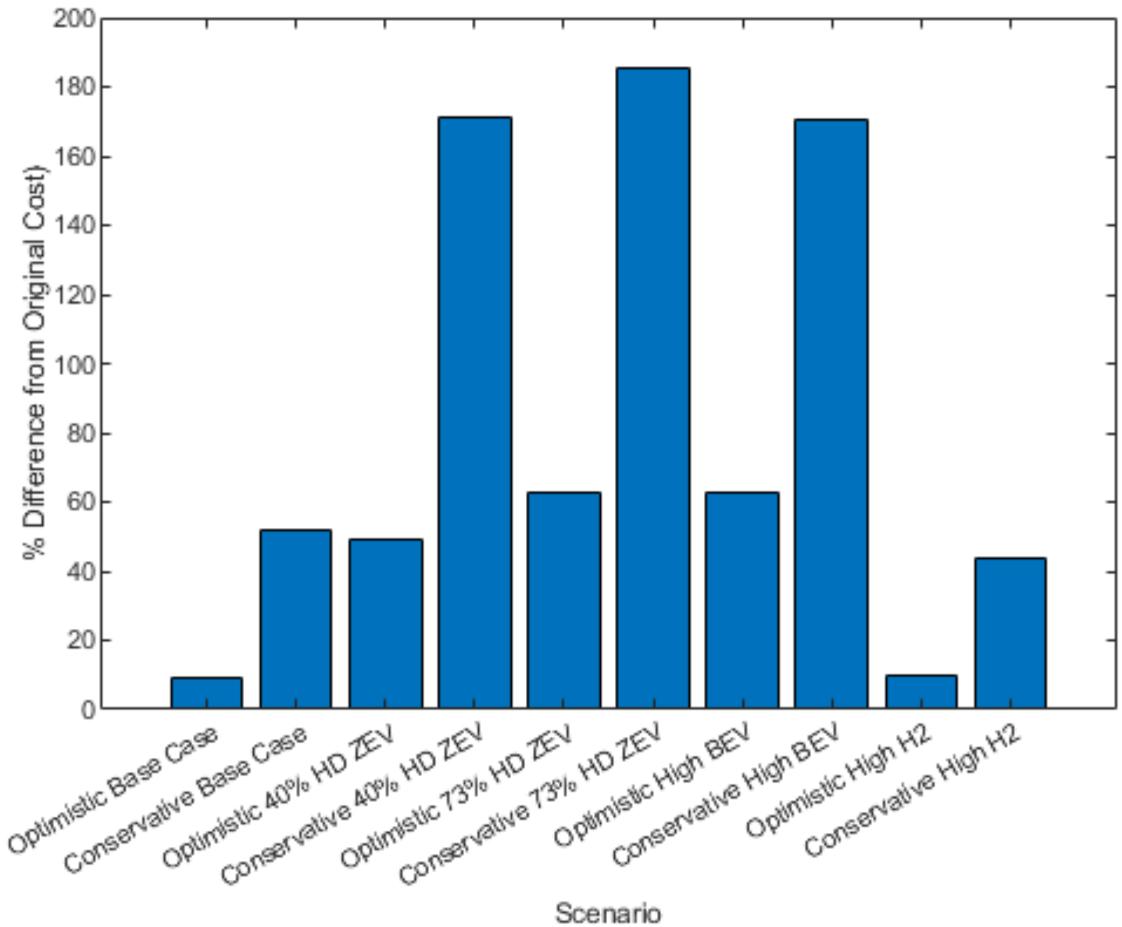

Figure 34: Relative cost increases for each HDV scenario associated with the optimistic and conservative charging infrastructure analyses.

The conservative cases all cost more than their optimistic counterparts because they implement larger numbers of chargers. Figure 34 in particular highlights the benefits of investing in both BEV and FCEV infrastructure, as the High H2 scenario (which invests most heavily in FCEVs) suffers the lowest relative increase of all of the HDV scenarios. This indicates that the High H2 scenario's economy is less sensitive to BEV charging infrastructure vehicle to charger ratios, and therefore capacity demands and cost fluctuations.

B. Refinery Scenarios

1. System Cost

In the refinery scenarios, renewable capacity spanning for each scenario was not necessary because the change in load demand between each scenario was small (maximum 1.7%). The transportation load from the CPR base case scenario was used for the refinery scenarios to isolate the effects of different refinery pathways. The renewable capacity was kept constant at the base level used in the HDV cases for all of the refinery cases (174.14 GW solar, 91.3 GW wind). Figure 35 compares the total system costs of the refinery scenarios to the CPR base case scenario. The y axis is zoomed in on the top of the plot to highlight the relative costs of the scenarios for visual clarity, but Table 9 lists the raw values to illustrate how close together the cost results were. The largest percent difference between the scenario costs was 1.17% (RARO and RPWR). A small variation like this was expected because the refinery load that changes between scenarios is only 0.43% of the total electric load on the grid. With little variation between scenarios at such a small portion of demand, they are likely to generate similar results.

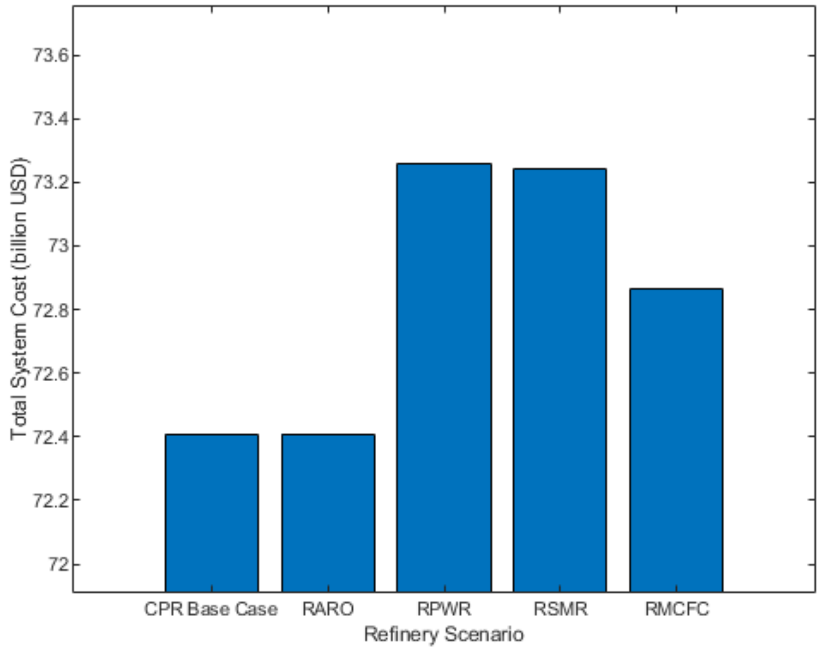

Figure 35: Total system cost of refinery scenarios in billions of USD, y axis shifted to show detail.

CPR Base Case	RARO	RPWR	RSMR	RMCFC
72.410	72.409	73.257	73.243	72.863

Table 8: Total system cost of refinery scenarios in billions of USD.

2. Technology Selection

a) Electrolyzer and Energy Storage Technology Mix

The energy storage and electrolyzer technology mix for the refinery cases can be found in Figure 36. As they are similar in value, Table 9 also lists the capacity value for each technology and scenario. In all the scenarios, more electrolyzer capacity than energy storage capacity was installed. The RMCFC scenario has the most hydrogen demand and the most combined electrolyzer and energy storage installed capacity. The combination of technologies in the

RMCFC case reinforces the conclusion from the HDV cases that increased hydrogen demand necessitates increased storage and electrolyzer capacity for flexibility. Since there is not a lot of variation in the results, it can be concluded that dramatic changes to the unit processes in refineries would not have a large effect on grid dynamics. That is a promising conclusion, as the main concern associated with electrification of cross-economy sectors is that the grid infrastructure could not handle the shift in demands.

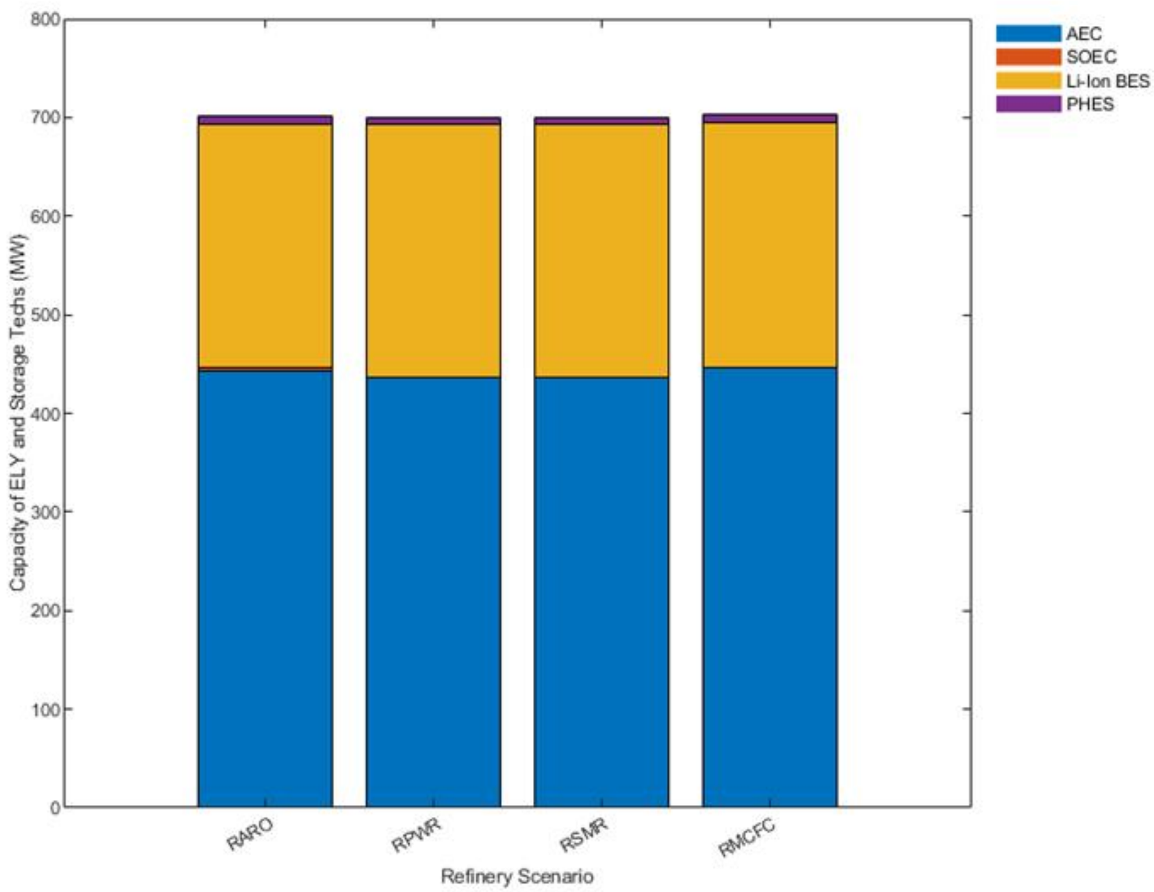

Figure 36: Refinery scenario electrolyzer and energy storage technology capacities.

Capacities (MW)	RARO	RPWR	RSMR	RMCFC
AEC	443.8	436.7	436.8	446.8
SOEC	0	2.0	0	0
Li-Ion BES	246.8	256.6	256.5	248.6
PHES	8.4	6.5	6.5	7.3

Table 9: Refinery scenario electrolyzer and energy storage technology capacities.

b) Hydrogen Energy Storage

The annual state of charge of hydrogen energy storage is show in Figure 37. The state of charge in all scenarios builds steadily in the spring and summer, stays high for most of the second half of the year, before discharging during winter when long duration storage is most utilized. With winter lows of intermittent renewable generation, hydrogen storage is shown here to help with the seasonal scale implications of a fully renewable electric grid.

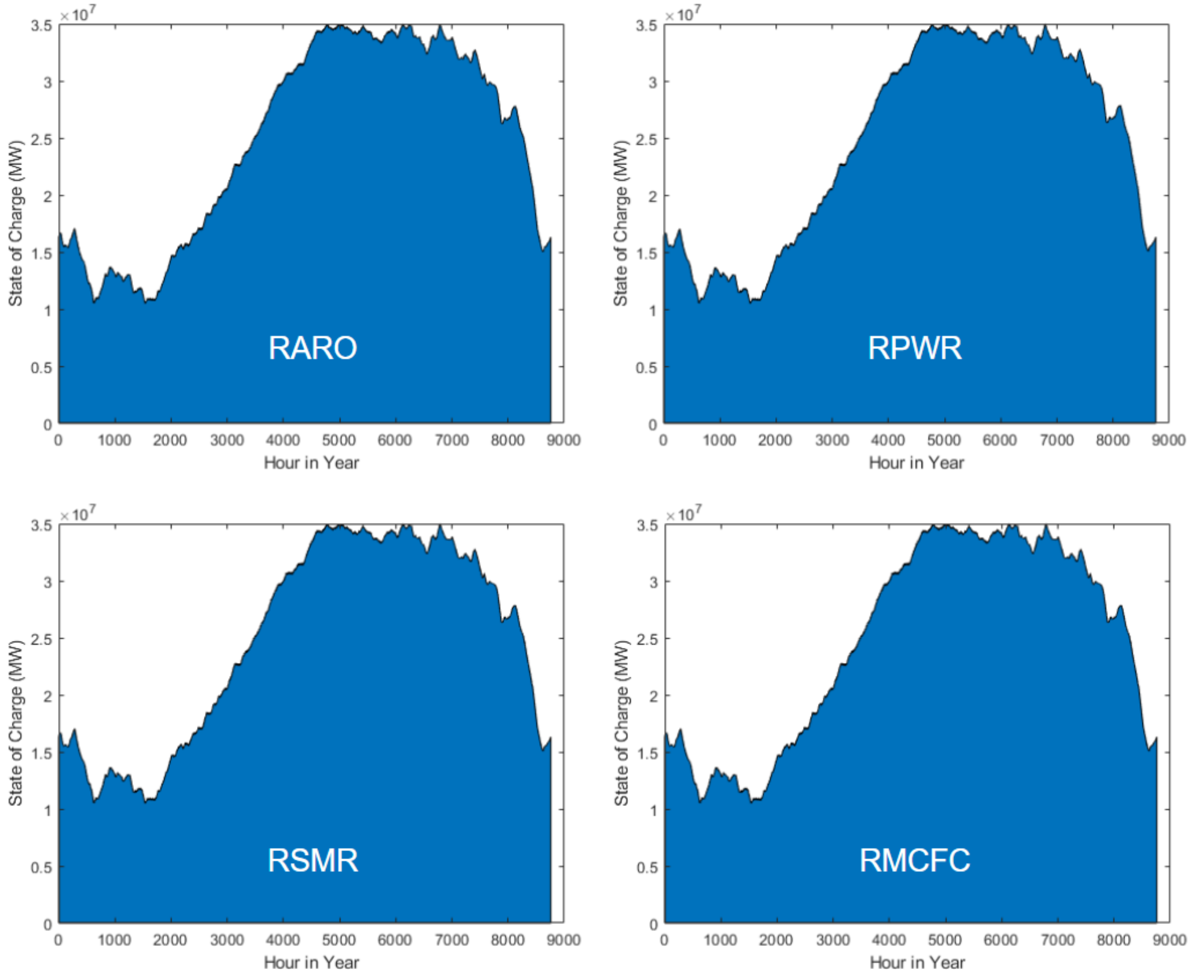

Figure 37: Hydrogen Energy Storage state of charge for refinery scenarios.

3. Emissions and Air Quality Analysis

a) GHG Emissions

The greenhouse gas emissions associated with each scenario are directly related to the extent to which they replace process units with fuel cell systems. The process units as-is produce GHGs as a result of combustion, and any steam demand in a refinery is currently generated by steam methane reformation. SMR produces 8-12 kg of CO_2 for every kg of hydrogen generated, while the hydrogen boiler used in this analysis produces none. The emissions are not offset to the electricity needed to generate the hydrogen due to the 100% zero emission grid assumption.

Ultimately, the RARO case, which retrofits all process units with MCFC systems, effectively removes all greenhouse gas emissions from the refining process associated with electric, fuel, and steam demands. As described in [58], all of the scenarios achieve 100% decarbonization, attributed to the MCFC's carbon capture capabilities.

b) Air Quality

Table 10 lists the effect of each refinery scenario on CAP emissions in California determined by [58]. The listed values are a useful reference, but do not align with the versions of the cases modeled in the report because the source used methane as the fuel cell fuel rather than hydrogen. As a result, the CAP emissions would be reduced by more than the percentages determined by the source report.

Scenario	**Percent Reduction**						
	NO_x (%)	SO_x (%)	PM (%)	CO (%)	VOC (%)	NH_3 (%)	CO_2 (%)
RARO	66	99	99	-16	99	---	100
RPWR	15	0.70	---	-2	37	---	100
RSMR	1	0.10	---	-6	6	---	100
RMCFC	59	99	99	-15	99	---	100

Table 10: Change in various GHG emissions by refinery scenario. [58]

Steam boilers and heaters are a large contributor to refinery CAP emissions, so the transition to hydrogen boilers and for steam and heat has a positive effect on sector emissions. Hydrogen fuel in place of methane fuel for refinery processes removes the CO pollution from the vicinity. CO reductions would not affect the spatial air quality modeling or secondary pollutants but can be a harmful primary pollutant. Primary PM comes from combustion in refineries. All of the modeled refinery scenarios eliminate combustion through the use of hydrogen fuel and hydrogen boilers, so remaining PM concerns from the original scenarios were solved with those shifts.

NO_x emissions were reduced by all, but not eliminated by any refinery scenario. (The total removal of combustion would be required to virtually eliminate NO_x emissions.) In spatial air quality modeling, the concentration of NO_x is an essential metric because it is involved in the generation of ozone and secondary PM. Figure 38 shows the spatial NO_x emissions reductions for four scenarios: (a) complete removal of CA refineries, (b) RARO, (c) RMCFC, and (d) RPWR. Complete removal has a large effect in northern California, and RARO and RMCFC have slightly smaller but notable effects in the same region. The RSMR case was not plotted in air quality analysis because its effect on emissions was negligible. Figure 38: NOx emissions in ton/day for (a) complete removal of CA refineries, (b) RARO, (c) RMCFC, (d) RPWR. [58]

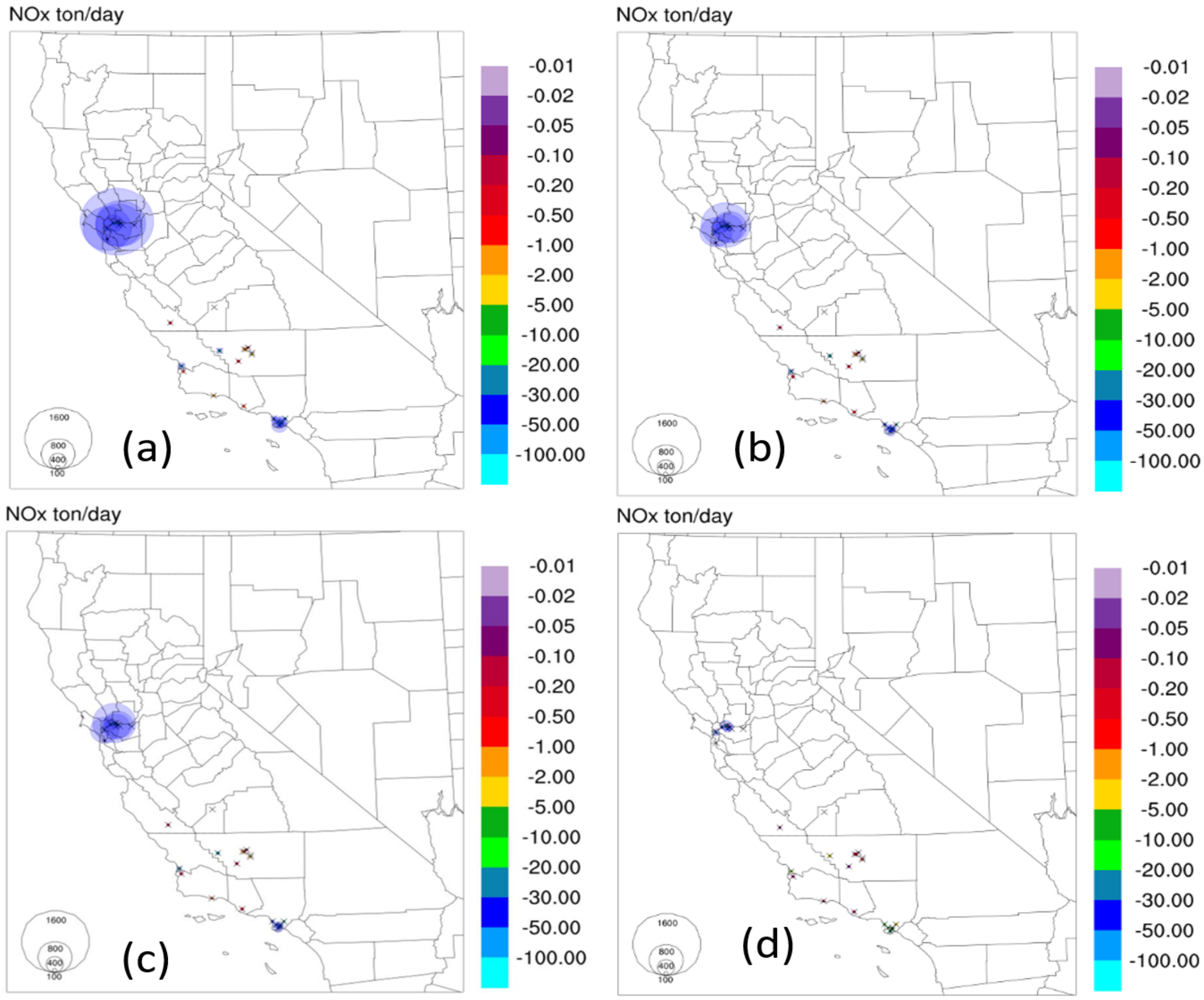

Figure 38: NOx emissions in ton/day for (a) complete removal of CA refineries, (b) RARO, (c) RMCFC, (d) RPWR. [58]

Spatial atmospheric chemistry and air quality results were modeled in CMAQ to analyze 8-hour ozone and 24-hour $PM_{2.5}$ concentrations to understand the potential health benefits of refinery fuel cell implementation. Figure 39 includes the 8-hour ozone concentration reductions for the same four cases as Figure 38 [58]. The theoretical removal of all refineries has the largest impact on ozone concentrations, especially in the San Joaquin Valley and inland (downwind) of San Francisco. RARO and RMCFC both achieve smaller but still considerable ozone reductions since they both replace all or most of the process units with zero emission fuel cells. Since

RPWR only replaces the power generation system, the majority of the ozone-causing emissions are not mitigated.

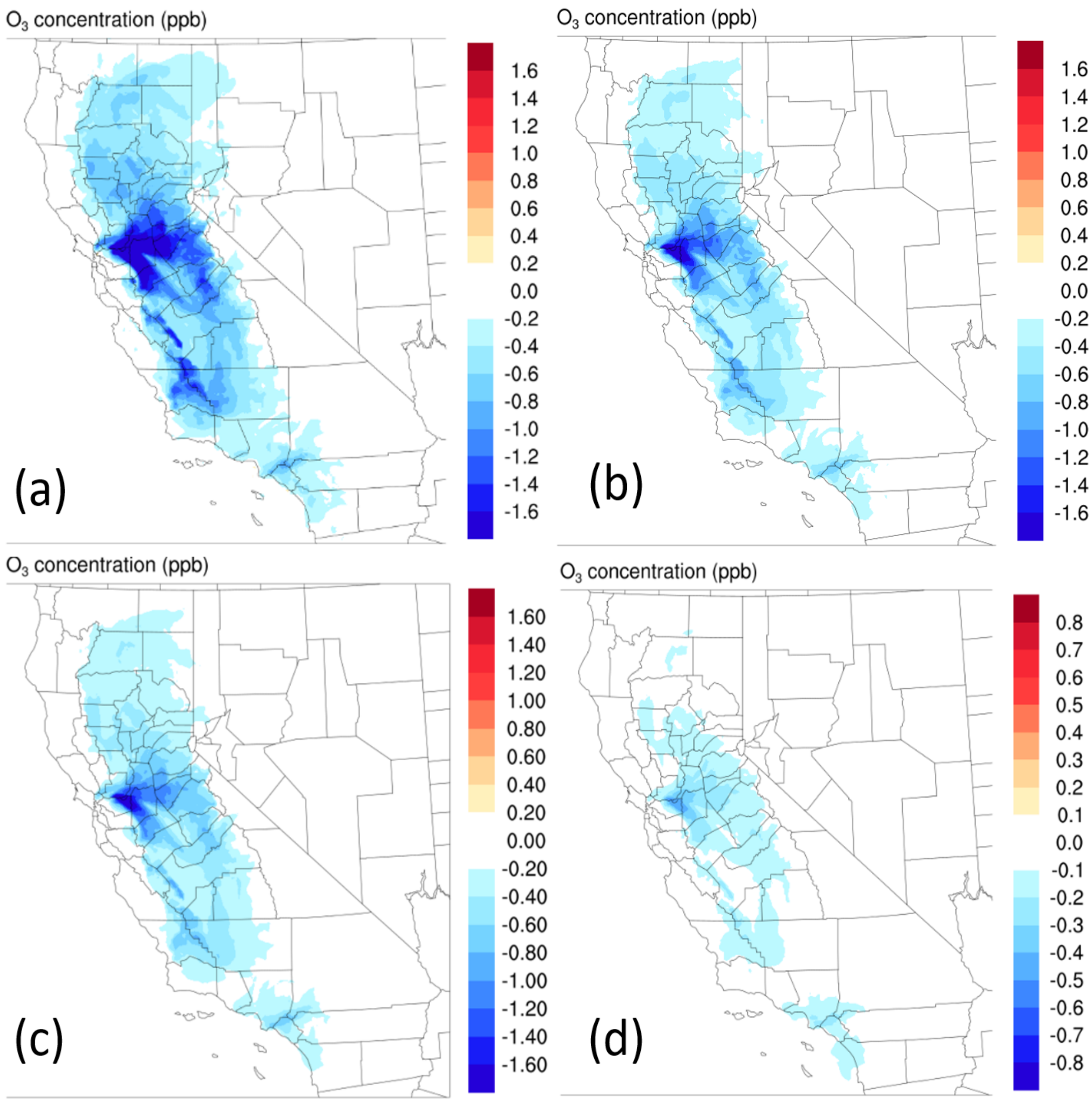

Figure 39: 8-hour ozone concentration reductions for (a) complete removal of CA refineries, (b) RARO, (c) RMCFC, (d) RPWR. [58]

In terms of $PM_{2.5}$, the RARO and RMCFC cases reduce concentrations about as well in magnitude and spatial spread as the upper bound complete removal of refineries case (see Figure 40). The RPWR map units are ng/m^3 rather than the μg/m^3 used for the other scenarios so that the changes would be visible, but they are much smaller deviations in RPWR than the other three cases.

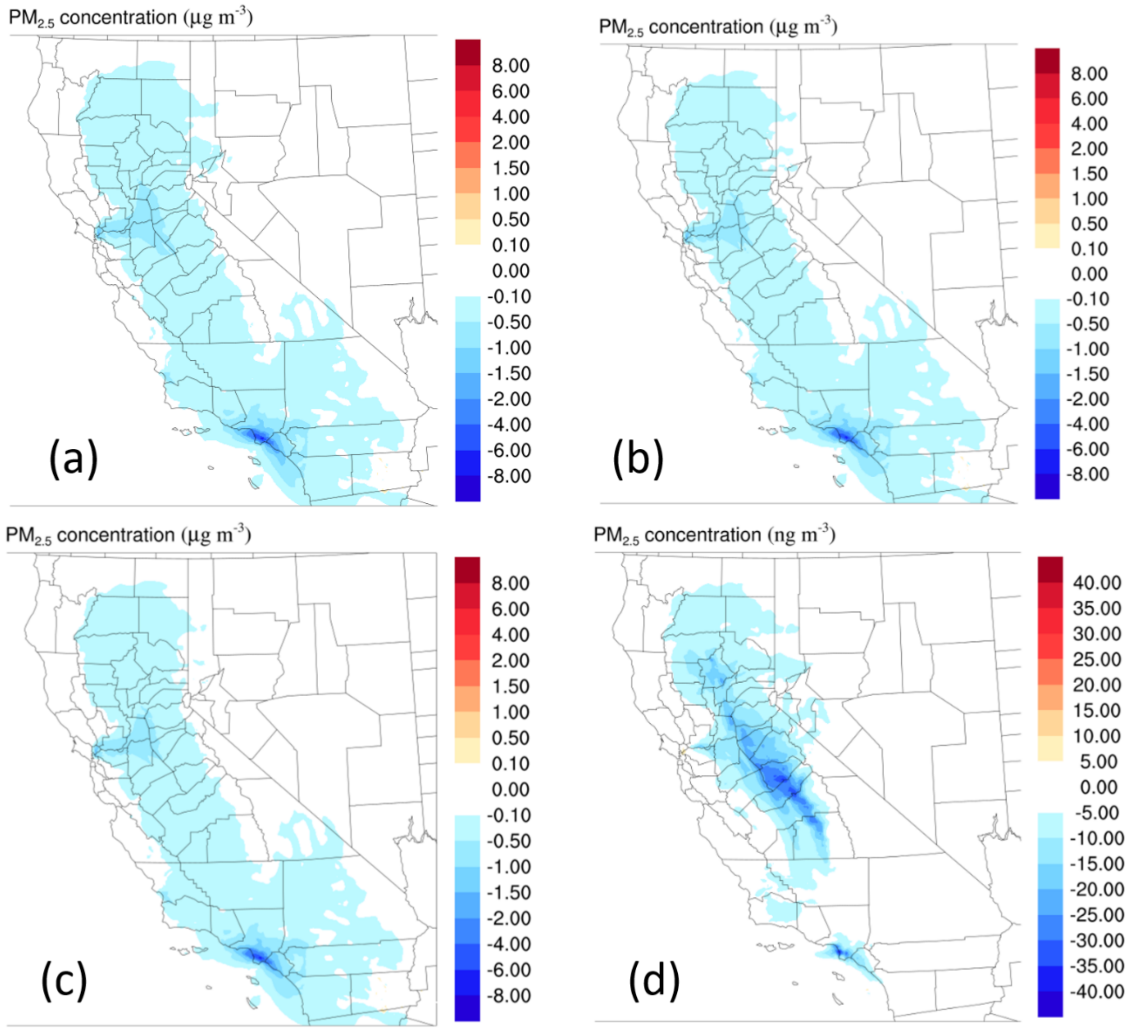

Figure 40: Reduction of PM2.5 concentrations in CA for (a) complete removal of CA refineries, (b) RARO, (c) RMCFC, (d) RPWR.[58]

C. Combined Scenarios

The goal of the combined scenarios was to assess the least cost pathways to electrify, decarbonize, and improve air quality implications of HDVs, refineries, and the electric grid as a cooperative system. To that end, the combined scenarios (listed in Table 4) that were modeled chose the RARO refinery case and the High BEV and High H2 HDV cases since they go the furthest in emissions and air quality improvement (refer to Table 4). The least cost renewable capacities for High BEV and High H2 were used in the model with the combined electric and hydrogen demands, resulting in two combined scenario runs: RARO + High BEV and RARO + High H2.

1. System Cost

The system costs for each combined scenario were comparable to their HDV constituent scenario. Figure 41 shows the multi-sector scenario total system costs alongside the CPR Base Case and each of the constituent refinery and HDV scenario costs. The optimistic charging infrastructure HDV scenario costs were used. In both scenarios, the costs for the combined cases are slightly lower than the HDV constituent scenario, though the margins are low (<0.0002%). The RARO scenario removes refinery electric demand, but its hydrogen demand is about 5 times greater than the High BEV hydrogen demand and about 2 times greater than the High H2 demand. Since the cost for the combined scenarios are slightly lower, that indicates that slightly reduced electric demand and increased hydrogen demand work compatibly in these cases to lower cost.

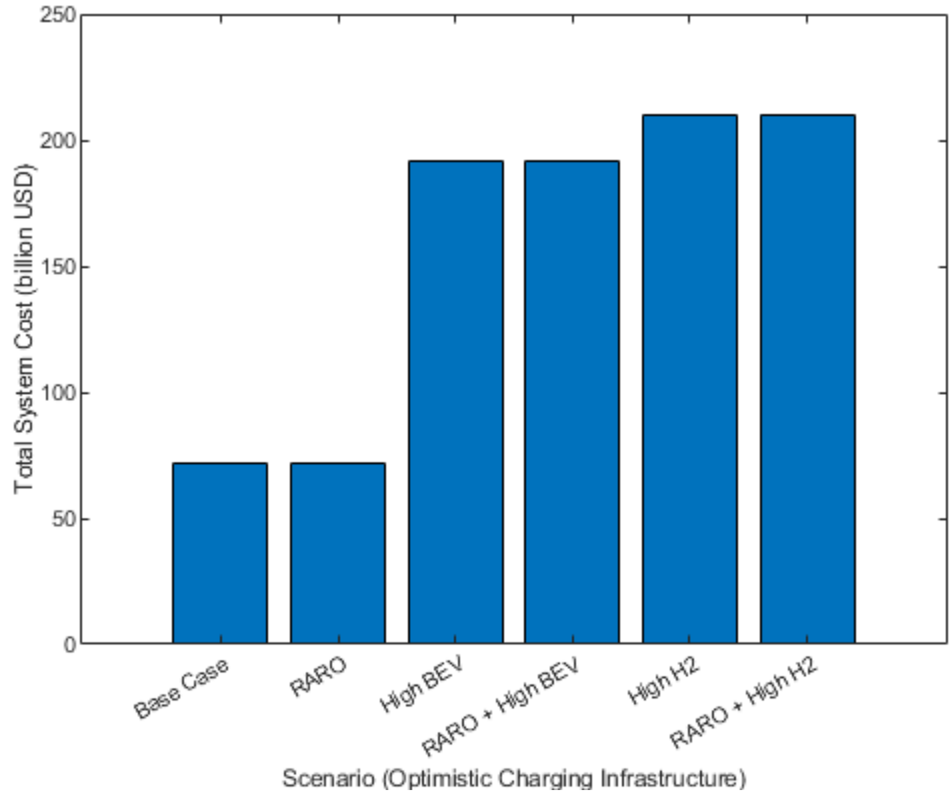

Figure 41: Total system cost of multi-sector scenarios in billions of USD with constituent scenarios for reference.

2. Technology Selection

a) Electrolyzer and Energy Storage Technology Mix

Grid-wide electrolyzer and energy storage technology capacities necessary to meet demand and minimize system cost for the combined scenarios and their constituent scenarios are compared in Figure 42. All scenarios require more grid-wide electrolyzer and energy storage capacity than the CPR base case scenario, a result of cross-sector electrification and increased demands. The RARO scenario has the highest hydrogen demand of the constituent scenarios, but with the additional FCEV hydrogen demand from the HDV scenarios, the two combined scenarios have the largest hydrogen demands of the plot below. Notably, the High BEV scenarios have lower total electrolyzer and energy storage capacities than the RARO case on its own. However, the larger electrolyzer capacity is likely a result of the combined HDV and refinery hydrogen demand. The High H2 scenario also has a larger hydrogen demand than the High BEV, so it requires higher energy storage capacities to promote grid flexibility and time to offset the hydrogen generation demand.

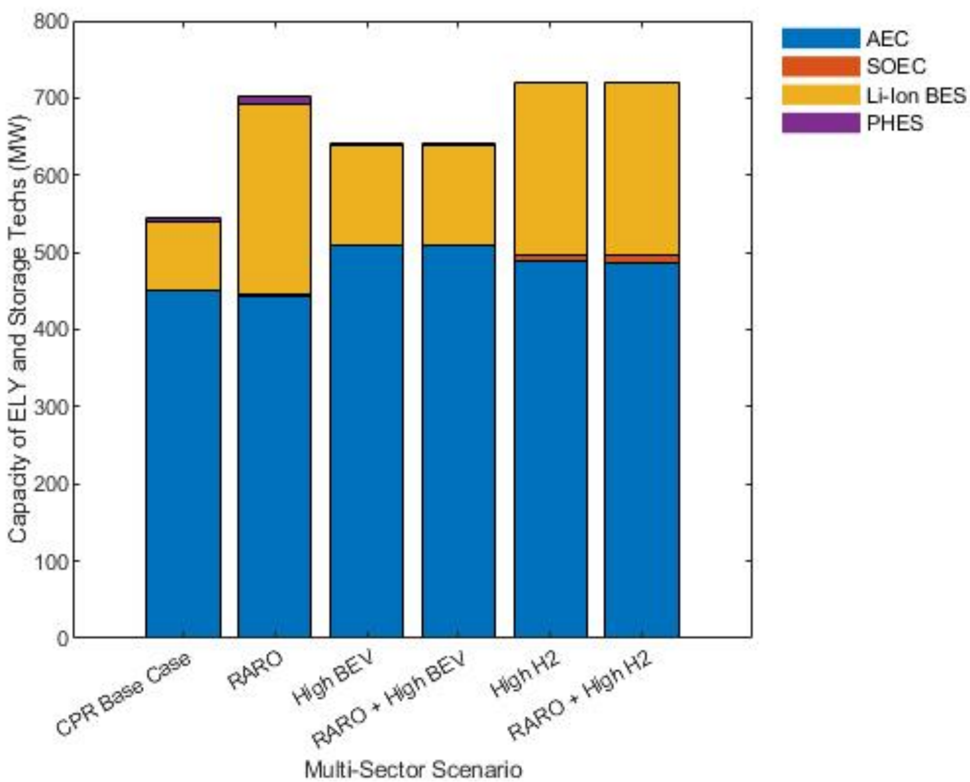

Figure 42: Multi-sector scenario electrolyzer and energy storage technology capacities in MW with constituent scenarios for reference.

To understand the extent to which each scenario utilizes its electrolyzer and energy storage technologies, a review of the total annual demand of the technologies, presented in Figure 43, is required. Even though RARO has a higher installed capacity, the demand figure shows that the HDV and combined scenarios use the technologies more throughout the year. Those cases more efficiently utilize the installed capacities, keeping the grid more balanced and low cost even in the event of much higher demands. The High H2 scenarios have a higher total capacity and total demand because their renewable capacity is 50% larger than that of the High BEV cases. More renewable capacity allows for the utilization of more otherwise curtailed renewables to charge batteries and/or generate hydrogen with these technologies. For example, the time series in Figure 44 show an example of a period in the year in which electrolyzers use electricity more frequently in the RARO + High H2 scenario than the RARO scenario. Even if they have similar installed capacities, higher frequency of use means that the grid is getting more value out of the installed technology.

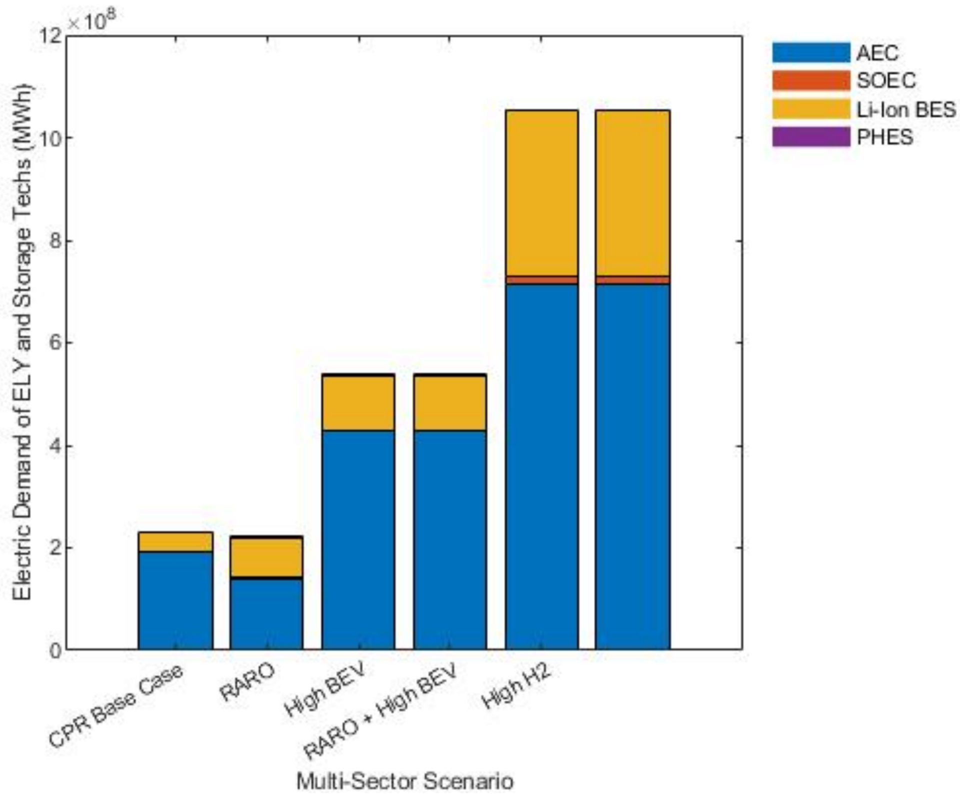

Figure 43: Multi-sector scenario electrolyzer and energy storage technology annual electric demand in MWh with constituent scenarios for reference.

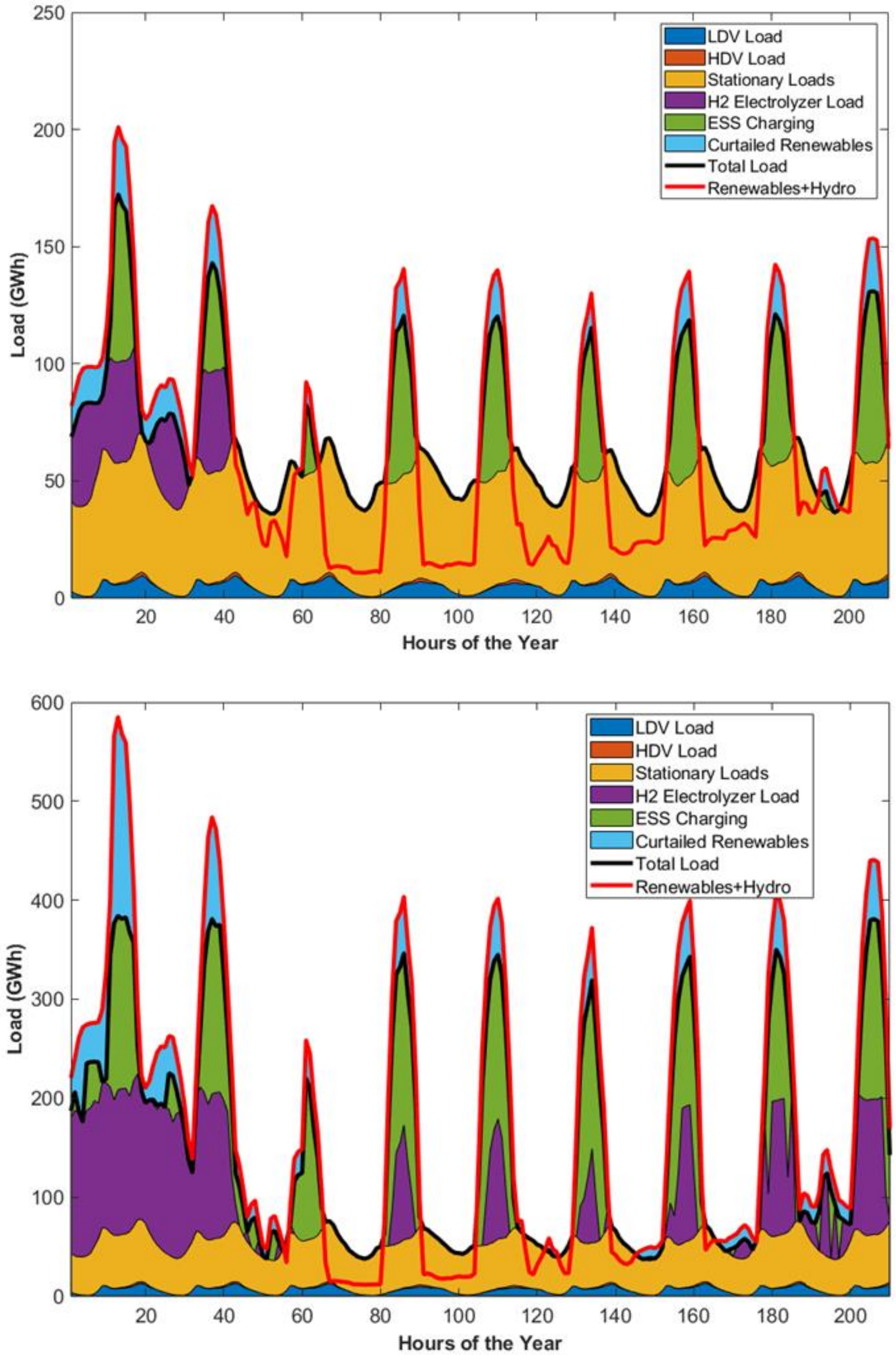

Figure 44: Generation and load time series for hours 241-450 in the year for the RARO case (top) and the RARO + High H2 case (bottom).

b) Hydrogen Energy Storage

Combining the RARO scenario with the High BEV and High H2 scenarios yields the hydrogen energy storage profiles in Figure 45. The shape of the combined scenario curves reflects the influence of the smoother, more gradual increase in state of charge generated by the RARO results. RARO + High BEV’s maximum state of charge increases by an order of magnitude, likely due to the large increase in hydrogen demand. The RARO + High H2 scenario results in the most use of hydrogen energy storage with the highest peak state of charge and greatest area under the curve (indicating greatest total electricity stored).

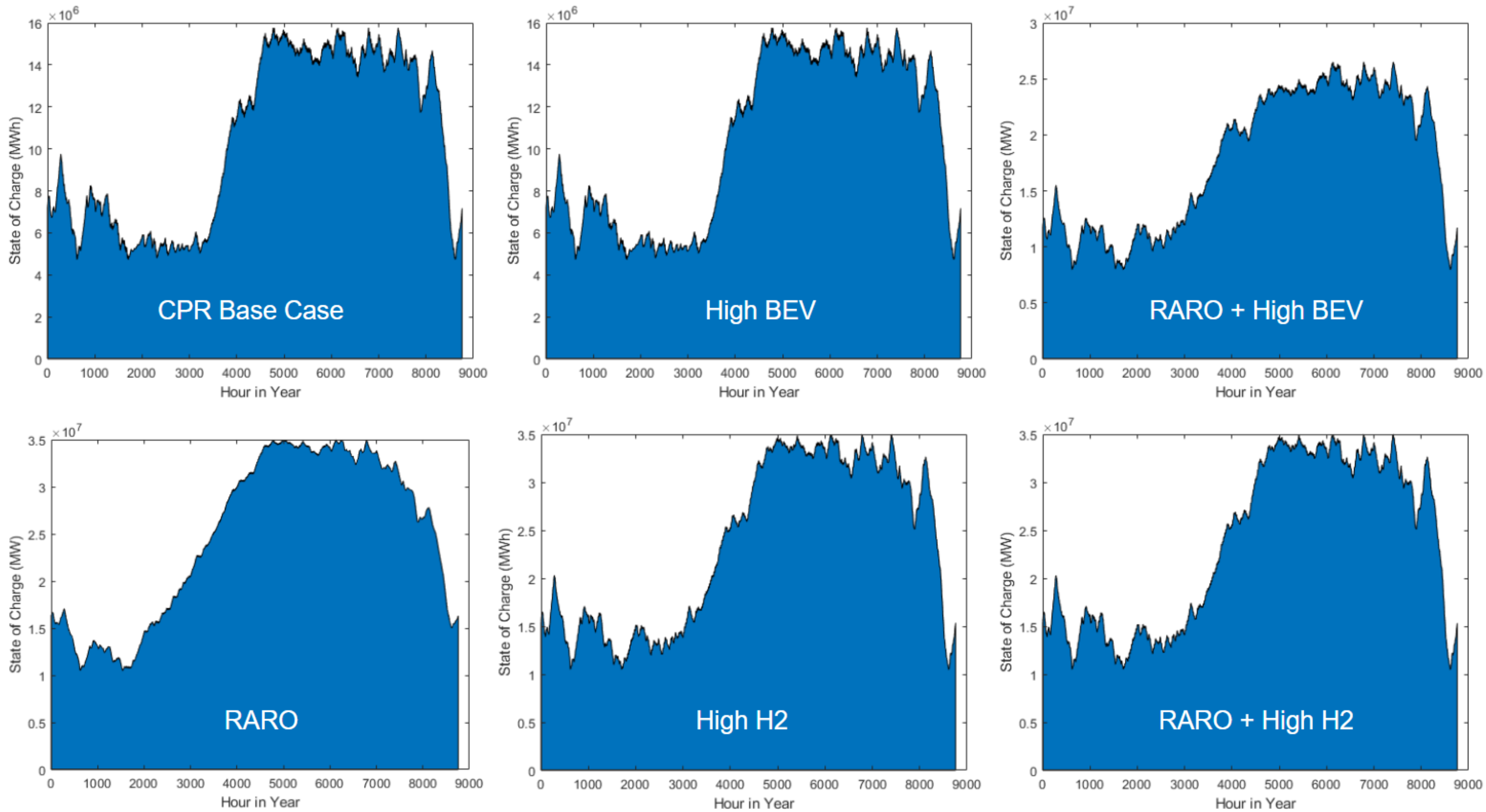

Figure 45: HES annual state of charge for combined cases and their constituent scenarios for reference.

3. Air Quality and Emissions Analysis

A considerable benefit of combining vehicle electrification and refinery decarbonization in the context of a 100% renewable electric grid is that the multi-sector scenarios also combine the emissions and air quality advantages of each. Table 11 lists the approximate lower limits of the maximum 24-hour $PM_{2.5}$ and 8-hour ozone concentration reductions in the state. The values for RARO and High BEV are from the maximum reductions in their air quality spatial analyses. For High H2, the values were calculated by adding the baseline reductions of the High BEV case to the additional concentration reductions identified as a result of a 100% renewable grid. Finally, the combined cases simply added the reductions from their constituent cases since the cause of the reductions do not overlap; the effects of each scenario were isolated in modeling.

	RARO	High BEV	High H2	RARO + High BEV	RARO + High H2
24-hour $PM_{2.5}$ Concentration Maximum Reduction ($\mu g/m^3$)	-1.8	-2.0	-4.0	-3.8	-5.8
8-hour Ozone Concentration Maximum Reduction (ppb)	-1.6	-10.0	-13.0	-11.6	-14.6

Table 11: 24-hour PM2.5 and 8-hour ozone concentration maximum reductions from constituent cases and calculated for combined cases.

VI. SUMMARY, CONCLUSIONS, AND RECOMMENDATIONS

A. Summary

The goal of this thesis was to establish cost optimal pathways in the energy sector to achieve the reduction of carbon and criteria pollutant emissions required to meet the 2045 California environmental targets with a focus on the following two major emission sectors: heavy-duty vehicles and refineries. It aimed to address the absence in the literature regarding (1) multi-sector analyses, (2) cost-based analyses, (3) consideration of current 100% RPS goals, and (4) accounting for both air quality and GHG emissions. The combination of these qualities provides a needed and more robust evaluation of the electrification of highly emitting sectors which affect electric grid dynamics and total grid system costs.

This work first analyzed previously established HDV and refinery scenarios and proposes steps to limit or, ideally, eliminate emissions from each subsector. Annual hourly electric and hydrogen demand curves for different technology rollouts (scenarios) were combined with a projected hourly grid demand for 2045, creating composite load demand input profiles for the cost-based optimization grid model HiGRID+. For each scenario, the input wind and solar generation capacities were spanned for each scenario to identify the least cost capacities for each input demand profile. For the HDV scenarios, optimistic and conservative vehicle to charger ratios were used to represent different levels of investment in vehicle charging infrastructure. GHG and CAP emissions for each scenario were calculated using literature-based emission factors and accounting for 100% RPS and the removal of natural gas as a fuel in refineries. Then, based on the emission reductions achieved by the subsector scenarios, two multi-sector scenarios were formed by combining the most effective refinery scenario with the two HDV scenarios that exhibited the highest reduction in emissions.

Based on the optimization, two multi-sector scenarios were identified that achieve most cost-effectively the 2045 California GHG and CAP emission reduction goals in the refinery and HDV subsectors assuming a 100% renewable electric grid.

B. Conclusions

- **Two scenarios provide the least cost pathways for multi-sector decarbonization and air quality improvements.**

  The two combined scenarios, "RARO + High BEV" and "RARO + High H2," incorporate the least cost wind and solar capacities for their respective HDV scenarios because the RARO refinery case does not add a significant amount of load that would require additional generation capacity. The multi-sector scenarios achieve almost complete HDV decarbonization (restricted due to legacy internal combustion vehicles still on the road) and complete refinery decarbonization. The air quality improvements of each of the sub-sector scenarios combined additively to those associated with a 100% renewable electric grid, a change that could improve health outcomes in the regions with the highest primary and secondary pollutant reductions.

- **Too much or too little installed renewable capacity has a negative effect on total system cost.**

  In simulation, spanning renewable capacities showed that a balance between renewable generation capacity and load demand minimizes cost. That value has upper and lower limits due to the practical effects of installing too little or too much capacity on the grid. Too little capacity reduces flexibility by limiting the amount of otherwise curtailed electricity that can flatten the demand curve, driving cost up. Even with the capability of HiGRID+ to allocate excess renewables (greater than direct demand) for energy storage and hydrogen generation, there is still a point at which too much capacity causes wasted excess generation and results in money spent on renewable installation that is not needed to meet load demand and/or those excess renewable channels. The wind and solar capacities must allow for enough flexibility without over-generating and wasting resources.

- **VHD and total electrolyzer and energy storage capacity are directly related.** According to the outputs from the HDV scenarios, VHD and the required total electrolyzer and energy storage capacity are directly correlated. Since vehicle hydrogen can be produced at any time preceding the use of the hydrogen for fueling, increased VHD causes an increased need for electrolyzers to generate hydrogen to serve both VHD at all times and EHD when required. When plotted together as hourly profiles, electrolyzer demand and energy storage discharge often aligned with each other and the renewable generation peaks. As a result, excess renewable generation is directly used for electrolytic hydrogen generation and battery electric energy storage.
- **The total cost of BEV implementation is driven by charging infrastructure buildout, while the total cost of FCEV implementation is driven by the cost of vehicle hydrogen fuel.**

  The investigation into conservative and optimistic vehicle-to-charger ratios showed that charging infrastructure buildout is the primary influence on the cost of BEV penetration. The more that vehicles can share charging stations, the less expensive it is to achieve a high BEV fleet penetration. The cost of FCEV implementation is primarily influenced by the cost of hydrogen fuel, which is in turn driven by hydrogen production costs and the penetration of green hydrogen generation technologies. The cost of both scenarios is similar.

- **Replacing refinery processes with fuel cell systems (primarily MCFCs for the added carbon capture benefit) can significantly reduce refinery emissions while not affecting the demand on the utility grid.**

  All four of the refinery scenarios involved the retrofit of some, if not all in the case of RARO, refinery process units with SOFCs or MCFCs. However, since refinery load is a small portion of total load demand, altering that demand had little effect on the optimization output and, as a result, the electric grid technology mix and cost. For the RARO scenario and the RMCFC scenario to a lesser extent, key GHG and CAP emissions were reduced by the shift to fuel cell process systems. Refinery fuel cell retrofits present a subsector transition that can reduce emissions without a large change in grid system cost and technology rollout pathways.

C. Suggestions for Further Work

- Identify and explore which factors most restrict the selection of hydrogen as an energy storage technology.
- Model for intermittent years before 2045 with the goal to provide specific, actionable policy recommendations.
- Model the full thermodynamic analysis of a refinery operating with fuel cell retrofits using hydrogen fuel from the beginning instead of converting methane fuel calculations to hydrogen approximations.
- Conduct air quality analyses for the refinery cases using hydrogen instead of methane as the fuel.
- Conduct air quality analyses for the optimized cases to evaluate the spatial air quality impacts of the multi-sector load shift approaches more accurately.

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